THE CHEMICAL COMPONENTS OF TOBACCO AND TOBACCO SMOKE

SECOND EDITION

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Foreword

The following pages are an attempt to update a situation with regard to the composition of tobacco and tobacco smoke that has existed for almost five decades. Although it is suspected that the chemical components of tobacco and tobacco smoke may have been cataloged in-house at various U.S. and foreign tobacco companies as well as by various governmental agencies, no such catalog has been published since the 1968 review by the highly competent tobacco scientist R.L. Stedman of the U.S. Department of Agriculture (3797). One article published by a tobacco company prior to that of Stedman was a 1963 referenced monograph on tobacco and tobacco smoke components by Philip Morris, Inc. (2939). Its monograph was submitted to the 1964 Advisory Committee for use in preparation of its 1964 report to the U.S. Surgeon General. The Philip Morris monograph had been preceded by the 1959 published review by Johnstone and Plimmer (1971). In subsequent years, several tobacco and tobacco smoke publications dealt with specific types or classes of components, e.g., the 1964 compilation of the polycyclic aromatic hydrocarbons (PAHs) in tobacco smoke by Elmenhorst and Reckzeh (1139), the 1969 review by Neurath on the nitrogen-containing components identified in tobacco smoke (2724), and the 1977 review by Schmeltz and Hoffmann on the nitrogen-containing components in both tobacco and tobacco smoke (3491). Several catalogs of the chemical components of only tobacco smoke have been published, e.g., the 1954 article by Kosak (2170), but the most recent one was that of Ishiguro and Sugawara (1884) in 1980. Since the 1968 Stedman article in which about 1200 tobacco and smoke components were listed, the number of identified tobacco and tobacco smoke components has increased sevenfold to almost 8600, a number that includes only about 500 of the many thousands of enzymes identified in the tobacco plant.

The references cited for a particular tobacco and/or tobacco smoke component may deal with its identification or with a variety of topics pertinent to the particular component. Such topics may include such simple items as the isolation and identification of a component, its characterization by classical chemical means such as the definition of the structure of solanesol isolated from flue-cured tobacco by Rowland et al. (3359), or the characterization of a component by spectrographic means such as UV, IR, NMR, MS, and chromatographic retention time, e.g., the identification by Snook et al. of many PAHs (3756–3758) and aza-arenes (3750) in cigarette mainstream smoke (MSS). Many references cited herein describe the search for and elucidation of the precursor in tobacco of a particular component in cigarette MSS (3616), e.g., the saturated aliphatic hydrocarbon precursors of the PAHs, including benzo[*a*]pyrene (B[*a*]P); the quantitation of the component on a per gram of tobacco basis or on its per cigarette MSS yield, particularly if the component is considered a health problem; and the improvements/developments in analytical technology to determine the per cigarette MSS and/or sidestream smoke (SSS) yield of the component. Also included in citations for a particular MSS, SSS, and environmental tobacco smoke (ETS) component are the publications of results of experimental studies on its biological activity plus discussions and/or assertions of its toxicity and/or tumorigenicity. While their number is much fewer than the opposite point of view, included are references to studies on the inhibition of adverse biological activity of a tobacco smoke component by another smoke component, e.g., the inhibition of mouse-skin tumorigenicity of B[*a*]P by *n*-hentriacontane and *n*-pentatriacontane (4314, 4336), the inhibition of *N*-nitrosodimethylamine (NDMA) mutagenicity by nicotine (2327a, 2327b), the inhibition of mouse-skin tumorigenicity of dibenz[*a,h*]anthracene (DB[*a,h*]A) by benz[*a*]anthracene (B[*a*]A) (3814), both classified as significant tobacco smoke tumorigens. Also cited are reports on the controversies over the extrapolation of the biological effect of a specific component administered individually vs. its biological effect when it is the component in a highly complex mixture such as MSS and is administered to a different species, by a different route, and at a dose level far in excess of its level in the complex mixture (1318a, 3300, 3627). Lastly, many studies are cited in which cigarette design technologies were generated to control the per cigarette MSS yield of FTC "tar" and one or more specific components of concern, e.g., reconstituted tobacco sheet, expanded tobacco, ventilated filters, filter-tip, and cigarette paper additives.

While some of the citations may seem obscure to a reader newly involved in tobacco and/or smoke research, they are included to elucidate the historical background and relationship to more recent studies, e.g., publications pertinent to 2-methyl-1,3-butadiene (isoprene), a fairly plentiful component of the vapor phase cigarette smoke. The publications include the 1913 report by Staudinger et al. (25A68) that pyrolysis of isoprene yielded a "tar." In 1918, the procedure to successfully generate tumors by animal skin painting was described (4361). Five years later, Kennaway (2073–2076) demonstrated the tumorigenicity of the pyrolysate "tar" from isoprene, and much later, Badger et al. (143) recorded the PAH content of an isoprene pyrolysate. Another example includes a series of references to the research results reported by Roffo that a tobacco "destructive distillate" was tumorigenic (3322, 3325), contained B[*a*]P (3316), and the B[*a*]P content and tumorigenicity of the "destructive distillate" were reduced by organic-solvent extraction of the tobacco prior to destructive distillation (3327).

Our goal was to present to the reader as many pertinent references that we could find for a particular component and permit the reader to decide which references to study. For some components, dozens of references are available, for other components only one or two. The multireferenced components are usually those considered to be involved in the health problems connected to tobacco smoking. Since the publication of the first edition of this book in late 2008, we have added to our Alphabetical Component Index and the appropriate major chapter tables nearly a thousand reported components of tobacco and/or tobacco smoke. References pertinent to these newly cataloged components and the earlier reported ones have been included in the Bibliography and in the appropriate major chapter tables devoted to functionality.

We express our deep appreciation to several scientific staff members of the Verband der Cigaretten-Industrie and the Beiträge zur Tabakforschung International. They reviewed the initial chapter of the draft of the first edition of our opus and made many meaningful suggestions and pointed out the need for several corrections. Most of their input was applied to that chapter and eventually extended to subsequent chapters as we wrote them. One needed correction that was described was a problem with the electronic address for a specific reference. It was found to be inaccessible at the time of the review. That was corrected, since the reference had multiple electronic addresses, the inaccessible one was replaced with an accessible and operative one. However, the finding triggered an examination of all the electronic addresses cited in the Bibliography section. Of the nearly 900 such addresses, three more were found to be inaccessible. Fortunately, each was part of a reference with multiple electronic addresses, and the inaccessible address for each was replaced with an accessible one.

We apologize to the reader for the omission not only of any tobacco or tobacco smoke component from the catalog but also any significant reference by one or more competent investigators who provided information pertinent to one or more specific components.

Acknowledgments

During the many years that this tobacco and tobacco smoke component catalog was being prepared, numerous components were discussed with colleagues, many of whom were involved either in tobacco and/or tobacco smoke research within the tobacco industry or outside of it. Much meaningful information was obtained during the many discussions, and such information has been incorporated into our effort. We greatly appreciate the input not only from those colleagues who are still with us but also from those who are not.

In the first group, we are extremely grateful to Fred W. Best, Michael F. Borgerding, N.M. Chopra, Christopher R.E. Coggins, William M. Coleman III, Lawrence C. Cook, James T. Dobbins Jr., Michael F. Dube, Curt R. Enzell, Charles R. Green, Paul Kotin, Brian M. Lawrence, Chin K. Lee, John C. Leffingwell, Robert A. Lloyd, Jr., William C. Luffman, Dwo Lynm, C.D. McGee, Alan B. Norman, Charles W. Nystrom, Michael W. Ogden, John H. Reynolds IV, Charles H. Risner, Charles E. Rix, Joseph N. Schumacher, Stephen B. Sears, Jeffery I. Seeman, Carr J. Smith, Thomas W. Stamey, Jr., David E. Townsend, and Jack L. White.

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We also wish to express our gratitude to those who, over the years, have provided us with much information on scientific publications and presentations. They include Charles W. Nystrom, Nell W. Sizemore, and the late Frank G. Colby, William W. Menz, and John J. Whalen. Particularly meaningful over the past decade has been the information provided by the extremely diligent Helen S. Chung of the R.J. Reynolds R&D Scientific Information Division.

One of us (T.A.P.) wishes to especially thank Patricia F. Perfetti for the encouragement and faith she has showed me as my wife, best friend, faithful colleague, and my partner in many happy and productive years of scientific research.

Authors

Alan Rodgman, MA, PhD, MCIC: Most of the original text of the following biography was written in 2003 for Alan Rodgman's nomination for the Tobacco Science Research Conference Lifetime Achievement Award. He was recipient of the 2003 award. In several places, the nominator's paragraphs have been slightly modified to include additional, more recent information plus a more recent picture than the 2003 one has been provided. The author of the 2003 nomination wrote:

> For here we are not afraid to follow truth wherever it may lead, nor to tolerate any error so long as reason is left free to combat it.
>
> **Thomas Jefferson, 1820**

The words penned long ago by Jefferson epitomize the life and professional career of Alan Rodgman.

For one year short of a half century, Dr. Rodgman has been at the forefront of tobacco science. His increasingly rare combination of keen scientific intellect, unceasing productivity, sense of tobacco science history, and unfailing attention to clear, concise, timely communication make him an ideal choice for the Tobacco Science Research Conference's (TSRC's) Lifetime Achievement Award. Not only has Alan Rodgman made his own prodigious, personal scientific contributions to tobacco and smoke chemistry and their related toxicology, but his mentoring of associates and many other tobacco scientists have allowed him to amplify his contributions far beyond those capable of any one man. Dr. Rodgman's professional "family tree" reads as a "Who's Who" in tobacco science.

Alan Rodgman was born in 1924 in Aberdare, Glamorgan County, Wales, to Arch and Margaret Llewellyn Rodgman. The family moved to Toronto, Ontario, Canada, in 1928. There he was educated at the grade and collegiate level. Because of the early death of his father when Rodgman was ten years old, he worked after school and on Saturdays at the children's and adult department of a local branch of the Toronto Public Library from 1937 to 1942. In 1945, Alan Rodgman entered the University of Toronto as recipient of the two highest mathematics, physics, and chemistry scholarships awarded in competition in 1942. Because of a University of Toronto rule on retaining no more than two competitive scholarships, a third chemistry and physics scholarship awarded to Rodgman reverted to the next highest candidate. The three-year period between earning the scholarships and their implementation was spent on active duty as a volunteer in the Royal Canadian Navy during World War II, with service on the North Atlantic Ocean.

Between 1945 and 1949, at the University of Toronto, Rodgman was awarded eight additional scholarships—one in mathematics, physics, and chemistry in 1946 and seven in chemistry in 1947, 1948, and 1949. His bachelor's thesis on *N*-nitrosamines in 1949, master's thesis on kinetics of the original Diels–Alder reaction in 1951, and doctoral thesis on oxymercuration–deoxymercuration in 1953 were conducted with Dr. George F. Wright* as his advisor. Rodgman taught the laboratory aspect of analytical chemistry during the first year of his master's period. His master's and doctoral research formed part of 11 publications coauthored between 1952 and 1959 with Dr. Wright who, by the way, from 1954 to 1959, preceded Dr. Dietrich Hoffmann as Dr. Ernst L. Wynder's tobacco smoke chemistry colleague.

Rodgman married Doris Curley in June 1947. They have three sons (Eric, Paul, and Mark), three daughters-in-law (Melody, Ella, and Sara), and seven grandchildren.

While pursuing his chemistry degrees, Rodgman conducted carcinogenesis and anticarcinogenesis research from 1947 to 1953 during summers, winter evenings, and weekends with Dr. Wilbur R. Franks, cancer research professor at the Banting and Best Department of Medical Research, University of Toronto. He conducted such research full-time to mid-1954 after receiving his doctorate in June 1953. Rodgman's first three scientific publications (on anticarcinogenesis) in 1947 and 1948 preceded the receipt of his bachelor's degree in chemistry in 1949. From 1951 to mid-1954, he also taught organic and physical chemistry plus mathematics for physical chemistry in evening courses sponsored by the Chemical Institute of Canada.

In mid-1954, Rodgman joined the Research Department of the R.J. Reynolds Tobacco Company as a senior research chemist. In October 1954, he initiated its program on cigarette smoke composition, personally conducting the laboratory research until 1967 and actively directing it and environmental tobacco smoke studies thereafter until 1987. Following successive promotions from senior research chemist to section head to division manager, he became director of research in 1976, and after an R&D reorganization in

* The lack of a period after Dr. Wright's middle initial is not a typographical error.

1980, he was appointed director of fundamental research. Rodgman became an American citizen in 1961.

After more than 60 years, Rodgman is still a member of the American Chemical Society and the Chemical Institute of Canada. Until 2006, he had been a member of the New York Academy of Sciences for over 40 years and also a member of Sigma Xi. He served on the editorial board of *Tobacco Science* as member and vice chairman (1963–1967); on the editorial board of *Beiträge zur Tabakforschung International* (1976–1987); on the Industry Technical Committee, Council for Tobacco Research (1955–1960); on the CORESTA Scientific Commission (1982–1985); and on several U.S. government committees, e.g., the Tobacco Working Group of the National Cancer Institute's Smoking and Health Program on the Less Hazardous Cigarette (1976–1977) and the U.S. Technical Study Group of the Cigarette Safety Act of 1984 (1984–1987). From 1960 to 1987, Rodgman served on numerous Tobacco Chemists' Research Conference (TCRC) committees. In 1972, he was involved in various aspects of the joint CORESTA/TCRC Conference in Williamsburg, Virginia. In 1976, he persuaded his company's management to continue its CORESTA membership. In the early 1980s, when a host site for the 1982 CORESTA Symposium did not materialize, Rodgman was instrumental in arranging for his company to sponsor the symposium in Winston-Salem, North Carolina. He served as its vice chairman.

Rodgman was the chairman for the 38th TCRC symposium entitled "Design of Low-'Tar' Cigarettes" held in 1984. On the occasion of TCRC's 50th conference in 1996, he coauthored with Charles R. Green a comprehensive review and presentation entitled "The Tobacco Chemists' Research Conference: A Half Century Forum for Advances in Analytical Methodology of Tobacco and Its Products." The following year at the 51st conference, he prepared a symposium paper and presentation on "FTC 'tar' and nicotine in cigarette mainstream smoke: A retrospective." In addition, Dr. Rodgman has presented many other original research papers at the conference.

In the journal *Tobacco Science*, he has published 13 scientific papers on tobacco smoke composition. Additionally, the 1986 volume of *Tobacco Science* was dedicated to Dr. Rodgman to honor his prolific career. In addition to serving as a reviewer for manuscripts submitted to *Tobacco Science* and *Beiträge zur Tabakforschung International*, Rodgman has served as a reviewer not only for manuscripts submitted to several other journals including *Recent Advances in Tobacco Science*, *Journal of Analytical and Applied Pyrolysis*, *Food and Chemical Toxicology*, and the *Journal of Organic Chemistry* but also for the page proofs of several well-known books on tobacco-related topics.

From 1954 to retirement and from retirement to 2004, Rodgman was involved in consulting activities on the scientific aspects of litigation against R.J. Reynolds Tobacco Company. Over 13,000 pages of his contributions are available at http://tobaccodocuments.org/bliley_rjr/list. Many of the more recent contributions were the consequence of the "Master Settlement" between the states and tobacco companies. Additionally, he has been a major contributor to the scientific content of *Beiträge zur Tabakforschung International*, both through submitted papers and as a volunteer editor. Dr. Rodgman has mined the wealth of documents previously considered proprietary to clarify the intent and content of tobacco and smoke research conducted by himself, his colleagues, and other scientists. The papers authored/coauthored by Rodgman during the last two decades include publications on environmental tobacco smoke (3255a); FTC "tar" and nicotine in cigarette mainstream smoke (3258); tobacco smoke components (3260); polycyclic aromatic hydrocarbons (3262, 3306a, 3306b, 5077); phenols (3712); "smoke pH" (3261); "IARC Group 2A carcinogens" (3713) and "IARC Group 2B carcinogens" (3714) reported in cigarette mainstream smoke; the effects of additives on cigarette mainstream smoke properties (3263, 3264, 3266); the problems with lists of tumorigens (3265, 3300, 5557); various tobacco substitutes (1375a); and the effect of expansion of tobacco on cigarette mainstream smoke properties (1375b).

At the 2002 CORESTA Congress held in New Orleans, Dr. Rodgman coauthored with Charles R. Green an invited speaker symposium paper entitled "Toxic chemicals in cigarette mainstream smoke—Hazard or hoopla." In this paper, the authors critically examined the proper listing and prioritizing of toxic chemicals in cigarette mainstream smoke. Moreover, the authors pointed to a number of disconcerting chemical and biological limitations in existing knowledge, which calls into question the veracity of such listed strategies for their oft-stated purposes. This example is included in Alan Rodgman's nomination to illustrate his lifelong pursuit of the truth.

In summary, there is no question that Alan Rodgman has dedicated his professional life to the achievement of the highest standards for tobacco science. Even with this nomination and the accompanying materials, it is impossible to convey to an outsider the tremendous impact that this person has made to our knowledge of tobacco and its smoke. Although his own personal scientific accomplishments are by themselves worthy of TSRC's Lifetime Achievement Award, the amplification of his life's work through influence on many other tobacco scientists is difficult to quantify. Beyond his many professional achievements is a man who is widely respected and personally liked both within and outside the tobacco science community.

Because his philosophy on publication authorship differed substantially from that of many academic, government agency, and health organization investigators, Rodgman did not insert his name as coauthor on the many articles on tobacco and smoke composition presented at conferences and/or published in peer-reviewed journals by his staff members. If he had done what many supervisors do, his list of publications between 1960 and 1987 would be increased by almost 200. However, his contributions to many of the studies are described in the Acknowledgment section of many of his staff/colleagues' publications.

Thomas Albert Perfetti, PhD was born in 1952 in Jeannette, Pennsylvania, the second son of Ruth Peters and Bruno Massimo Perfetti. He was one of five children. Perfetti received his elementary education in several schools in the Pittsburgh area. In 1970, he entered Indiana University of Pennsylvania (IUP). He earned a bachelor of science degree in chemistry in 1974. During his stay at IUP, he conducted cell transport research with Dr. Richard Hartline and synthesized numerous radiopharmaceuticals. Perfetti's first publication was on the preferential uptake of *d*-α-amino adipate by *Alcaligens denitrificans* in 1975.

In 1974, he entered the Virginia Polytechnic Institute and State University (VPI-SU), Blacksburg, Virginia. His doctoral thesis (1977), under Dr. Michael Ogliaruso, was on the electronic effects associated with the Woodward–Hoffman Rules. While pursuing his doctoral degree in physical organic chemistry, Perfetti worked as a research fellow for NASA, taught at organic chemistry labs, and tutored undergraduates. In 1976, Perfetti won the President's Award for Distinguished Teaching at VPI-SU.

Perfetti married Patricia Ann Finley, who graduated with him from the Chemistry Department at IUP, in 1975. They have two sons, Michael and David. The family now resides in Winston-Salem, North Carolina.

In late 1977, Dr. Perfetti joined the R.J. Reynolds Research Company (RJRT) as a research chemist. There, he initiated several research programs on tobacco and smoke chemistry, cigarette design, sensory science, flavor chemistry, and analytical method development. Perfetti was promoted from senior research chemist (1979), to senior staff scientist (1984), then to master scientist (1986), and finally to principal scientist (1991). He is a recognized expert in the areas of nicotine and menthol chemistry and in the area of innovation. As principal scientist, he worked with R.J. Reynolds-Nabisco and R.J. Reynolds International on corporate program development and program management issues. He also acted as a liaison on patent acquisitions, patent applications, and consulting activities on the scientific aspects of litigation against RJRT. Much of his career was spent in the laboratory, although he served as the manager of several divisions. Dr. Perfetti retired from RJRT in 2003. In that same year, he and his wife started Perfetti & Perfetti, LLC, a scientific consulting firm in Winston-Salem, North Carolina. Their company has done quite well with numerous national and international clients.

Perfetti has served as a reviewer for *Tobacco Science,* the *Journal of Food and Chemical Toxicology*, and *Beiträge zur Tabakforschung International*. He served on several Tobacco Chemists' Research Conference committees and contributed to two of its symposia (1987, 1993), one of which he chaired (1993).

Perfetti is a member of the American Chemical Society (ACS). He has served as assistant historian to the Division of the History of Chemistry. He is a member and fellow of the American Institute of Chemists and is a certified professional chemist. He was a cofounder and past president of the North Carolina Chromatography Discussion Group and former chairman of the Education Committee of the Central North Carolina Section of the ACS. Dr. Perfetti has been cited in *Who's Who in America*, *Who's Who in Science and Technology*, in the *International Directory of Distinguished Leadership*, and *Who's Who in American Leaders in America*. In 1993, Dr. Perfetti was presented with the Distinguished Alumni Award, Indiana University of Pennsylvania. In 1995, he and several other RJRT scientists were given the George Land World-Class Innovator Award for outstanding work in instilling the principles of innovation at RJRT Research and Development.

Over the last 32 years, Perfetti has made over 60 presentations and published numerous papers in peer-reviewed journal in the areas of biochemistry, tobacco and smoke chemistry, sensory perception, mathematics, and innovation. During his career at RJRT, he prepared more than 250 formal company research reports. He has written chapters for two books and has developed and presented five courses in the areas of cigarette design and innovation. Dr. Perfetti has 38 U.S. patents and hundreds of foreign patents.

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Introduction

> History balances the frustration of how far we have to go with the satisfaction of how far we have come. It teaches us tolerance for the human shortcomings and imperfections which are not uniquely of our generation, but of all time.
>
> **Lewis F. Powell, Jr. Associate Justice of the Supreme Court of the United States (1972–1987)**

INTENT OF THE WORK

Years from now, just as we were surprised how paltry was the number of identified tobacco smoke components cataloged in 1954 by Kosak (2170), others will no doubt have similar remarks concerning this catalog. We hope the reader will be satisfied rather than frustrated with the progress that has been made by tobacco scientists over the last 50+ years in furthering our knowledge base of components identified in tobacco and tobacco smoke. It should be noted the last published detailed catalog of tobacco and tobacco smoke components was that of Stedman (3797) in 1968.

CHEMICAL COMPOSITION OF TOBACCO

The Master Catalog, collected over a 50-year period, is our tabulation of all the information on the components identified in tobacco and smoke. The Master Catalog contains all of the information on components in tobacco and tobacco smoke that is contained in each chapter of this book as well as the information in the Bibliography and Alphabetical Component Index sections of this book. During the creation of this book, the information contained in the Master Catalog was searched to extract all of the components by functional group (alcohols, esters, aldehydes, etc.) to be included in the separate tables for each chapter of this book. The Bibliography was separated from the Master Catalog as a separate section of this book. An Alphabetical Components Index was created as a ready resource for readers to access particular information on each component and to locate the chapters and tables in the book chapters where that class of components is discussed. The original Master Catalog that we developed as such is not part of this book but was subdivided into numerous tables of components identified in tobacco and tobacco smoke by chemical functionality, the Bibliography, and the Alphabetical Components Index. This edition of our book catalogs nearly a thousand more tobacco and/or tobacco smoke components than were listed in the First Edition. Also, nearly a thousand more references pertinent to the newly reported components and to the previously reported ones are listed in the Bibliography.

The following, discussed in detail in Chapter 28, is a summary of the overall change in the number of components in our Index during the past 4 years, from 2008 to date:

Index Date	Tobacco Smoke	Tobacco	Tobacco and Tobacco Smoke	Subtotal	Smoke Isomers	Total
2012	6010	5595	2215	9390	192	9582
2008	5315	4994	1879	8430	192	8622

Tobacco is a fascinating organism. This plant, as all plants do, takes the simplest of molecules (carbon dioxide, nitrogen, and water), light, and a series of metals (as micronutrients) and through a sophisticated internal process converts these materials to complex molecules for plant growth regulation and maintenance. Tobacco has been called a chemical factory. It has been cultivated for the purpose of collecting nicotine for use as an insecticide and for starting material for numerous commercial chemicals such as the pyridines. More recently, it has been studied as a source of plant protein [Fraction 1 (F-1) and Fraction 2 (F-2) protein] (3974c). There are many different botanical classifications for tobacco plants. The genus *Nicotiana* has over 60 known species; each has been examined as to its genetic, physiological, botanical, and chemical characteristics (3972, 3973). Two tobacco species are grown commercially: *Nicotiana rustica* primarily for nicotine and solanesol collection; *Nicotiana tabacum* for use as in cigarette, pipe, cigar, snuff, and chewing tobaccos.

To date, nearly 5700 components have been identified in tobacco. The total appears at the end of the Alphabetical Components Index and represents an increase of more than 700 over the 4994 listed in the earlier version of our catalog [see p. 1784 in (5078)]. This number does not include the nontobacco components listed as added flavorants by Doull et al. (1053) and Baker and Bishop (172a) or the hundreds of enzyme and other proteinaceous components listed in our Master Catalog. This is a tremendous achievement compared to the number of tobacco components reported as 3044 in 1988 by Roberts (3215), reported as 2549 tobacco compounds in 1982 by Dube and Green (1067), the 200 identified compounds reported in 1960 (2338), the 199 organic compounds and 21 inorganic elements reported as identified in tobacco in 1959 (1971), and the accounting of less than 10 tobacco constituents by Frankenburg (1221) in 1946. It should be noted that in the classification by Frankenburg, the tobacco constituents listed were not individual compounds but classes of compounds such as alkaloids, proteins (soluble and insoluble fractions), nitrate-nitrogen, and amino nitrogen. It is estimated that literally tens of thousands of unidentified compounds are yet to be discovered in tobacco. This estimate is based upon

the assumptions that there has already been thousands of organic, inorganic, and organometallic compounds identified in tobacco, that each plant contains hundreds of extremely complex compounds, e.g., various types of DNA and RNA, numerous types of complex enzymes, proteins, sugar, and amino acid oligomers, needed for plant growth, regulation, and maintenance, and that numerous fragments of these complex molecules have already been reported in tobacco.

If it were not for scientists' curiosity and the tremendous advances in analytical chemistry over the last 50–60 years, the need for this revised version of our 2008 catalog of compounds in tobacco and tobacco smoke would not be critical. Over the last 50–60 years, literally tens of thousands of scientific articles on varied topics in tobacco and tobacco smoke science have been written. Our understanding of these two areas of science has advanced tremendously in the recent past. As noted by Knipling [see Preface in Tso (3974c)],

> Pioneering tobacco research was the foundation of plant science at the dawn of modern development, in such areas as light, nutrition, genetics, growth control, disorders and metabolism. Tobacco research led to current advancements in plant biotechnology. In addition, tobacco plant research contributed significantly to public health research in radioactive elements, mycotoxins, and air pollutants. However, public support for tobacco research has today greatly declined to almost total elimination because of a sense of political correctness … tobacco is one of the most valuable research tools, and is a most abundant source of scientific information. Research with tobacco plants will contribute far beyond the frontiers of agricultural science: tobacco can be a source of food supply with nutrition value similar to that of milk; tobacco can be a source of health supplies including medical chemicals and various vaccines; tobacco can be a source of biofuel. All we need is to treat tobacco with respect; the use of tobacco is only in its initial stages.

For over 50 years, our Master Catalog of components identified in tobacco and smoke has been in the process of assembly. Each component has one or more corresponding references. The tobacco literature was diligently searched for components identified in tobacco and tobacco smoke. As new components in tobacco and tobacco smoke were reported by R.J. Reynolds Tobacco (RJRT) Co. R&D personnel and in the published scientific literature, they were entered into the Master Catalog. Data on components in mainstream smoke (MSS), sidestream smoke (SSS), and environmental tobacco smoke (ETS) were collected from studies on the smokes from a variety of tobacco types and blends and numerous forms of smoking articles, e.g., cigarettes, cigars, cigarillos, pipes. Data on tobacco components were collected from studies on numerous species of *Nicotiana* (primarily *N. tabacum*). The tobacco component data were collected from studies not only on all stages of plant development (seed to harvested plant) but also from tobacco processed in various ways (aged, fermented [various degrees], steamed, cut, rolled, expanded, converted to reconstituted sheet [by various methods], treated with additives) prior to use as a smoking material.

The Master Catalog contains an enormous variety of species from nearly every class of chemical components. We have separated and combined the identified components in tobacco and tobacco smoke into classes of components, e.g., hydrocarbons, alcohols, acids, esters, aza-arenes, and each class will be discussed in a separate chapter. For the reader's information, tobacco and tobacco smoke components possessing multifunctional groups will appear in each of the appropriate chapter lists but will be only tallied once as a tobacco component and/or a tobacco smoke component. For example, 2-furancarboxylic acid (2-furoic acid) is listed in the carboxylic acid chapter and the ether chapter; 4-hydroxy-3-methoxybenzaldehyde (vanillin) is listed in each of the aldehyde, ether, and phenol chapters. Also as an amendment to the First Edition of our catalog where multifunctional components were inserted into several major chapter tables, in this edition, the multifunctional components are listed in the Index as being cited in all the major chapter tables where they occur.

The Master Catalog and the chapters on the various classes of tobacco components do contain some items not identified as tobacco components per se. They include items that (1) are not identified components of untreated tobacco and/or its smoke but are individual compounds added to the tobacco in a flavor formulation to improve consumer acceptability of commercial products,* (2) are the pesticides, herbicides, nematicides, growth control agents, etc. (or their residues), that improve the agronomic situation for tobacco cultivation or have been found on tobacco, (3) are mycotoxic products of microorganisms found on tobacco plants, e.g., aflatoxins, and (4) thermal degradation products from (1), (2), and (3) found in tobacco smoke. Many of the components in (1) were identified as added tobacco ingredients in the reports by Doull et al. (1053), Baker and Bishop (172a), and Baker et al. (174b). Many of the components in (2) are retained in the tobacco after harvesting and curing, are transferred intact to the smoke, and in some cases, are degraded to compounds not usually expected in tobacco smoke. As noted previously, the items in (1) and (3) were not included in the 4200 identified tobacco components discussed earlier. As noted previously, the items in (1) and (3) were not included in the 4200 identified tobacco components discussed earlier. Also not included in our Master Catalog are the additives comprising mixtures from naturally occurring products, e.g., alfalfa extract, basil oil, honey. These will be discussed in the chapter on tobacco additives.

During the 1920s and 1930s, plant nutrition was an active area of research and tobacco served as the model in much of that work. The results of research on nitrogen assimilation,

* Among the flavor formulation compounds listed as tobacco ingredients by Baker and Bishop (172a), Baker et al. (174b), and Doull et al. (1053) was a substantial number of compounds reported as identified components of additive-free tobacco and/or its smoke [see Tables 1, 5, and 7A in (3266)]. That number was increased recently because of the identification of several additional listed flavor formulation compounds in flue-cured tobacco by Peng et al. (2917a) and in Perique tobacco by Leffingwell and Alford (2339a).

light as a factor in nitrogen fixation, and how weather contributed to nutrient uptake contributed greatly to our understanding of plant science. All these advancements seem trivial today in light of the sophisticated work in genomics but were nonetheless initially due to the pioneering work of scientists working with tobacco (3972, 3973).

The presence of some microelements in tobacco was reported as early as 1921. Today, nearly all of the common elements including alkali, alkali earth, heavy metal, and rare elements have been reported to be present in tobacco, e.g., Al, As, Ba, B, Cs, Cr, Co, Cu, F, Au, I, Pb, Li, Mg, Mn, Hg, Mo, Ni, Pt, Po, Ra, Rb, Se, Si, Ag, Sr, S, Ta, Ti, Sn, U, V, and Zn. Many heavy metal radioactive components have been reported in tobacco including those from the uranium series, e.g., ^{234}U, ^{226}Ra, ^{228}Ra, ^{222}Rn, ^{210}Po, and others, e.g., ^{38}Cl, ^{46}Sc, ^{134}Ce, ^{59}Fe, ^{40}K. The presence of such elements in tobacco may be accidental, acquired from soil or from other sources. Scientists curious to understand the role of these assorted elements conducted research studies from the 1920s in order to understand the role of each element in plant growth and development. The effect of boron on plant growth was first noted in 1929, zinc in 1942, and copper in 1942. The concept of metals as catalysts in plant growth advanced the areas of chemical catalysis and its use in industrial fermentation (3972, 3973). The transfer of elements, particularly some of the metallic ones noted earlier, from tobacco to its smoke has been studied since the mid-1950s, e.g., Cogbill and Hobbs (769).

Elemental isotopes have also been used in tobacco research for over 50 years. Studies with single, double, and even triple labeled compounds incorporating ^{15}N, ^{3}H, and ^{14}C were reported by personnel at the U.S. Department of Agriculture (USDA) in the early 1950s in their studies on plant metabolism (3972, 3973).

Tobacco is a very labor-intensive and sensitive crop. Hundreds of agronomic and physical processing steps occur from seed planting to final use in commercial products. The type of tobacco (flue-cured, burley, MD, Oriental) as well as dark air-cured tobacco and various cigar tobaccos and how the tobacco is produced and cured affect the type and level of chemical compounds in tobacco leaf and in smoke. Among the chemicals applied to tobacco are insecticides, acaricides, miticides, nematicides, and growth control agents, e.g., sucker-control and yellowing agents. These were developed to control pests and plant growth, to reduce labor, and ultimately to produce a better, healthier, and more profitable crop. Their number and types are large. Over the years, new chemical agents were developed and commercialized as others were either banned or found to be less effective. Nonetheless, some pesticide residues remain in the soil and are often transported to the plant. All the commercial pesticides (as well as herbicides) are tested thoroughly and can be safely used (822a). As an example, today, the most widely used sucker-control agents are fatty compounds, including fatty acids, alcohols, esters, and some of their derivatives. These sucker-control agents significantly inhibit axillary growth without causing undesirable side effects to the plant or the public (3972, 3973).

The genetic makeup of tobacco includes 25,000–50,000 genes. The gene mapping of tobacco is being conducted in the Plant Pathology Department, North Carolina State University Centennial Campus, College of Agricultural and Life Sciences, Raleigh, NC, in a project known as the Tobacco Genome Initiative (TGI). Its goal is to sequence and catalog more than 90% of the genome of cultivated tobacco, *N. tabacum*. Although tobacco has been cultivated for more than 500 years and is a crop of great economic significance, relatively little information exists on its genome structure and organization.

A complete tobacco gene catalog will provide information needed to investigate the physiological and genetic processes in the plant kingdom, in general, and in *N. tabacum* specifically. Understanding the genetic processes occurring within the tobacco plant could potentially provide valuable information on ways to reduce the harm associated with cigarette smoking and also provide information on agronomic traits associated with disease and pest resistance genes for use in improving traditional and molecular breeding projects aimed at enhancing the performance of tobacco as a crop. The plants within the agriculturally important *Solanaceae* family which includes tobacco, tomato, potato, eggplant, and pepper crop plants will all benefit from gene discovery in *N. tabacum*.

Available for public use are additional databases that contain listings of enzymes, enzymatic pathways, and reaction products of metabolic and catabolic processes occurring in tobacco species. Many of these are listed as references in our chapter catalogs:

- GenBank (tobacco): For references, see http://www.ncbi.nlm.nih.gov/Genbank/index.html (1282a).
- BRENDA: The Comprehensive Enzyme Information System, entry of hydroxymethylglutaryl-CoA reductase (NADPH) (EC-Number 1.1.1.34) Nicotiana, Kyoto Encyclopedia of Genes and Genomes (KEGG) Link 00100 Steroid Biosynthesis, see http://www.genome.jp/dbget-bin/show_pathway?map00100+1.1.1.34 (429c).
- BRENDA: The Comprehensive Enzyme Information System; http://www.genome.jp/dbget-bin/show_pathway?map00500+2.4.1.35 (429b).
- KEGG; see Kanehisa, M. and S. Goto: KEGG: Kyoto Encyclopedia of Genes and Genomes; *Nucleic Acids Res.* 28 (2000) 27–30 (429b).
- Lyon, G.D.: Host pathogen interactions & crop protection; Metabolic pathways of the diseased potato at http://www.scri.sari.ac.uk/publications/annualreports/98Indiv/21Metabo.pdf (429b).

Plant scientists have long known that all organic components are dynamic in nature and change in numerous ways when present in biological systems. Chemical, catalytic, enzymatic, and bacteriological processes occur continuously during plant

growth in the field and until these biological processes are quenched at harvest and during processing. Tobacco scientists have extensively studied the metabolism and catabolism occurring in *Nicotiana* plants because the change or formation of each compound may affect its final quality and thus its usability. Organic compounds are formed, transformed, and interact during plant growth in the field, during postharvest handling processes of curing, aging, and fermentation, during manufacturing, including interaction with additives, and during blending (3972, 3973).

The chemical composition of the tobacco determines the chemical composition and yield of components in its tobacco smoke. For example, leaf protein (F-1 and F-2 protein) is abundant in tobacco and turns over and decomposes continuously to produce a vast array of protein subunits, amino acids, and amino acid oligomers (3974c).

Tobacco leaf protein by itself contributes little to smoking quality, but it is a major precursor of hundreds of tobacco smoke components, e.g., numerous nitrogenous compounds, amino acids. Similarly, other major tobacco components such as the carbohydrates, carboxylic acids, pigments, polyphenols, fatty compounds, phytosterols, and many primary or secondary compounds play a significant role in producing a myriad of tobacco smoke compounds (3972, 3973).

Tobacco has been used in one form or another in civilized society for nearly five centuries. Eventually in the late nineteenth century, investigations as to its composition began, but they were not particularly numerous. The major driving force in the escalation in the mid-twentieth century of studies on tobacco composition was the attempt to define (1) its components that contributed to the consumer acceptability of the taste and aroma of tobacco itself and its smoke and (2) the precursors in tobacco of the toxicants in its smoke.

The latter investigations were triggered by the following events: (1) The publication from 1950 to 1953 of the results from several retrospective studies on lung cancer in smokers and nonsmokers [Doll and Hill (1027), Mills and Porter (2556), McConnell et al. (2515), Sadowsky et al. (3375a), Schrek et al. (3529), Wynder and Graham (4306b)]. The results suggested an association between cigarette smoking and cancer of the lung, particularly the lung cancer tumor type defined as squamous cell carcinoma. (2) The 1953 presentation and publication by Wynder et al. (4306a) of their findings on the production of malignant tumors in a susceptible strain of mice skin painted daily with massive doses of solutions of cigarette smoke condensate (CSC) supposedly generated under conditions simulating the human smoking of a cigarette. These statistical and biological findings augmented by the results of additional similar studies led to an escalation in the research to define the composition of cigarette smoke and to determine which of its components were responsible for the observed biological response. When a particular class of components—the polycyclic aromatic hydrocarbons (PAHs)—was considered responsible, studies escalated to define the precursors in tobacco of the PAHs in its smoke.

Previous detailed reports on the composition of tobacco included those issued by Brückner in 1936 (451), Latimer in 1955 (2270), Johnstone and Plimmer in 1959 (1971), Shmuk in 1961 (3657), Stedman in 1968 (3797), Roberts et al. in 1975 (3224), Schmeltz and Hoffmann on nitrogen-containing tobacco components in 1977 (3491), and Enzell et al. on terpenoid-derived tobacco components between 1976 and the late 1980s (1149, 1150, 1156, 4089, 4090). One thing has become apparent since the mid-1950s: No other consumer product that involves a complex mixture has been defined in such detail as tobacco and/or its smoke, e.g., the number of components identified to date in tobacco is almost twice that of the number identified in coffee.

In the last 90 years, tobacco scientists have spent considerable time and effort determining and reporting on the chemical composition of tobacco. One of the first attempts at estimating the mass balance of the major and minor constituents of tobacco was that of Hobbs in 1972 (1665). Hobbs stated the following in his review:

> In order to understand; even approximately, the bearing of the various physicochemical processes on the character of the generated (*smoke*) aerosol it is essential to know in some detail the composition of the tobacco from which the aerosol is produced … It will be recognized that the use of different blending quantities of the several varieties of tobacco, or of different processing methods can markedly influence the quantitative composition of (*tobacco*), … but the differences are likely to be more quantitative than qualitative. (1665)

In his review, Hobbs included a figure illustrating the approximate chemical composition of blended cigarette tobacco. Figure 0.1 is a representation of those same data.

Table 4.1 summarizes the numbers of carboxylic acids and amino acids identified to date in tobacco and tobacco smoke. Their listing and references are presented in subsequent chapter tables (Tables 4.3 and 4.10).

The data that Hobbs used were collected over many years by scientists at Liggett and Myers Tobacco Company. Hobbs' data were subsequently reproduced by Green (1351, 1352b), in tabular form, see Table 0.1. Hobbs' original figure showed the approximate chemical composition of blended cigarette tobacco (at ~12% moisture). The data from Green (1351, 1352b) were calculated on a dry weight basis.

The data in Table 0.1 show three columns. The original data by Hobbs (1665) are in the second column. Hobbs' data included water, humectants, and flavorants on the tobacco. Column three is the same data as in column two, but the data were recalculated to remove water, the added humectants, and the applied flavorants. As can be seen in column three, the carbohydrates (sugars, celluloses, pectic substances, starch, and pentosans) represent nearly 41% of the dry weight of tobacco. Lignin accounts for about 4% of the weight. The tobacco protein and amino acids represent about 10% of the dry tobacco weight. The volatile bases and alkaloids make up about 4% of the tobacco weight. Waxes and resins (the ether extractable portion of tobacco) represent about 10% of the dry tobacco weight. Metals (6%) and inorganic ions (1.8%) make up another 7.8% of the tobacco weight. The phenolics

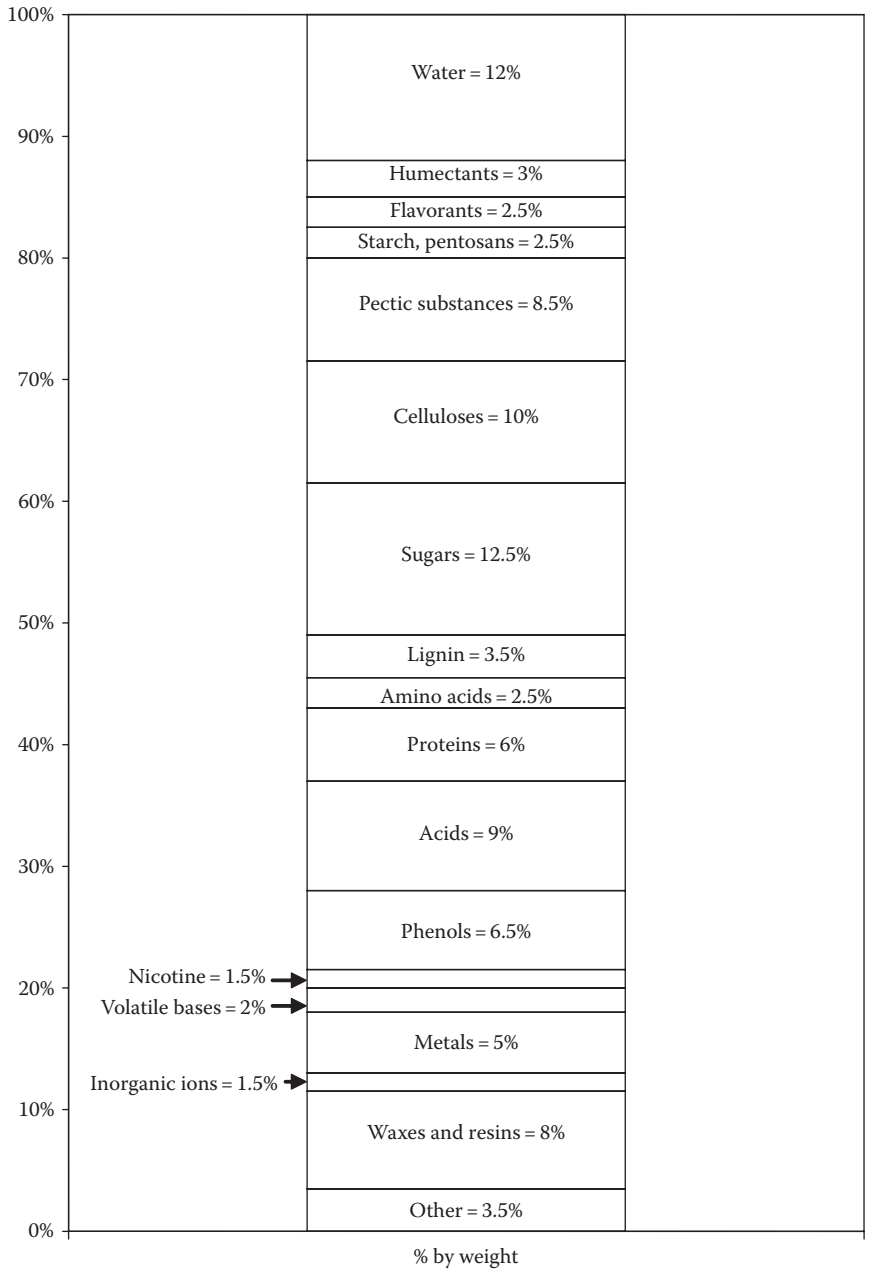

FIGURE 0.1 Approximate chemical composition of blended cigarette tobacco (1665).

and acids represent about 8% and 11% of the dry tobacco weight, respectively. Together, these tobacco constituents account for about 96% of the dry weight of tobacco. Hobbs (1665) added a category called "others" (at about 4%) which accounted for the remaining unaccounted for weight. Much of the "other" category was believed to be composed of dirt, sand, and other intractable materials.

To date, as indicated on the last page of our Alphabetical Component Index, 5596 separate components have been identified in tobacco. Table 0.2 contains three columns of information: the classification of the tobacco component(s), the average concentration of the component(s) in percent (%) dry weight of tobacco, and references to tables in the second edition of this book [Green (1351) and others that support the concentration data]. There are four broad classes of tobacco components in Table 0.2: hydrocarbons, oxygen-containing components, nitrogen-containing components, and miscellaneous components.

It must be noted that the majority of compounds found in tobacco are multifunctional. For example, polyfunctional *O*-containing compounds are counted in each functional group, e.g., propanoic acid, 2-hydroxy- (lactic acid) appears in the alcohol section and the acid section; benzoic acid, 4-hydroxy-3-methoxy- (vanillic acid) appears in the acid section, the phenol section, and the ether section. In Table 0.2, care was taken to count each tobacco isolate in only one of the component categories. Every attempt was made not to duplicate any of the 5596 tobacco compounds identified to date in tobacco. To accomplish this, a method for segregation of compounds, particularly those that were multifunctional,

TABLE 0.1
Approximate Chemical Composition of Blended Cigarette Tobacco (1665, 1351, 1352b)

Component	Wet Weight Blended Cigarette Tobacco, %	Dry Weight Tobacco (Only)[a], %
Carbohydrates		
Sugars	12.5	15.15
Celluloses	10.0	12.12
Pectic substances	8.5	10.36
Starch, pentosans	2.5	3.03
Water	12.0	0
Proteins and amino acids		
Proteins	6.0	7.27
Free amino acids	2.5	3.03
Bases		
Volatile bases	2.0	2.42
Nicotine	1.5	1.81
Waxes and resins	8.0	9.69
Metals	5.0	6.06
Phenols	6.5	7.87
Acids	9.0	10.90
Lignin	3.5	4.24
Humectants	3.0	0
Flavorants	2.5	0
Inorganic ions	1.5	1.81
Others	3.5	4.24
Total	100	100

[a] Percent dry weight = minus water, humectants, and added flavorants.

was used. The hierarchical system chosen for the segregation of the chemicals was patterned after the organization of chemical compounds in Beilstein [Heller (1990)]. That is, compounds without functional groups (i.e., the hydrocarbons) were followed by hydroxyl compounds, oxo compounds, carboxylic acids, amines, etc. As in Beilstein, the concept of parents and derivatives was followed. For example, phenol would be considered a parent. All substituted phenols were grouped with phenol as derivatives. Although, the strict rules used in Beilstein were not always applied, all of the 5596 compounds were accounted for in a logical manner.

The second column of data in Table 0.2 lists the average concentration of tobacco compounds. The values listed were obtained from several sources. Primarily, the concentration data were obtained from the present text, Rodgman and Perfetti (5078), Green (1351, 1352b), Hobbs (1665), various reports from the RJRT Company database (www.rjrtdoc.doc), Demole et al. (937–943), Dickerson et al. (965), Leffingwell (2337–2339, 2339a, 2339b, 2341), Lloyd et al. (2389), Roberts et al. (3215, 3219), Schumacher (3550, 3560, 3561), Schlotzhauer et al. (3458), Stedman (3797), Tso (3973, 3974a), Weeks (4159), and from years of personal experience (TAP) in tobacco science. In most cases, concentrations of the largest tobacco compounds (those greater than 0.05%) were obtained from literature sources. Although in a few cases, particularly those classes of compounds that had low to very low (0.001%–0.000001%) concentrations, e.g., anhydrides, quinones, oxazoles, aza-arenes, the concentrations were estimated.

Column three of Table 0.2 contains references to tables of data in this text and/or papers by Green (1351, 1352b) and others.

The chemical class of compounds in tobacco that has the largest mass is the oxygen-containing compounds (75.70%), followed by the nitrogen-containing compounds (12.98%), miscellaneous compounds (10.61%, including the category "Others" at 1.21%), and finally the hydrocarbons (0.71%). Within the oxygen-containing components, the largest single subclass of chemical components was the carbohydrates at 40.2%. There are 15.15% sugars, 12.12% celluloses, 10.36% pectins, and 3.03% starch. There are 9.8% carboxylic acids and 9.0% lipids (waxes) and resins in tobacco. In the lipids (waxes) and resins category, about 60% of the weight is lipids and 40% is resins. The lipids and resins category contain those compounds that prior to the 1950s were collected as part of the alcohol-ether-soluble fraction of tobacco. The phenolic category contains 8.3% of the dry mass of tobacco. About 2.25% of the weight of the phenolic category is lignin. The remainder of the weight from the oxygen-containing class of tobacco is composed of alcohols, phytosterols (and their derivatives), aldehydes, ketones, amino acids, esters, lactones, anhydrides, quinones, and ethers, ranging in levels from 2.0% to 0.0001% by weight of the dry mass of tobacco.

The two largest categories of compounds that contribute to the nitrogen-containing class of chemicals found in tobacco are the proteins and amino acids (6.4%) and the nitrogen heterocyclic compounds, which includes numerous types of tobacco alkaloids and related compounds (6.5%). The remainder of the weight from the nitrogen-containing class of tobacco is composed of amides, imides, *N*-nitrosamines, nitroalkanes, nitroarenes, nitrophenols, lactams, oxazoles, and aza-arenes. The mass of all of these remaining nitrogen-containing compounds represents only 0.08% of the dry weight of tobacco.

The third largest class of components found in tobacco was called "miscellaneous components" because it includes a broad range of chemical classes: sulfur-containing compounds; halogen-containing compounds; metals, nonmetals, and ions; pesticide residues; and the unknown components called "others." In the third class, the largest contributors to tobacco mass are the metals, nonmetals, and ions (7.2%). The halogen-containing compounds contribute 1.5% of the dry tobacco weight. Sulfur-containing compounds contribute 0.7% of the dry tobacco weight, and approximately 1.21% of the dry tobacco weight is compounds grouped as "others." Pesticide residues in tobacco contribute very little to the total tobacco mass (0.00001%).

The last class of components identified in tobacco is the hydrocarbons (alkanes, alkenes, alkynes, alicyclics, monocyclic aromatics, and polycyclic aromatics). The total mass of the hydrocarbons is only 0.71% of the dry weight of tobacco. The largest contributors to mass from this class of components are

TABLE 0.2
Distribution and Approximate Composition of Tobacco

Classification of the Tobacco Component	Average Concentration, %	Tables in Present Text and Other References
Hydrocarbons		
Alkanes	0.32	Table 1.10
Alkenes and alkynes	0.09	Table 1.11
Alicyclics	0.22	Table 1.12
Monocyclic aromatic	0.08	Table 1.13
Polycyclic aromatic	0.0001	Table 1.19, Stepanov et al. (5567)
Subtotals	0.71	
Oxygen-Containing Components		
Alcohols	1.7	Table 2.5
Phytosterols and derivatives	0.2	Table 2.7
Aldehydes	1.4	Table 3.12
Ketones	1.8	Table 3.13
Carboxylic acids	9.8	Table 4.3
Lipids (waxes) and resins	9.0	Green (1352b)
Amino acids	2.0	Table 4.10
Esters	0.9	Table 5.3
Lactones	0.001	Table 6.2
Anhydrides	0.0001	Table 7.1
Carbohydrates	40.2	Table 8.3
Celluloses: 13.3%		
Pectins: 11.4%		
Sugars: 14.1%		
Starch: 1.4%		
Total: 40.2%		
Phenols	8.3	Table 9.22
Lignin: 2.25%		
All other phenolics: 6.05%		
Quinones	0.001	Table 9.24
Ethers	0.4	Table 10.2
Subtotals	75.70	
Nitrogen-Containing Components		
Nitriles	0.0001	Table 11.2
Proteins, enzymes, and amines	6.4	Tables 12.2 and 22.2
Amides	0.06	Table 13.1
Imides	0.02	Table 14.1
N-Nitrosamines	0.002	Table 15.8
Nitroalkanes, nitroarenes, and nitrophenols	0.00001	Table 16.1
Nitrogen heterocyclic components (volatile bases) 4.5%	6.5	Tables17.1, 17.3, 17.5, 17.6, 17.8, and 17.10
[Monocyclic four-membered *N*-containing ring compounds, monocyclic five-membered *N*-containing ring compounds, compounds with multiple monocyclic five-membered *N*-containing ring, monocyclic six-membered *N*-containing ring compounds, compounds with a six-membered *N*-containing ring and a second five-membered *N*-containing ring, compounds with two or more six-membered *N*-containing rings]		
Alkaloids: 2.0%		
Lactams	0.0001	Table 17.13
Oxazoles	0.00001	Table 17.14
Aza-arene, aza-arene derivatives, and *N*-heterocyclic amines	0.000001	Tables 17.21, 17.23, and 17.31
Subtotals	12.98	

(*continued*)

TABLE 0.2 (continued)
Distribution and Approximate Composition of Tobacco

Classification of the Tobacco Component	Average Concentration, %	Tables in Present Text and Other References
Miscellaneous Components		
Sulfur-containing	0.7	Table 18.1
Halogen-containing and fixed gases	1.5	Table 18.4, Table 19.5
Metal, nonmetals, and ions	7.2	Tables 20.5 and 20.6
Pesticide residues	0.00001	Table 21.3, Binkley (5037)
All other compounds	1.205577	
Subtotals	10.61	
Grand total	100.00	

the alkanes (0.32%) and the alicyclics (0.22%). The alkenes and alkynes (0.09%), the monocyclic aromatics (0.08%), and the polycyclic aromatics (0.000002%) round out the other hydrocarbons that contribute to the dry weight of tobacco.

Figure 0.2 illustrates the approximate chemical composition of tobacco based on the data of Table 0.2.

Table 0.3 is a comparison of the reported concentrations of chemicals found in tobacco from Hobbs (1665) compared to similar data entries in Table 0.2 of this report.

There is close agreement between the estimates of the gross compositional tobacco data reported by Hobbs (1665) in 1972 *vs*. the data of Table 0.2. The differences between the Hobbs' data and the data of Table 0.2 could be from differences in tobacco types tested or from improvements in analytical separation, detection, and quantification technologies. The differences in the subtotals for carbohydrates, proteins, and amino acids; Hobbs' classification of bases; and most of the other chemical classes are generally different by less than 1–2 weight percent. Under the classification of "Others" for the data of this report (column three), there is about 2.9% dry weight of tobacco (i.e., 4.1%–1.2% [from Table 0.2] = 2.9%) that represents hundreds of minor tobacco constituents not accounted for in the components listed in column one of this table. It is quite remarkable how qualitatively similar the data are between the Hobbs data and those from Table 0.2. As Hobbs (1665) mentioned in 1972, any "differences (*in the chemical composition of tobacco*) are likely to be more quantitative than qualitative."

Because of the excellent fractionation and identification technologies developed during the early 1950s, the compositions of tobacco and tobacco smoke, both classified as highly complex mixtures, have been defined more completely than the composition of any other highly complex commercial product such as coffee. By year-end 1953, the many years of research by scientists using classical chemical techniques to define the composition of tobacco and its smoke provided meaningful information on the nature of over 300 tobacco components and fewer than 100 tobacco smoke components. Those involved in the pre-1954 research not only provided the cornerstone of our knowledge of the two compositions but also deserve the gratitude of their successors for the early information generated on tobacco and its smoke. This article is our tribute to those researchers who generated much meaningful knowledge on the composition of tobacco and tobacco smoke prior to 1954 despite the now known fractionation and analytical limitations of the so-called classical chemical techniques. It also notes the similarity of some of the early and more recent research results obtained on the chemical and biological properties of smoke condensate and several of its components from tobacco with those obtained by Roffo in the 1930s on a destructive distillate of tobacco.

The compilation of the catalog on the more than 8400 chemical components identified in tobacco and tobacco smoke provided an excellent assessment of the caliber of the research conducted since its escalation in the mid-1950s. The classical chemical analysis used before that date to isolate and characterize a component of a complex mixture was gradually augmented post-1953 by the inclusion of many different, new, and highly efficient separation and analytical technologies. Various types of chromatography coupled with various spectral technologies such as ultraviolet, infrared, nuclear magnetic resonance, and mass provided the means to identify more complex structures of components isolated in much lesser amounts than could be done by using the classical chemical approach. For example, inclusion of such technologies resulted in the increase of the number of identified chemical components in tobacco smoke from the fewer than 100 reported by Kosak in 1954 (2170) to the more than 5200 cataloged recently by Rodgman and Perfetti (5078). The manifold scientific skills generated and employed during those more than 50 years of research obviously deserve great commendation.

In the early part of the twentieth century until the mid 1950s, there was limited interest in the relationship between the majority of identified chemicals in tobacco and tobacco smoke and the varied asserted health issues associated with smoking in general, compared to the time after the mid-1950s. This limited interest may have been due to a lack of understanding of how to interpret the chemical data collected on the complex mixtures of tobacco and tobacco smoke in relation to biological endpoint data. On the other hand, early tobacco research concentrated on a greater understanding of the alkaloids in tobacco.

In early tobacco research, nicotine and other related tobacco alkaloids were regarded as toxic constituents of

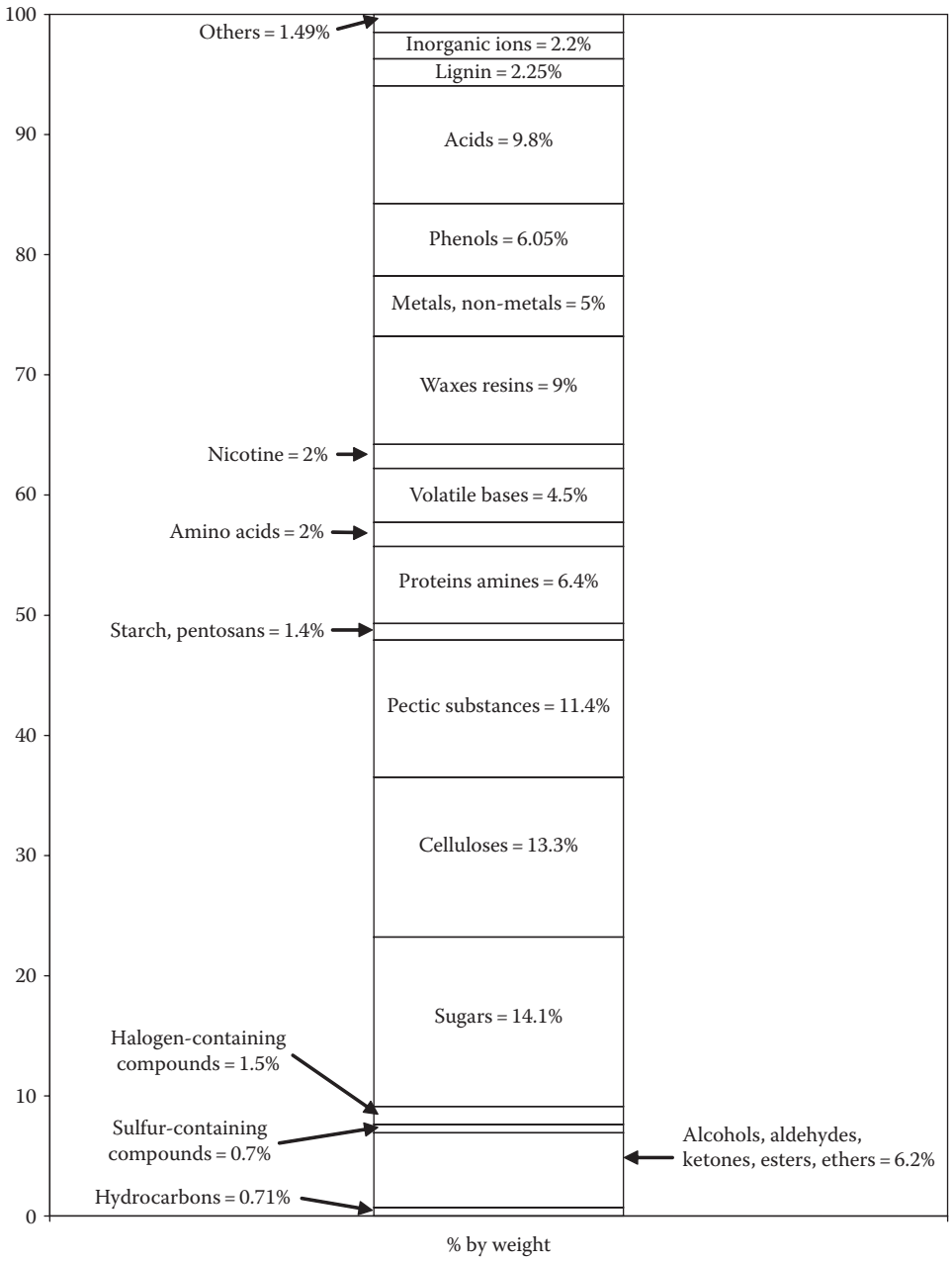

FIGURE 0.2 Approximate chemical composition of tobacco.

tobacco, and their presence in smoke was considered a health concern. Tobacco alkaloids were also important as raw materials for pesticides and as sources of raw material for the chemical industry. As a result, considerable effort was focused in the early years of tobacco research on nicotine and related tobacco alkaloids. This work included the development of new analytical determinations for tobacco alkaloids and tests to measure its toxicity and dependence of nicotine for smokers. Work in the area of breeding new tobacco lines was focused on two directions. Efforts were directed at developing low nicotine or nicotine-free tobaccos for health reasons and secondly, in the direction of tobaccos extremely high in nicotine, as a raw material for pesticides, chemicals, and pharmaceuticals.

During our cataloging of the chemical components of tobacco and tobacco smoke, it became apparent that the chemical research conducted on them from early in the 1800s to September 1953, the date of submission of the Kosak's manuscript for publication, also deserved considerable commendation. Considerable skill in classical chemical methods was used to isolate and characterize the tobacco and smoke components known by late 1953. In this article, the results of that research are summarized in an attempt to illustrate that not only should they not be minimized or disregarded but also the investigators who generated such meaningful results deserve considerable credit.

One of the stimuli cited by Kosak (2170) for the generation of his 1954 catalog of tobacco smoke components was the brief

TABLE 0.3
Comparison of Hobbs (1665) Data on Approximate Chemical Composition of Blended Cigarette Tobacco Compared to Similar Data of Table 0.2

Component	Hobbs Tobacco Data Dry Weight Basis, %	Dry Weight Tobacco Data from Table 0.2, %[a]
Carbohydrates		
Sugars	15.15	14.1
Celluloses	12.12	13.3
Pectic substances	10.36	11.4
Starch, pentosans	3.03	1.4
Subtotal	40.66	40.2
Proteins and amino acids		
Proteins, enzymes, and amines	7.27	6.4
Free amino acids	3.03	2.0
Subtotal	10.3	8.4
Bases		
Volatile bases	2.42	4.5
Nicotine	1.81	2.0
Subtotal	4.23	6.5
Lipids (waxes) and resins	9.69	9.0
Metals	6.06	5.0
Phenols	7.87	6.05
Acids	10.90	9.8
Lignin	4.24	2.25
Inorganic ions	1.81	2.2
Others	**4.24**	**4.1**
Total	100	100

1952 published report by Graham et al. (5202) on the induction of tumors in laboratory animals repeatedly painted with large doses of cigarette smoke tar, a report that was followed in early 1953 by a presentation at the American Association for Cancer Research (4306a) and then by a detailed publication in a peer-reviewed scientific journal in late 1953 (4306a). Wynder et al. (4306a) described many of the early studies on the effects of exposure of laboratory animals to various tars, including those derived from tobacco by smoking or extraction [E. Hoffmann et al. (1813), Helwig (1617, 5221), Bogen and Loomis (377), Cooper et al. (813), Campbell (579, 581), Schürch and Winterstein (3563), Taki (3865), Sugiura (5415), Flory (1206, 5178), and Shubik (3663)]. An early study reported in 1911 by Wacker and Schmincke (5446) preceded the development and description of the procedure to induce cancer in laboratory animals by skin painting with coal tar in 1915–1918 by Yamagiwa and Ichikawa (4361). As noted by Wynder et al. (4306a), each of the tobacco tar studies conducted after the Yamagiwa–Ichikawa reports suffered from one or more deficiencies such as a low number of daily or weekly paintings, low tar-painting dosage, inadequate smoking procedure for tar collection, and the like. However, seldom discussed is the fact that the Wynder et al. study involved a cigarette smoking procedure (35 mL puff, 2 s puff, 3 puff/min) different from the one in vogue since its elucidation (35 mL puff, 2 s puff, 1 puff/min) by Bradford et al. in 1936 (423b). Tripling the puff/min not only substantially increases the per-cigarette-tar yield but also drastically alters its composition, with substantial increases in several smoke components with known tumorigenicity to mouse skin, e.g., PAHs benzo[*a*]pyrene (B[*a*]P) and dibenz[*a,h*]anthracene (DB[*a,h*]A).

Other reports that triggered interest in the biological properties and chemical composition of CSC were the numerous publications between 1950 and 1953 on the epidemiology of lung cancer and cigarette smoking. They were presented in 1950 by Wynder and Graham (4306b), Doll and Hill (1026a), Levin et al. (2355), Mills and Porter (2556), and Schrek et al. (3529). These were followed in 1952 and 1953 by similar extensive studies conducted by Doll and Hill (1027), McConnell et al. (2515), Koulumies (4250), Lickint (5266), and Sadowsky et al. (3375a). It should be noted that the prospective method did not replace retrospective studies. Both approaches have their advantages and disadvantages. In the retrospective study, interviewers record the habits of smokers and controls; the prospective studies are better suited to survey larger groups of diseased and controls in terms of their environment, their behaviors, and specific diseases they contract.

Preceding these 1950–1953 epidemiological studies were several reported from 1912 to 1950, but in their 1950 report, Graham and Wynder (4306b) described in general several of the deficiencies of the earlier epidemiological studies, e.g., small sample size, lack of a control population, statistical procedure, tumor definition. Among the earlier studies were reports and/or comments on respiratory tract cancer by Adler (5096) in 1912, by Tylecote (5425) in 1927, by Lickint (5265) in 1935, by Arkin and Wagner (5101) in 1936, by Kennaway and Kennaway (5239, 5240) in 1936 and 1947, by Roffo (3322) in 1937, by Müller (5297) in 1939, by Ochsner and DeBakey (5316, 5317) in 1940 and 1941, and by Schairer and Schöninger (5370) in 1943.

The reports by Ochsner and DeBakey subsequently led to an interesting situation in the content of several U.S. Surgeon Generals' reports on smoking and health. From the late 1930s through the late 1960s, Ochsner, at that time one of the few eminent lung cancer surgeons in the United States, authored or coauthored over 40 articles and three books in which it was repeatedly asserted that the major cause of lung cancer was cigarette smoking. Despite his number of publications between the late 1930s and late 1963, the 1964 Advisory Committee to the U.S. Surgeon General (3999) and the 1979 (4005) and 1982 (4011) U.S. Surgeon Generals cited only one 1939 Ochsner-authored publication (5314) and one of his authored books, the 1954 edition (5315) on the relationship between lung cancer and cigarette smoking. Was the limitation of the citations of Ochsner's publications on cigarette smoking and lung cancer possibly due to either or both of the following situations?

1. Despite the repeated assertion that the major cause of lung cancer was cigarette smoking, Ochsner et al. frequently included other comments in the same articles, e.g., (a) the cause of the increasing incidence of cancer of the lung is not definite [see

p. 212 in (5317)], (b) the etiology of bronchogenic carcinoma is unknown (5320), and (c) the etiological picture (for bronchogenic carcinoma) is obscure. It is probable that there are a number of etiological factors in the production of this disease (5134).

2. Despite the repeated assertion that the major cause of lung cancer was cigarette smoking, the data on patients undergoing lung resection in the Ochsner Clinic because of lung cancer were summarized in several Ochsner et al.'s reports as follows: (a) In 129 resected cases, no factor was found which might bear a significant relationship to the occurrence of the disease. Neither occupation nor smoking habits, which some reports, including our own, have stressed as of possible etiological significance, seem of any special significance in this particular series (5318). (b) In the analysis of 147 resected cases, no etiological factor was found to bear a significant relationship to the occurrence of the disease. Both occupation and smoking, which had been particularly emphasized by some observers as possible etiological factors and which we were inclined previously to consider more seriously, were found to have no special significance in this analysis (5319).

CHEMICAL COMPONENTS OF TOBACCO AND TOBACCO SMOKE IDENTIFIED PRIOR TO 1954

Many components were identified in tobacco and/or tobacco smoke prior to the issuance of the 1954 Kosak's report (2170), the numerous epidemiological studies on tobacco smoking and respiratory cancer, and the 1953 report of tumor induction in laboratory animals by cigarette-tar painting (4306a). Most of the pre-1954 characterizations of such components were accomplished by the so-called classical chemical procedures. The components are listed in Table 0.4 with the identification and confirmation listed chronologically. If more than one study on a specific component was reported in a given year, the investigators in that year are listed alphabetically.

Examination of the data in Table 0.4 reveals the many investigators who contributed much meaningful information on tobacco and/or smoke composition prior to year-end 1953. They include the following: Brückner, Burkhard, Eulenberg, Frankenburg, Gabelya, Garner, Gottscho, Kipriyanov, Kissling, Kobel Lehmann, Molinari, Neuberg, Pfyl, Pontag, Preiss, Pyriki, Roffo, Schöller, Shmuk, Späth, Thoms, Vohl, and Wenusch. Each of them deserves much tribute for their contributions. Several of them continued to contribute to our knowledge of the composition of tobacco and/or tobacco smoke after 1953, e.g., Frankenburg, Garner, Gottscho, and Pyriki.

Compared to the fewer than 100 tobacco smoke components listed by Kosak (2170), Table 0.4 contains 325 chemical components identified and studied in tobacco prior to the publication of the Kosak's article. Included in 383 entries in Table 0.4 (as they were in the Kosak's tabulation) are several components originally assumed to be individual alkaloid-related components but subsequently were found to be known compounds or mixtures of known compounds, e.g., anodmine, gudham, lathrein, lohitam, obelin, poikiline, α-socratine, β-socratine, and γ-socratine (4208, 4209, 4210, 4211, 4213). They were not included in the count of the 325 identified tobacco components. The eventual characterization of anodmine, gudham, lathrein, lohitam, obelin, and the three socratines was described in 1955 by Kuffner et al. (2224). Their characterization of these supposedly alkaloid-related components was summarized by Johnstone and Plimmer (1971) in their 1959 review of tobacco and tobacco smoke composition. They wrote in 1959

> The constitution of these bases remained unknown until recently when investigators having access to original specimens were able to elucidate the identities of some of them by application of modern analytical techniques. γ-Socratine was found to be identical with *l*-nornicotine, and a crude mixture of α- and β-socratine (the only sample available), was shown to consist mainly of nicotyrine and 2,3′-dipyridyl with small quantities of nicotinic acid, nornicotine, and possibly anatabine (2224).

While noting that both ammonia and nicotine were previously identified as tobacco smoke components, Kosak elected not to list references to them because their number of references, in his opinion, was too numerous to list. Also the number of references to carbon dioxide and carbon monoxide was limited by Kosak (2170). Table 0.4 lists many of the pre-1954 references to ammonia, nicotine, carbon dioxide, and carbon monoxide in tobacco and/or tobacco smoke. Included in Table 0.4 are several pesticide residues, e.g., arsenic/arsenic (As) oxide, Toxaphene®, Lindane®, Parathion®, DDT, and TEPP (tetraethyl pyrophosphate), plus several pesticide residue degradation products, e.g., *o*,*p*′-DDD and *m*,*p*′-DDD, identified by Vinzant in 1951 (5439). Listed in Table 0.4 are a few compounds used as flavorants on tobacco products, most notably menthol which, however, occurs naturally in trace amounts in several tobacco types. Table 0.4 also cites numerous references to pre-1954 studies of a general nature. These include references to arsenical insecticides, alkaloids, aliphatic acids, aliphatic hydrocarbons amino acids, bases, tobacco distillates, tobacco fats, chlorophyll degradation products, enzymes (general information), hydrocarbons, hygroscopic agents, paraffins, pigments, sugars, tobacco combustion products, tobacco (general), tobacco smoke (general), and triglycerides. These items are not included in the total of 325.

Among metals, nonmetals, and ions, Kosak in his 1954 catalog listed only arsenic plus four ions as smoke components, and Kosak questioned the identification of each of the latter. Examination of Table 0.4 reveals that over 50 metals, nonmetals, and ions were identified in tobacco prior to late 1953. However, it was post-1953 when a concerted effort was made to determine the transfer of numerous metals from tobacco to tobacco smoke during the smoking process, e.g., the 1957 study by Cogbill and Hobbs (769). The references

TABLE 0.4
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
75-07-0	Acetaldehyde	1908 Brasch and Neuberg (5135)	1926 Neuberg and Kobel (2702a)
		1909 Brasch (5136)	1931 Neuberg and Burkard (2702)
		1931 Neuberg and Burkard (2702)	1936 Dixon et al. (5165)
		1933 Pfyl (2936)	
		1954 Kosak (2170)	
	Acetate	1939 Roffo (**D**) (3324, 5359)	
		1954 Kosak (2170)	
64-19-7	Acetic acid	1843 Zeise ([i]) (**Dr**) (4406)	1871 Vohl and Eulenberg (4064)
		1871 Vohl and Eulenberg (4064, 4065)	1884 Takayama (5419)
		1892 Abeles and Paschkis (18)	1909 Garner (1276)
		1929 Gabelya and Kipriyanov (**Dr**) (1263)	1924 Shmuk (5381)
		1931 Neuberg and Burkard (2702)	1929 Balabucha-Popzova (5114)
		1937 Bradford et al. (424)	1929 Shmuk (3655b)
		1939 Roffo (**D**) (3324, 5359)	1931 Yamafuji (5478)
		1950 Peterson (2934)	1935 Koenig (2154)
		1951 Garner (5189)	1936 Dixon et al. (5165)
		1952 James and Martin (1917)	1941 Sabetay et al. (3374)
		1954 Kosak (2170)	1951 Garner (5189)
	Acids, aliphatic	1931 Neuberg and Burkard (2702)	1930 Shmuk and Piatnicki (3655b)
		1937 Wenusch and Schöller (4214)	1931 Yamafuji (5478)
		1940 Haag (5207)	1943 Venkatarao et al. (4042b)
		1954 Kosak (2170)	1953 Wada and Kobashi (5447)
	Acids, amino-		1951 Roberts and Wood (5353)
			1952 Frankenburg and Gottscho (1223)
			1953 Pearse and Novellie (2911c)
			1953 Zacharius and Frankenburg (4398c)
	Acids, nonvolatile		1914 Garner et al. (5194)
			1931 Vickery and Pucher (5433)
			1933 Pucher and Vickery (3001a)
			1951 Garner (5189)
	Acids, phenolic	1939 Roffo (**D**) (3324, 5359)	
		1954 Kosak (2170)	
7440-34-8	Actinium		1937 Drobkov (5167)
56-41-7	*L*-α-Alanine		1952 Frankenburg and Gottscho (1223)
			1953 Pearse and Novellie (2911c)
			1953 Zacharius and Frankenburg (4398c)
107-95-9	β-Alanine		1953 Pearse and Novellie (2911c)
			1953 Zacharius and Frankenburg (4398c)
	Aldehydes		1953 Ross (3335)
	Alkaloids, tobacco or tobacco smoke	1931 Shmuk and Kolesnik (3659)	1901 Pictet and Rotschy (5332, 5333)
		1939 Wenusch (5457)	1908 Pictet and Court (4837a)
		1953 Latimer (2269)	1931 Ehrenstein (1116)
			1938 Marion (5271)
			1939 Späth and Kuffner (3761)
			1941 Jackson (17B18)
			1948 Frankenburg (1221)a
			1952 Badgett et al. (5111)
			1953 Tso and Jeffrey (3983a)
7429-90-5	Aluminum	1952 Bailey (160)	1932 Eisenmenger (5170)
			1938 McMurtrey and Robinson (5285)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
			1938 Morgan and Street (5291)
			1944 LeCompte (20A57)
			1951 Garner (5189)
	Amines, aliphatic	1929 Gabelya and Kipriyanov (**Dr**) (1263)	
7664-41-7	Ammonia	1857 Vogel (4060, 4061)	1885 Müller-Thurgen (5298)
		1858 Vogel (4062)	1894 Behrens (5126)
		1871 Vohl and Eulenberg (4064, 4065)	1908 Pictet and Court (4837a)
		1879 Périgord (2928)	1914 Garner et al. (5194)
		1880 LeBon (2326)	1928 Shmuk (5382)
		1899 Thoms (3909)	1929 Gabelya and Kipriyanov (1263)
		1900 Thoms (3910)	1930 Smirnov and Izvoshtshikov (5396)
		1902 Pontag (2973)	1936 Dixon et al. (5165)
		1903 Pontag (2973)	1936 Preiss (2987)
		1908 Biederbeck (5129)	1937 Fromm (1244)
		1908 Lee (5263)	1939 Gaertner (5186)
		1908 Lehmann (2342a)	1939 Shmuk (5389)
		1909 Lehmann (2343)	1948 Pyriki (3022)
		1910 Toth and Krampera (3934)	1950 Molinari (2607)
		1911 Vaubel (4041)	1951 Garner (5189)
		1912 Anonymous (5099, 5100)	1952 Hough et al. (1835b)
		1928 Shmuk (5382)	1952 Jensen (1941)
		1929 Bogen (375)	
		1929 Gabelya and Kipriyanov (**Dr**) (1263)	
		1929 Koperina (2161)	
		1931 Gavrilov and Koperina (1277)	
		1931 Haley et al. (1489)	
		1931 Shmuk and Kolesnik (3659)	
		1932 Barta and Toole (197, 198)	
		1932 McNally (2524)	
		1933 Pfyl (2937)	
		1934 Barta (195)	
		1936 Bogen (376)	
		1936 Preiss (2986–2988)	
		1937 Bradford et al. (424)	
		1939 Dittmar (985–987)	
		1939 Roffo (**D**) (3324, 5359)	
		1939 Shmuk (5389)	
		1948 Pyriki (3022)	
		1950 Peterson (2934)	
		1951 Garner (5189)	
		1952 Larsen (2263)	
		1954 Kosak (2170)	
	Ammonium salts	1936 Cuvelier (5159)	
	Ammoresinol		1936 Späth and Zajic (3763)
9000-92-4	Amylase		1913 Oosthuizen and Shedd (5323)
			1937 Matsumina (5275)
			1942 Ward (5449)
			1946 Garner (5188)
			1951 Garner (5189)
			1951 Nakai and Inaba (5301)
			1953 Barrett et al. (5123)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]**	**Tobacco**
	Anabaseine		1939 Henry (5222)
	Anodmin = mixture of basic components of tobacco and its smoke (2224)	1935 Wenusch and Schöller (4210, 4211) 1936 Wenusch and Schöller (5462) 1954 Kosak (2170)	1935 Wenusch and Schöller (4210, 4211)
120-12-7	Anthracene	1939 Roffo (**D**) (3323, 3324, 5359) 1953 Cooper and Lindsey (818) 1954 Kosak (2170)	
7440-36-0	Antimony		1934 Heffer et al. (20A26)
147-81-9	Arabinose		1929 Gabelya and Kipriyanov (1263)
7004-12-8	Arginine		1933 Vickery et al. (5436) 1935 Vickery et al. (5435) 1951 Garner (5189) 1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
7440-38-2	Arsenic	1922 Leitch and Kennaway (5264) 1927 Remington (3104) 1932 McNally (2524) 1934 Gross and Nelson (1430) 1935 Bastedo (5124). 1945 Thomas and Collier (3899) 1947 Griffon and Delga (1395) 1950 Daff and Kennaway (889, 5160) 1951 Daff et al. (889a) 1952 Goulden et al. (5201) 1953 Monnet and Dupont (2609) 1954 Kosak (2170)	1905 Boening (373) 1922 Leitch and Kennaway (5264) 1927 Remington (3104) 1928 Popp (2978, 5338) 1934 Carey et al. (5142) 1935 McMurtrey (5281) 1938 McMurtrey (5283) 1939 Barksdale (5119) 1940 Barksdale (5120) 1941 McMurtrey (5284) 1942 Vucetich and Carratala (4070) 1944 Vincent (5438) 1947 Griffon and Delga (1395) 1950 Daff and Kennaway (889, 5160) 1951 Daff et al. (889a) 1951 Garner (5189) 1951 Oliver (5322) 1952 Bunce (5139) 1953 Monnet and Dupont (2609) 1953 Wolff et al. (4273)
1327-53-3	Arsenic oxide (As_2O_3)	1927 Remington (3104) 1932 McNally (2524) 1934 Gross and Nelson (1430) 1935 Bastedo (5124) 1945 Thomas and Collier (3899) 1947 Griffon and Delga (1395) 1950 Daff and Kennaway (889, 5160) 1951 Daff et al. (889a) 1952 Goulden et al. (5201) 1953 Monnet and Dupont (2609) 1954 Kosak (2170)	1905 Boening (373) 1927 Remington (3104) 1928 Popp (2978, 5338) 1934 Carey et al. (5142) 1935 McMurtrey (5281) 1938 McMurtrey (5283) 1940 Barksdale (5120) 1941 McMurtrey (5284) 1942 Vucetich and Carratala (4070) 1947 Griffon and Delga (1395) 1950 Daff and Kennaway (889, 5160) 1951 Daff et al. (889a) 1951 Garner (5189) 1953 Monnet and Dupont (2609)
	Arsenical insecticides		1901 Marlatt (5272) 1908 Marlatt (5273)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
50-81-7	Ascorbic acid		1947 Maton (2489) 1951 Lona and Porzio-Giovanola (5267a) 1951 Tombesi (3922)
7006-34-0	Asparagine		1894 Behrens (5126) 1937 Vickery et al. (5437) 1951 Garner (5189) 1952 Frankenburg and Gottscho (1223) 1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
56-84-8	Aspartic acid		1952 Frankenburg and Gottscho (1223) 1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
275-51-4	Azulene	1947 Ikeda (1857) 1954 Kosak (2170)	
7440-39-3	Barium		1913 McHargue (5278) 1913 Traetta-Mosca (5422) 1916 Artis and Maxwell (5103) 1916 Knight (5245) 1921 Headden (5218)
	Bases	1940 Haag (5207)	1931 Yamafuji (5478) 1934 Nito and Kitamura (5311)
100-52-7	Benzaldehyde	1931 Neuberg and Burkard (2702) 1954 Kosak (2170)	
	Benzenamine, alkyl- {coridine}		1871 Vohl and Eulenberg (4064)
	Benzenamine, alkyl- {rubidine}		1871 Vohl and Eulenberg (4064)
	Benzenamine, alkyl- {viridine}		1871 Vohl and Eulenberg (4064)
	Benzenamine, 4-(1,1-dimethylethyl)- {parvoline}		1871 Vohl and Eulenberg (4064)
53-19-0	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDD; *o,p′*-TDE}		1951 Vinzant (5439)
4329-12-8	Benzene, 1-chloro-3-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*m,p′*-DDD}		1951 Vinzant (5439)
789-02-6	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDT}		1951 Vinzant (5439)
50-29-3	Benzene, 1,1′-(2,2,2-trichloroethylidene) bis[4-chloro- {*p,p′*-DDT}		1951 Vinzant (5439)
100-21-0	1,4-Benzenedicarboxylic acid {terephthalic acid}		1946 Frankenburg (5180)
120-80-9	1,2-Benzenediol {catechol}	1893 Kissling (5243) 1936 Molinari (2605) 1950 Molinari (2607)	1935 Koenig (2154)
123-31-9	1,4-Benzenediol {hydroquinone}		1952 Volgunov (5440)
100-51-6	Benzenemethanol {benzyl alcohol}	1939 Wenusch (4202)	1939 Wenusch (4202)
65-85-0	Benzoic acid {benzenecarboxylic acid}	1931 Neuberg and Burkard (2702) 1939 Wenusch (4202) 1940 Haag (5207) 1954 Kosak (2170)	
99-50-3	Benzoic acid, 3,4-dihydroxy- {protocatechuic acid}		1929 Shmuk (3655b)
149-91-7	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}		1929 Shmuk (3655b)
59-02-9	2*H*-1-Benzopyran-6-ol,3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)- {α-tocopherol}		1945 Riemenschneider et al. (3155)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
92-61-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin}		1948 Best (5127) 1953 Johanson (5235)
21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		1935 Kurilo (5255) 1937 Kurilo (5256) 1950 Howard et al. (1837a)
117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetrin}		1935 Kurilo (5255) 1936 Neuberg and Kobel (2704a) 1950 Howard et al. (1837a)
153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin}		1931 Hasegawa (5217) 1935 Kobel and Neuberg (2153a) 1935 Neuberg and Kobel (5304) 1936 Neuberg and Kobel (2704a, 5305) 1944 Couch and Krewson (5156, 5157) 1944 Griffith et al. (5204) 1947 Couch (828b) 1949 Badgett et al. (5110) 1951 Garner (5189) 1951 Nio and Wada (5310)
480-10-4	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glycoside}		1953 Wada (4072a)
50-32-8	Benzo[*a*]pyrene	1937 Roffo (**D**) (3316) 1939 Roffo (**D**) (3323–3325, 5359) 1941 Roffo (**D**) (3326) 1942 Roffo (**D**) (3327) 1954 Kosak (2170)	
8001-35-2	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated {Toxaphene®}		1951 Vinzant (5439)
507-70-0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *endo*- {borneol}		1941 Sabetay et al. (3374)
366-18-7	2,2′-Bipyridine		1901 Pictet and Rotschy (5332) 1928 Shmuk (5382)
581-50-0	2,3′-Bipyridine		1928 Shmuk (5382) 1936 Späth and Zajic (3763) 1939 Späth and Biniecki (5403) 1946 Frankenburg (1221) 1952 Frankenburg and Gottscho (1223) 1953 Tso and Jeffrey (3983a)
581-49-7	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (S)- {*l*-anatabine}		1937 Späth and Kesztler (5406, 17B55) 1946 Frankenburg (1221) 1948 Shmuk (5390) 1953 Tso and Jeffrey (3983a)
5953-51-5	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-methyl-, (S)-		1937 Späth and Kesztler (5407) 1946 Frankenburg (1221)
7440-69-9	Bismuth		1934 Heffer et al. (20A26)
7440-42-8	Boron	1952 Bailey (160)	1923 Warrington (5450) 1926 Sommer and Lipman (5402) 1927 Swanback (5417) 1929 McMurtrey (5279) 1934 Van Schreven (5429) 1935 McMurtrey (5281)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
			1938 McMurtrey (5283)
			1938 McMurtrey and Robinson (5285)
			1938 Morgan and Street (5291)
			1941 McMurtrey (5284)
			1950 Steinberg (5413)
			1951 Garner (5189)
			1952 Lashkevvich (5261)
123-72-8	Butanal	1908 Brasch and Neuberg (5135)	
		1909 Brasch (5136)	
		1931 Neuberg and Burkard (2702)	
		1954 Kosak (2170)	
107-89-1	Butanal, 3-hydroxy- {aldol}	1931 Neuberg and Burkard (2702)	
107-85-7	1-Butanamine, 3-methyl- {isoamyl amine}		1911 Ciamician and Ravenna (5147)
			1928 Shmuk (5382)
110-15-6	Butanedioic acid {succinic acid}	1939 Roffo (**D**) (3324, 5359)	1924 Shmuk (5381)
		1954 Kosak (2170)	1929 Shmuk (3655b)
			1930 Shmuk (5384)
6915-15-7	Butanedioic acid, hydroxy- {malic acid}		1809 Vauquelin5430
			1884 Takayama (5419)
			1894 Behrens (5126)
			1904 Kissling (5244)
			1924 Shmuk (5381)
			1929 Shmuk (3655b)
			1931 Yamafuji (5478)
			1930 Shmuk (5384)
			1935 Koenig (2154)
			1937 Pucher et al. (5342)
			1939 Shmuk (5389)
			1951 Bacon et al. (5109)
			1951 Garner (5189)
			1952 Bacon et al. (5109)
			1953 Phillips and Bacot (2947c)
			1953 Wright and Burton (5477)
16426-50-9	Butanedioic acid, hydroxy-, calcium salt		1937 Pucher et al. (5342)
			1951 Garner (5189)
869-06-7	Butanedioic acid, hydroxy-, magnesium salt		1937 Pucher et al. (5342)
			1951 Garner (5189)
585-09-1	Butanedioic acid, hydroxy-, potassium salt		1937 Pucher et al. (5342)
			1951 Garner (5189)
431-03-8	2,3-Butanedione	1935 Neuberg and Kobel (2704)	1929 Schmalfuss and Barthmeyer (5371)
		1939 Schmalfuss (3475)	1932 Schmalfuss and Schmalfuss (5372)
		1950 Schmalfuss (3475)	1935 Neuberg and Kobel (2704)
		1953 Sasaki (3413)	
		1954 Kosak (2170)	
107-92-6	Butanoic acid	1843 Zeise (4406)	1871 Vohl and Eulenberg (4064)
		1871 Vohl and Eulenberg (4064, 4065)	1909 Garner (1276)
		1900 Thoms (3910)	1924 Shmuk (5381)
		1904 Thoms (3912)	1929 Shmuk (3655b)
		1931 Neuberg and Burkard (2702)	
		1935 Wenusch (4185)	

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
		1951 Garner (5189)	
		1952 James and Martin (1917)	
		1954 Kosak (2170)	
56-12-2	Butanoic acid, 4-amino- {4-aminobutyric acid}		1952 Frankenburg and Gottscho (1223)
			1953 Pearse and Novellie (2911c)
			1953 Zacharius and Frankenburg (4398c)
503-74-2	Butanoic acid, 3-methyl- {isovaleric acid}		1946 Frankenburg (5180)
2055-23-4	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)- {pseudooxynicotine}		1939 Henry (5222)
71278-11-0	1-Butanone, 4-amino-1-(3-pyridinyl)- {poikiline}		1948 Wenusch (4207)
538-79-4	3-Buten-1-amine, *N*-methyl-4-(3-pyridinyl)- {metanicotine, nicotimine}		1928 Shmuk (5382)
			1948 Shmuk (5390)
110-17-8	2-Butenedioic acid (*E*)- {fumaric acid}	1939 Roffo (**D**) (3324, 5359)	1924 Shmuk (5381)
		1954 Kosak (2170)	1929 Shmuk (3655b)
			1930 Shmuk (5384)
7440-43-9	Cadmium		1934 Heffer et al. (20A26)
7440-70-2	Calcium	1952 Bailey (160)	1907 Garner (5187)
			1928 Bailey and Anderson (5113)
			1935 Koenig (2154)
			1950 Steinberg (5413)
			1951 Garner (5189)
			1952 Bacon et al. (5109)
			1953 Bortner and Hamilton (5133)
7440-44-0	Carbon		1934 Garner et al. (5192, 5193)
			1951 Garner (5189)
124-38-9	Carbon dioxide	1843 Zeise (4406)	1909 Boekhout and de Vries (5132)
		1899 Thoms (3909)	1934 Garner et al. (5192, 5193)
		1900 Thoms (3910)	1936 Dixon et al. (5165)
		1901 Habermann (1466)	1951 Garner (5189)
		1903/04 Moir (2571)	
		1904 Habermann (1468)	
		1909 Lehmann (2343)	
		1914 Bush (5140)	
		1922 Armstrong and Evans (90)	
		1929 Bogen (375)	
		1929 Gabelya and Kipriyanov (**Dr**) (1263)	
		1938 Saruta (3412)	
		1938 Wenusch and Schöller (4215)	
		1939 De Voogd and Van der Linden (957)	
		1939 Roffo (**D**) (3324, 5359)	
		1939/40 de Campos (920)	
		1940 Haag (5207)	
		1949 Fishel and Haskins (1202)	
		1952 Larsen (2263)	
		1954 Kosak (2170)	
75-15-0	Carbon disulfide		1951 Garner (5189)
630-08-0	Carbon monoxide	1843 Zeise (4406)	
		1871 Vohl and Eulenberg (4064, 4065)	
		1874 Krause (2183)	
		1877 Schwarz (3564)	
		1879 Périgord (2928)	
		1880 LeBon (2326)	

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
630-08-0	Carbon monoxide (cont.)	1884 Fokker (1208) 1899 Thoms (3909) 1899 Wahl (4078a) 1900 Thoms (3910) 1901 Habermann (1466) 1902 Pontag (2973) 1903 Pontag (2973) 1903 Spitta (5411) 1903/04 Moir (2571) 1904 Habermann (1468) 1907 Marcelet (2457) 1907 Tani (3870) 1907 Toth (3929) 1908 Fleig (1205) 1908 Lee (5263) 1908 Lehmann (2342a) 1908 Marcelet (2457) 1908 Toth (3929) 1909 Garner (1276) 1909 Lehmann (2343) 1911 Marcelet (2457) 1914 Bush (5140) 1920 Hartridge (1541) 1922 Armstrong and Evans (90) 1923 Baumberger (217) 1923 Heinz (5219) 1923 Jones et al. (1977) 1929 Bogen (375) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1929 Schöller (3522) 1932 McNally (2524) 1934 Ehrismann and Abel (1119) 1934 Leikola and Rautavaara (2347) 1934 Waser and Stähli (4143) 1935 Bastedo (5124) 1935 Wenusch and Schöller (4212) 1936 Bogen (376) 1937 Saruta (3412) 1937 Tsumura (3987) 1938 Roffo (3317) 1938 Saruta (3412) 1938 Wenusch and Schöller (4215) 1939 De Voogd and Van der Linden (957) 1939 Roffo (**D**) (3324, 5359) 1939/40 de Campos (920) 1940 Haag (5207) 1942 Hukusima (1847) 1949 Copenhaver and Bigelow (5154) 1949 Fishel and Haskins (1202) 1951 Garner (5189)	

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
		1951 Obersteg and Scoch-Kanter (5313) 1954 Kosak (2170)	
463-79-6	Carbonic acid		1928 Shmuk (5382)
10361-29-2	Carbonic acid, ammonium salt	1939 Roffo (**D**) (3324, 5359)	
584-08-7	Carbonic acid, dipotassium salt {potash}		1894 Behrens (5126) 1935 Koenig (2154)
13717-00-5	Carbonic acid, magnesium salt		1923 Garner et al. (5195, 5197) 1951 Garner (5189)
7235-40-7	β,β-Carotene {β-carotene, all-*trans*}		1939 Nagel (5300) 1947 Jeffrey and Griffith (1927a) 1951 Garner (5189) 1952 Jensen (1941)
127-40-2	β,ε-Carotene-3,3′-diol {xanthophyll, lutein}		1939 Nagel (5300) 1951 Garner (5189)
9001-05-2	Catalase		1936 Dixon et al. (5165) 1937 Matsumina (5275) 1938 Hukusima (5231) 1946 Garner (5188) 1951 Garner (5189) 1951 Nakai and Inaba (5301) 1953 Brown and Steinberg (5137)
9012-54-8	Cellulase		1950 Tracey (5421) 1953 Barrett et al. (5123)
9004-34-6	Cellulose		1934 Pyriki (5344) 1935 Koenig (2154) 1936 Brückner (451) 1951 Garner (5189)
483-17-0	Cephalin		1939 Shabanov (5375)
7440-45-1	Cerium		1950 Yamagata (5479)
7440-46-2	Cesium		1862/63 Grandeau (20A25) 1913 Traetta-Mosca (5422)
16887-00-6	Chloride	1954 Kosak (2170)	1892 Nessler (5302) 1894 Behrens (5126) 1899 Pritchard (5337) 1923 Garner et al. (5195) 1925 Krevs (5252) 1928 Bailey and Anderson (5113) 1935 Koenig (2154) 1941 Ward (5448) 1950 McEvoy (5277) 1951 Garner (5189) 1951 Mosley et al. (5293)
479-61-8	Chlorophyll a		1939 Nagel (5300) 1951 Garner (5189)
519-62-0	Chlorophyll b		1939 Nagel (5300) 1951 Garner (5189)
1406-65-1	Chlorophyll a and b		1935 Koenig (2154) 1939 Nagel (5300) 1950 Steinberg (5413) 1951 Bacon et al. (5108) 1951 Garner (5189)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
			1952 Bacon et al. (5109) 1952 Jensen (1941)
	Chlorophyll degradation products	1937 Wenusch (5456) 1939 Roffo (**D**) (3324, 5359) 1954 Kosak (2170)	
57-88-5	Cholest-5-en-3-ol (3β)- {cholesterol}	1928 Kennaway and Sampson (2080) 1938 Roffo (25A54) 1939 Roffo (4A03, 25A57) 1941 Roffo (25A58) 1943 Kirby (5242) 1949 Falk et al. (1171)	1928 Kennaway and Sampson (2080) 1938 Roffo (25A54) 1939 Roffo (4A03) 1941 Roffo (25A58) 1943 Kirby (5242) 1949 Falk et al. (1171) 1934 Heffer et al. (20A26)
7440-47-3	Chromium		1936 Johnson (1951) 1934 Heffer et al. (20A26)
7440-48-4	Cobalt		1952 Nicholas (5308) 1953 Nicholas and Thomas (5309)
7440-50-8	Copper	1952 Bailey (160)	1934 Heffer et al. (20A26) 1937 Manns et al. (5270) 1938 McMurtrey and Robinson (5285) 1950 Swanback (5417) 1951 Garner (5189) 1952 Lashkevvich (5261) 1953 Brown and Steinberg (5137)
57-12-5	$Cyanide^{-}$	1932 McNally (2524) 1954 Kosak (2170)	
608-73-1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {Lindane®}		1951 Vinzant (5439)
327-97-9	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl] oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid; 3-*O*-caffeoylquinic acid}		1909 Gorter (5200) 1930 Shmuk and Piatnicki (3655b) 1933 König and Dörr (5246) 1935 Koenig (2154) 1939 Shmuk (5389) 1951 Garner (5189) 1951 Roberts and Wood (5353) 1953 Pearse and Novellie (2911c)
77-95-2	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy- {quinic acid}		1929 Shmuk (3655b) 1930 Shmuk (3655b, 5383) 1939 Shmuk (5389) 1951 Garner (5189)
89-78-1	Cyclohexanol, 5-methyl-2-(1-methylethyl)- {menthol} Pre-1954, considered as a flavorant applied to and identified on tobacco and found in its smoke; subsequently identified as naturally occurring in several different additive-free tobaccos (2339a, 2389, 2544, 3560, 3561) and its mechanism of formation as an isoprenoid defined (1156, 4090)	1941 Haggard and Greenberg (1482) 1952 Rakieten et al. (3072b)	1941 Haggard and Greenberg (1482)
498-40-8	Cysteic acid		1953 Zacharius and Frankenburg (4398c)
52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto-}		1951 Garner (5189) 1951 Sharmon (5376) 1953 Zacharius and Frankenburg (4398c)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]**	**Tobacco**
24645-67-8	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-}		1951 Garner (5189)
56-89-3			1951 Sharmon (5376)
			1953 Zacharius and Frankenburg (4398c)
334-48-5	Decanoic acid {capric acid}	1952 James and Martin (1917)	
	Decarboxylase, α-ketoglutaric acid		1953 Barrett et al. (5123)
	Deoxyribonucleic acid		1953 Silberger and Skoog (5395)
9004-53-9	Dextrin		1934 Pyriki (5344)
			1942 Ward (5449)
			1951 Garner (5189)
			1953 Phillips and Bacot (2947c)
9000-92-4	Diastase		1914 Garner et al. (5194)
			1942 Ward (5449)
			1951 Garner (5189)
	Distillate, destructive, tobacco	1937 Roffo (**D**) (3316)	
		1939 Roffo (**D**) (3324, 5359)	
	Distillate, dry, tobacco	1826 Unterdorden (**Dr**) (5427)	
		1843 Zeise (**Dr**) (4406)	
		1930 Gabelya and Kipriyanov (**Dr**) (1263)	
143-07-7	Dodecanoic acid {lauric acid}	1952 James and Martin (1917)	
	Emulsin		1913 Oosthuizen and Shedd (5323)
			1951 Garner (5189)
	Enzymes, general		1950 Holden (1814a)
			1951 Bacon et al. (5108)
			1952 Bacon et al. (5109)
75-04-7	Ethanamine	1871 Vohl and Eulenberg (4064, 4065)	1871 Vohl and Eulenberg (4064)
62-49-7	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl- {choline}		1932 Nottbohm and Mayer (2808a)
			1933 Vickery et al. (5436)
			1935 Vickery et al. (5435)
			1951 Garner (5189)
460-19-5	Ethanedinitrile {cyanogen}	1910 Toth (3932)	
		1911 Toth (3932)	
144-62-7	Ethanedioic acid {oxalic acid}	1938 Wiley et al. (5467)	1884 Takayama (5419)
			1894 Behrens (5126)
			1904 Kissling (5244)
			1924 Shmuk (5381)
			1929 Shmuk (3655b)
			1935 Koenig (2154)
			1939 Shmuk (5389)
			1951 Bacon et al. (5108)
			1952 Bacon et al. (5109)
			1953 Wright and Burton (5477)
563-72-4	Ethanedioic acid, calcium salt		1894 Behrens (5126)
			1937 Pucher et al. (5342)
			1951 Garner (5189)
107-21-1	1,2-Ethanediol {ethylene glycol}	1938 Forbes and Haag (1209)	1938 Wiley et al. (5467)
		1949 Reif (3100)	1954 Kosak (2170)
		1954 Kosak (2170)	
64-17-5	Ethanol		1926 Neuberg and Kobel (2702a)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]**	**Tobacco**
111-46-6	Ethanol, 2,2′-oxybis- {diethylene glycol} A tobacco additive applied to and identified in tobacco and its smoke	1945 McNally et al. (5286) 1951 Garner (5189) 1954 Kosak (2170)	1937 Haag (5206) 1937 Holck and Carlson (5228) 1938 Newman (5307) 1945 McNally et al. (5286) 1952 Küchle et al. (5254). 1954 Kosak (2170)
350-03-8	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine, methyl 3-pyridyl ketone}		1952 Frankenburg and Gottscho (1223) 1953 Tso and Jeffrey (3983a)
74-86-2	Ethyne {acetylene}	1934 Ehrismann and Abel (1119) 1949 Copenhaver and Bigelow (5154) 1949 Fishel and Haskins (1202) 1954 Kosak (2170)	
	Fat, tobacco		1883 Kissling (2101)
	Fluorescent components	1932 Hirst (1657)	1948 Best (5127) 1951/52 Mizukami (5289) 1953 Johanson (5235)
7782-41-4	Fluorine	1948 Spira (5410)	
50-00-0	Formaldehyde	1904 Thoms (3912) 1904 Trillat (3963, 5423) 1905 Trillat (3963) 1909 Lehmann (2343) 1926 Neuberg and Kobel (2702a) 1927 Neuberg and Ottenstein (2706) 1931 Neuberg and Burkard (2702) 1932 McNally (2524) 1935 Bastedo (5124) 1954 Kosak (2170)	1929 Neuberg and Kobel (2703)
64-18-6	Formic acid	1871 Vohl and Eulenberg (4064, 4065) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1931 Neuberg and Burkard (2702) 1937 Bradford et al. (424) 1940 Haag (5207) 1951 Garner (5189) 1952 James and Martin (1917) 1954 Kosak (2170)	1871 Vohl and Eulenberg (4064) 1924 Shmuk (5381) 1929 Shmuk (3655b) 1930 Shmuk (5384) 1930 Shmuk and Kashirin (5393) 1931 Neuberg and Burkard (2702) 1935 Koenig (2154) 1936 Dixon et al. (5165)
57-48-7	*D*-Fructose {levulose}		1884 Attfield (5105) 1929 Balabucha-Popzova (5114) 1934 Pyriki (5344) 1934 Shmuk (5387) 1942 Ward (5449) 1951 Bacon et al. (5108) 1951 Garner (5189) 1952 Bacon et al. (5109) 1953 Pearse and Novellie (2911c)
	Furan derivative	1935 Schürch and Winterstein (3562) 1954 Kosak (2170)	
98-01-1	2-Furancarboxaldehyde	1904 Thoms [opium study] (5420) 1912 Anonymous (5099, 5100) 1914 Bush (5140) 1929 Bogen (375) 1933 Molinari (2604)	1903 Jetta (5234) 1909 Boekhout and de Vries (5132) 1926 Neuberg and Kobel5303 1939 Wenusch (4202)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
		1935 Bastedo (5124) 1936 Bogen (376) 1939 Roffo (**D**) (3324, 5359) 1939 Wenusch (4202) 1954 Kosak (2170)	
98-00-0	2-Furanmethanol {furfuryl alcohol}		1931 Hukusima and Ooike (1848) 1950 Molinari (2607)
59-23-4	*D*-Galactose		1929 Balabucha-Popzova (5114) 1929 Gabelya and Kipriyanov (1263)
526-99-8	Galactaric acid {mucic acid}		1929 Gabelya and Kipriyanov (1263)
14982-50-4	Galacturonic acid		1929 Balabucha-Popzova (5114) 1929 Gabelya and Kipriyanov (1263) 1931 Neuberg and Scheuer (5306) 1951 Garner (5189)
25990-10-7	Galacturonic acid, homopolymer		1929 Balabucha-Popzova (5114)
554-91-6	Gentiobiose		1943 Miller (5288)
	Globulin		1932 Vickery (5432)
498-07-7	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan}	1938 Wenusch (4199, 4200) 1954 Kosak (2170)	1950 Molinari (2607)
50-99-7	α-*D*-Glucose		1894 Behrens (5126) 1934 Pyriki (5344) 1935 Kurilo (5255) 1936 Neuberg and Kobel (2704a) 1942 Ward (5449) 1951 Bacon et al. (5108) 1951 Garner (5189) 1952 Bacon et al. (5109) 1952 Hough et al. (1835b) 1953 Pearse and Novellie (2911c)
57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose}		1894 Behrens (5126) 1942 Ward (5449) 1951 Bacon et al. (5108) 1951 Garner (5189) 1952 Bacon et al. (5109) 1953 Pearse and Novellie (2911c) 1953 Phillips and Bacot (2947c)
576-37-4	Glucuronic acid		1931 Yamafuji (5478)
6899-05-4	Glutamic acid		1952 Frankenburg and Gottscho (1223) 1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
56-85-9	Glutamine		1934 Vickery et al. (5434) 1937 Vickery et al. (5437) 1951 Garner (5189) 1952 Frankenburg and Gottscho (1223) 1953 Pearse and Novellie (2911c)
56-40-6	Glycine		1953 Zacharius and Frankenburg (4398c)
70-18-8	Glycine, *N*-(*N*-*L*-γ-glutamyl-*L*-cysteinyl)- {glutathione}		1935 Heiserich (5220)
	Glycolase		1951 Garner (5189)
	Glycosides		1932 Yamafuji (4360a) 1939 Shmuk (5389) 1952 Geissmann and Hinreiner (5199)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
	Gudham = mixture of basic components of tobacco and its smoke (2224)	1935 Wenusch and Schöller (4211) 1954 Kosak (2170)	1935 Wenusch and Schöller (4211)
9034-32-6	Hemicellulose		1934 Pyriki (5344) 1935 Koenig (2154) 1951 Garner (5189)
630-04-6	Hentriacontane	1843 Zeise (4406) 1892 Abeles and Paschkis (18) 1894 Kissling (2102) 1934 Wenusch (4184) 1935 Schürch and Winterstein (3562) 1937 Wenusch (4194) 1954 Kosak (2170)	1883 Kissling (2101) 1931 Hukusima and Oika (1848) 1934 Chibnall et al. (701) 1942 Pyriki (5345) 1951 Garner (5189)
502-73-8	16-Hentriacontanone	1935 Schürch and Winterstein (3562)	
593-49-7	Heptacosane		1934 Chibnall et al. (701) 1931 Hukusima and Oika (1848) 1935 Shirokaya (5380) 1937 Shmuk (5388) 1942 Pyriki (5345) 1951 Garner (5189)
111-14-8	Heptanoic acid	1952 James and Martin (1917)	
123-19-3	4-Heptanone {butyrone, dipropyl ketone}	1931 Neuberg and Burkard (2702) 1954 Kosak (2170)	1935 Neuberg and Kobel (2704)
57-10-3	Hexadecanoic acid {palmitic acid}		1931 Hukusima and Oika (1848) 1935 Shirokaya (5380) 1937 Salisbury (5367) 1937 Shmuk (5388) 1944 Venkatarao et al. (4042c) 1945 Riemenschneider et al. (3155) 1951 Garner (5189)
50-70-4	Hexane, hexahydroxy- {sorbitol, glucitol}		1931 Hasegawa (5216) 1936 Neuberg and Kobel (2705) 1946 Frankenburg (5180)
142-62-1	Hexanoic acid {caproic acid}	1871 Vohl and Eulenberg (4064, 4065) 1931 Neuberg and Burkard (2702) 1952 James and Martin (1917) 1954 Kosak (2170)	
71-00-1	Histidine		1931 Yamafuji (5478) 1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
	Hydrocarbons, aliphatic		1883 Kissling (2101) 1901 Thorpe and Homes (3914)
	Hydrocarbons, aliphatic C_{25}–C_{32}		1883 Kissling (2101)
	Hydrocarbons, aromatic	1949 Fishel and Haskins (1202) 1954 Kosak (2170)	
	Hydrocarbons, unsaturated	1949 Fishel and Haskins (1202) 1954 Kosak (2170)	
74-90-8	Hydrocyanic acid {hydrogen cyanide}	1858 Vogel and Reischauer (4063) 1870 Poggiale and Marty (2971) 1871 Vohl and Eulenberg (4064) 1880 LeBon (2326) 1882 Molnár (2608)	1871 Vohl and Eulenberg (4064) 1950 Molinari (2607) 1951 Garner (5189)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
74-90-8	Hydrocyanic acid {hydrogen cyanide} (cont.)	1899 Thoms (3909) 1900 Thoms (3910) 1901 Habermann (1466) 1902 Pontag (2973) 1903 Habermann (1467) 1903 Pontag (2973) 1903 Thoms (3911) 1908 Lee (5263) 1908 Lehmann (2342a) 1909 Habermann and Ehrenfeld (1469) 1909 Garner (1276) 1909 Lehmann (2343) 1912 Lehmann and Gundermann (2344) 1914 Bush (5140) 1923 Heinz (5219) 1934 Ehrismann and Abel (1119) 1934 Waser and Stähli (4143) 1938 Schöller (3524, 3525) 1939 Wenusch (4202) 1939/40 de Campos (920) 1948 Haag and Larson (5208) 1949 Fishel and Haskins (1202) 1951 Garner (5189) 1954 Kosak (2170)	
1333-74-0	Hydrogen	1929 Gabelya and Kipriyanov (**Dr**) (1263)	
7783-06-4	Hydrogen sulfide	1858 Vogel and Reischauer (4063) 1901 Habermann (1466) 1909 Garner (1276) 1909 Habermann and Ehrenfeld (1469) 1909 Lehmann (2343) 1913 Toth (3933) 1914 Bush (5140) 1932 McNally (2524) 1935 Wenusch (4187) 1938 Schöller (3525) 1938 Wenusch and Schöller (4215) 1939 De Voogd and Van der Linden (957) 1939 Wenusch (4202) 1949 Fishel and Haskins (1202) 1951 Garner (5189) 1954 Kosak (2170)	1913 Oosthuizen and Shedd (5323) 1950 Molinari (2607)
	Hydropectin		1929 Balabucha-Popzova (5114)
	Hygroscopic agents	1937 Ballenger and Johnson (5115) 1937 Haag (5206) 1938 Ballenger (5116) 1938 Forbes and Haag (1209) 1939 Ballenger (5117) 1940 Haag (5207) 1945 McNally et al. (5286) 1951 Garner (5189)	1934 Mulinos and Osborne (5295) 1935 Greenwald (5203) 1935 Mulinos and Osborne (5297) 1937 Holck and Carlson (5228) 1938 Wiley et al. (5467) 1952 Küchle et al. (5253, 5254)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
6917-35-7	Inositol		1930 Shmuk (5383, 5384) 1935 Neuberg and Kobel (2704) 1951 Garner (5189)
3615-82-5	myo-Inositol, hexakis(dihydrogen phosphate), calcium magnesium salt {phytin}		1930 Shmuk (5384) 1913 Oosthuizen and Shedd (5323)
9025-67-6	Inulase		
9001-57-4	Invertase		1913 Oosthuizen and Shedd (5323) 1936 Dixon et al. (5165) 1937 Matsumina (5275) 1946 Garner (5188) 1951 Garner (5189) 1951 Nakai and Inaba (5301) 1953 Barrett et al. (5123)
7553-56-2	Iodine		1930 Schwaibold (5373) 1935 McMurtrey (5281) 1938 McMurtrey (5283) 1941 McMurtrey (5284) 1953 Wolff et al. (4273)
7439-89-6	Iron	1952 Bailey (160)	1888 Fesca and Imai (5176) 1909 Boekhout and de Vries (5132) 1929 Coolhaas (5153) 1933 Starkenstein and Stejskal (5412) 1937 McMurtrey (5282) 1938 McMurtrey and Robinson (5285) 1946 LeCompte (5262) 1951 Garner (5189) 1953 Brown and Steinberg (5137)
7004-09-3	Isoleucine		1950 Steinberg (5413) 1953 Zacharius and Frankenburg (4398c)
	Isonicoteine		1914 Noga (5312)
	Lactase		1913 Oosthuizen and Shedd (5323) 1946 Garner (5188) 1953 Barrett et al. (5123)
63-42-3	Lactose		1952 Hough et al. (1835b)
	Lathrein = a mixture of basic components of tobacco and its smoke (2224)	1935 Wenusch and Schöller (4210) 1936 Wenusch and Schöller (5462) 1954 Kosak (2170)	1935 Wenusch and Schöller (4210)
7439-92-1	Lead	1952 Bailey (160)	1861 Creegan (5158) 1921 Cadenhead and Jacques (5141) 1927 Prat (5340) 1929/30 Reitzel (5350) 1934 Heffer et al. (20A26) 1952 Bunce (5139)
8002-43-5	Lecithins		1894 Behrens (5126) 1937 Shabanov (5374)
7005-03-0	Leucine		1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
9005-53-2	Lignin		1934 Pyriki (5344) 1951 Garner (5189) 1953 Phillips and Bacot (2947c)

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TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
9001-62-1	Lipase		1913 Oosthuizen and Shedd (5323) 1946 Garner (5188) 1951 Garner (5189)
7439-93-2	Lithium		1909 Ravenna and Zamorani 5347 1913 Traetta-Mosca (5422) 1921 Headden (5218) 1935 McMurtrey (5281) 1938 McMurtrey (5283) 1941 McMurtrey (5284) 1950 Yamagata (5479) 1951 Garner (5189)
	Lohitam = mixture of basic components in tobacco and its smoke (2224)	1935 Wenusch and Schöller (4210) 1936 Wenusch and Schöller (5462) 1954 Kosak (2170)	1935 Wenusch and Schöller (4210)
6899-06-5	Lysine		1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
7439-95-4	Magnesium	1952 Bailey (160)	1922 Garner et al. (5196) 1923 Garner et al. (5195) 1928 Bailey and Anderson (5113) 1931 Anderson et al. (5098) 1935 Koenig (2154) 1936 Anderson et al. (5097) 1937 McMurtrey (5282) 1941 Ward (5448) 1950 Steinberg (5413) 1951 Garner (5189) 1953 Bortner and Hamilton (5133)
69-79-4	α-Maltose		1934 Pyriki (5344) 1941 Pyriki (3018) 1942 Ward (5449) 1951 Garner (5189) 1952 Hough et al. (1835b)
7439-96-5	Manganese	1952 Bailey (160)	1910 Mach (5268) 1934 Heffer et al. (20A26) 1938 McMurtrey and Robinson (5285) 1941 Ward (5448) 1951 Garner (5189) 1953 Brown and Steinberg (5137)
3615-41-6	*L*-Mannose, 6-deoxy- {α-rhamnose}		1929 Shmuk (3655b)
8049-97-6	Melanin		1934 Shmuk and Shirokaya (3660)
7439-97-6	Mercury		1934 Heffer et al. (20A26) 1936 Kincaid (5241)
74-89-5	Methanamine {methylamine}	1929 Gabelya and Kipriyanov (1263) (**Dr**) 1954 Kosak (2170)	1928 Shmuk (5382)
75-50-3	Methanamine, *N,N*-dimethyl- {trimethylamine}	1929 Gabelya and Kipriyanov (1263) (**Dr**)	1929 Gabelya and Kipriyanov (1263) 1936 Späth and Zajic (3763) 1939 Späth and Biniecki (5403)
124-40-3	Methanamine, *N*-methyl- {dimethylamine}	1929 Gabelya and Kipriyanov (**Dr**) (1263)	1928 Shmuk (5382)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
107-43-7	Methanaminium, 1-carboxy-*N,N,N*-trimethyl-, inner salt {betaine}		1928 Shmuk (5382) 1933 Vickery et al. (5436) 1935 Vickery et al. (5435) 1934 Nito and Kitamura (5311) 1951 Garner (5189) 1952 Willaman (5468)
74-82-8	Methane	1871 Vohl and Eulenberg (4064, 4065) 1909 Lehmann (2343)	
67-56-1	Methanol	1909 Lehmann (2343) 1927 Neuberg and Ottenstein (2706) 1929 Neuberg and Kobel (2703) 1929 Shmuk and Kashirin (5392) 1931 Neuberg and Burkard (2702) 1932 McNally (2524) 1939 Roffo (**D**) (3324, 5359) 1939 Wenusch (4202) 1951 Garner (5189) 1954 Kosak (2170)	1926 Neuberg and Kobel (2702a) 1929 Balabucha-Popzova (5114) 1929 Neuberg and Kobel (2703) 1929 Shmuk and Kashirin (5392) 1931 Neuberg and Burkard (2702) 1931 Neuberg and Scheuer (5306) 1936 Lokschina (2394) 1939 Shmuk (5389) 1951 Garner (5189)
63-68-3	*L*-Methionine		1951 Sharmon (5376) 1953 Zacharius and Frankenburg (4398c)
7439-98-7	Molybdenum		1939 Arnon and Stout (5102) 1947 Kozlowska (5251) 1953 Brown and Steinberg (5137)
9047-56-7	Mutase		1926 Neuberg and Kobel (2702a)
9033-12-9	Mutase, ketone-aldehyde		1951 Garner (5189)
7440-02-0	Nickel	1952 Bailey (160)	1934 Heffer et al. (20A26) 1952 Nicholas (5308) 1952 Hunter and Vergnano (5232) 1952 Shira and Kodaira (5379)
	Nicoteine = nornicotine + anatabine		1914 Noga (5312) 1928 Ehrenstein (1116) 1928 Shmuk (5382) 1935 Späth and Zajic (5409) 1936 Späth et al. (3762) 1939 Henry (5222)
	Nicotoine		1914 Noga (5312)
14797-55-8	Nitrate	1932 McNally (2524) 1954 Kosak (2170)	1894 Behrens (5126) 1951 Garner (5189)
7697-37-2	Nitric acid		1894 Behrens (5126)
7757-79-1	Nitric acid, potassium salt		1894 Behrens (5126)
7727-37-9	Nitrogen	1877 Schwarz (3564)	1934 Garner et al. (5192, 5193) 1951 Garner (5189)
630-03-5	Nonacosane		1934 Chibnall et al. (701)
112-05-0	Nonanoic acid	1952 James and Martin (1917)	
	Obelin = ammonia (2224)	1935 Wenusch and Schöller (4210, 4211) 1936 Wenusch and Schöller (5462) 1954 Kosak (2170)	1928 Shmuk (5382) 1929 Gabelya and Kipriyanov (1263) 1935 Wenusch and Schöller (4210, 4211) 1950 Molinari (2607)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
506-21-8	9,12-Octadecadienoic acid {linoleic acid}		1937 Salisbury (5367)
			1937 Shmuk (5388)
			1944 Venkatarao et al. (4042c)
			1945 Riemenschneider et al. (3155)
			1951 Garner (5189)
57-11-4	Octadecanoic acid {stearic acid}		1937 Salisbury (5367)
			1944 Venkatarao et al. (4042c)
			1945 Riemenschneider et al. (3155)
			1951 Garner (5189)
463-40-1	9,12,15-Octadecatrienoic acid {linolenic acid}		1935 Shirokaya (5380)
			1944 Venkatarao et al. (4042c)
112-80-1	9-Octadecenoic acid {oleic acid}		1937 Salisbury (5367)
			1937 Shmuk (5388)
			1944 Venkatarao et al. (4042c)
			1945 Riemenschneider et al. (3155)
			1951 Garner (5189)
78-70-6	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool}		1941 Sabetay et al. (3374)
124-07-2	Octanoic acid {caprylic acid}	1871 Vohl and Eulenberg (4064, 4065)	1941 Sabetay et al. (5363)
		1952 James and Martin (1917)	1946 Frankenburg (5180)
372-75-8	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline}		1953 Zacharius and Frankenburg (4398c)
9035-73-8	Oxidase		1910 Betting (5128)
			1913 Oosthuizen and Shedd (5323)
			1928 Shmuk (5382)
			1941 Roberts (5352)
			1946 Garner (5188)
			1951 Garner (5189)
			1953 Barrett et al. (5123)
9029-44-1	Oxidase, ascorbate		1953 Brown and Steinberg (5137)
9001-16-5	Oxidase, cytochrome c		1953 Barrett et al. (5123)
7782-44-7	Oxygen	1954 Kosak (2170)	1950 Molinari (2607)
79-83-4	Pantothenic acid		1952 Jensen (1941)
	Paraffins	1893 Kissling (5243)	1901 Thorpe and Homes (3914)
9025-98-3	Pectase		1946 Garner (5188)
			1951 Garner (5189)
9046-40-6	Pectic acid		1884 Takayama (5419)
			1929 Balabucha-Popzova (5114)
			1931 Neuberg and Scheuer (5306)
			1951 Garner (5189)
			1953 Phillips and Bacot (2947c)
9000-69-5	Pectin		1903 Jetta (5234)
			1929 Balabucha-Popzova (5114)
			1929 Gabelya and Kipriyanov (1263)
			1931 Neuberg and Scheuer (5306)
			1934 Pyriki (5344)
			1935 Koenig (2154)
			1951 Garner (5189)
			1953 Phillips and Bacot (2947c)
9047-18-1	Pectinic acid		1929 Gabelya and Kipriyanov (1263)
	l-Peganin		1936 Späth and Zajic (3763)
109-52-4	Pentanoic acid {valeric acid}	1871 Vohl and Eulenberg (4064, 4065)	1871 Vohl and Eulenberg (4064)
		1929 Gabelya and Kipriyanov (**Dr**) (1263)	1929 Gabelya and Kipriyanov (1263)
		1931 Neuberg and Burkard (2702)	1947 Sabetay and Panouse (5364)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]**	**Tobacco**
		1952 James and Martin (1917) 1954 Kosak (2170)	
105-43-1	Pentanoic acid, 3-methyl-		1947 Sabetay and Panouse (5364)
96-22-0	3-Pentanone	1927 Neuberg and Ottenstein (2706) 1931 Neuberg and Burkard (2702) 1954 Kosak (2170)	1935 Neuberg and Kobel (2704)
116001-96-8	Pentosan		1903 Jetta (5234) 1914 Garner et al. (5194) 1935 Koenig (2154) 1953 Phillips and Bacot (2947c)
	Pentose		1931 Neuberg and Scheuer (5306) 1934 Pyriki (5344) 1951 Garner (5189)
	Pentosenucleic acid		1953 Silberger and Skoog (5395)
	Peptide		1937 Vickery et al. (5437) 1951 Garner (5189)
9003-99-0	Peroxidase		1910 Betting (5128) 1937 Matsumina (5275) 1951 Garner (5189) 1951 Nakai and Inaba (5301) 1953 Barrett et al. (5123) 1953 Brown and Steinberg (5137)
85-01-8	Phenanthrene	1939 Roffo (**D**) (3324, 5359) 1954 Kosak (2170)	
	Phenanthrene derivative	1939 Roffo (4A03)	
108-95-2	Phenol	1871 Vohl and Eulenberg (4064, 4065) 1914 Bush (5140) 1936 Bogen (376) 1936 Molinari (2605) 1940 Haag (5207) 1947 Ikeda (1857) 1952 Rayburn (3090) 1953 Rayburn et al. (3090) 1954 Kosak (2170)	1871 Vohl and Eulenberg (4064) 1939 Wenusch (4202) 1950 Molinari (2607) 1953 Rayburn et al. (3090)
90-05-1	Phenol, 2-methoxy- {guaiacol}	1952 Rayburn (3090) 1953 Rayburn et al. (3090)	1939 Wenusch (4202) 1953 Rayburn et al. (3090)
97-54-1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}		1946 Frankenburg (5180)
97-53-0	Phenol, 2-methoxy-4-(2-propenyl)- {eugenol}		1941 Sabetay et al. (5363) 1946 Frankenburg (5180)
1319-77-3	Phenol, methyl- {cresol}	1936 Bogen (376)	
95-48-7	Phenol, 2-methyl- {*o*-cresol}	1952 Rayburn (3090) 1953 Rayburn et al. (3090)	
108-39-4	Phenol, 3-methyl- {*m*-cresol}	1952 Rayburn (3090) 1953 Rayburn et al. (3090)	1953 Rayburn et al. (3090)
	Phenols, structure unspecified	1954 Kosak (2170)	1934 Shmuk (5387) 1934 Shmuk and Shirokaya (3660)
63-91-2	Phenylalanine		1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
14265-44-2	Phosphate		1894 Behrens (5126) 1935 Koenig (2154)

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TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
	Phosphatase		1946 Garner (5188)
			1951 Garner (5189)
7803-51-2	Phosphine	1898 Cavalli (637)	
56-38-2	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®}		1951 Vinzant (5439)
7723-14-0	Phosphorus		1928 Bailey and Anderson (5113)
			1941 Ward (5448)
			1950 Steinberg (5413)
			1951 Garner (5189)
			1953 Bortner and Hamilton (5133)
	Phytosterols	1954 Kosak (2170)	1913 Traetta-Mosca (3942b)
			1935 Kobel and Neuberg (2153a)
			1935 Schürch and Winterstein (3562)
			1937 Shmuk (5388)
	Pigments		1935 Koenig (2154)
			1939 Nagel (5300)
110-89-4	Piperidine		1936 Späth and Zajic (3763)
535-75-1	2-Piperidinecarboxylic acid {pipecolic acid}		1953 Zacharius and Frankenburg (4398c)
	Poikiline = 1-Butanone, 4-amino-l-(3-pyridyl)-	1954 Kosak (2170)	1948 Wenusch (4207)
7440-09-7	Potassium	1952 Bailey (160)	1923 Garner et al. (5195)
			1928 Bailey and Anderson (5113)
			1950 Steinberg (5413)
			1951 Garner (5189)
			1953 Bortner and Hamilton (5133)
			1953 Wolff et al. (4273)
147-85-3	Proline		1952 Frankenburg and Gottscho (1223)
			1953 Pearse and Novellie (2911c)
			1953 Zacharius and Frankenburg (4398c)
78-98-8	Propanal, 2-oxo- {pyruvaldehyde, methyl-glyoxal}		1929 Kobel and Scheuer (2153b)
141-82-2	Propanedioic acid {malonic acid}		1953 Wada and Kobashi (5447)
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid}	1939 Roffo (**D**) (3324, 5359)	1884 Takayama (5419)
			1894 Behrens (5126)
			1904 Kissling (5244)
			1924 Shmuk (5381)
			1930 Shmuk (3655b)
			1930 Shmuk and Piatnicki (3655b)
			1931 Yamafuji (5478)
			1935 Koenig (2154)
			1939 Shmuk (5389)
			1951 Bacon et al. (5108)
			1952 Bacon et al. (5109)
			1953 Phillips and Bacot (2947c)
			1953 Wright and Burton (5477)
813-94-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, calcium salt		1937 Pucher et al. (5342)
			1951 Garner (5189)
3344-18-1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, magnesium salt		1937 Pucher et al. (5342)
			1951 Garner (5189)
6100-05-6	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, potassium salt		1937 Pucher et al. (5342)
			1951 Garner (5189)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
56-81-5	1,2,3-Propanetriol {glycerol} A tobacco additive applied to and identified in tobacco and its smoke; in 1964, it was identified as a component of additive-free, uncased tobacco (865)	1938 Forbes and (1209) 1945 McNally et al. (5286) 1951 Garner (5189) 1954 Kosak (2170)	1937 Holck and Carlson (5228) 1937 Shmuk (5388) 1945 McNally et al. (5286) 1946 Frankenburg (5180)
79-09-4	Propanoic acid {propionic acid}	1871 Vohl and Eulenberg (4064, 4065) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1952 James and Martin (1917)	1924 Shmuk (5381) 1929 Gabelya and Kipriyanov (1263) 1929 Shmuk (3655b)
50-21-5	Propanoic acid, 2-hydroxy- {lactic acid}		1953 Wada and Kobashi (5447)
	1-Propanone, 1-(3-pyridinyl)- {pyridyl ethyl ketone}	1919 Kissling (2107) 1935 Schöller 3523 1939 Wenusch (4202) 1954 Kosak (2170)	1928 Shmuk (5382)
67-64-1	2-Propanone {acetone}	1937 Wenusch (4194)	1871 Vohl and Eulenberg (4064)
107-02-8	2-Propenal {acrolein}	1932 McNally (2524) 1936 Bogen (376) 1937 Ribeiro (3126) 1954 Kosak (2170)	
331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid}	1939 Shmuk (5389)	1894 Behrens (5126) 1929 Shmuk (3655b) 1930 Shmuk (3655b, 5385) 1930 Shmuk and Piatnicki (3655b) 1935 Koenig (2154) 1939 Shmuk (5389) 1951 Garner (5189)
78990-62-2	Protease		1913 Oosthuizen and Shedd (5323) 1951 Garner (5189)
	Protein		1886 Mendel (5287) 1894 Behrens (5126) 1930 Smirnov and Izvoshtshikov (5396) 1933 Vickery et al. (5436) 1935 Koenig (2154) 1935 Vickery et al. (5435) 1951 Garner (5189)
20-73-0	1*H*-Purine		1950 Steinberg (5413)
73-24-5	1*H*-Purin-6-amine {adenine}		1931 Yamafuji (5478) 1933 Vickery et al. (5436) 1935 Vickery et al. (5435) 1934 Nito and Kitamura (5311) 1951 Garner (5189)
73-40-5	6*H*-Purin-6-one, 2-amino-1,7-dihydro- {guanine}		1935 Vickery et al. (5435) 1934 Nito and Kitamura (5311) 1951 Garner (5189)
69-93-2	1*H*-Purine-2,6,8(3*H*)-trione, 7,9-dihydro- {uric acid}	1937 Wenusch (5456) 1954 Kosak (2170)	
129-00-0	Pyrene	1953 Cooper and Lindsey (818)	
110-86-1	Pyridine	1871 Vohl and Eulenberg (4064, 4065) 1880 LeBon (2326) 1894/95 Brunton and Tunnicliffe (5138) 1899 Thoms (3909) 1900 Thoms (3910) 1903 Pontag (2973)	1871 Vohl and Eulenberg (4064) 1900 Eulenburg (5173) 1928 Shmuk (5382) 1929 Gabelya and Kipriyanov (1263) 1933 Dobrin (1020) 1936 Preiss (2987)

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TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
110-86-1	Pyridine (cont.)	1904 Thoms (3912) 1906 Warburg (4132) 1908 Lee (5263) 1908 Lehmann (2342a) 1909 Lehmann (2343) 1910 Toth and Krampera (3934) 1914 Bush (5140) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1932 McNally (2524) 1933 Pfyl (2937) 1935 Bastedo (5124) 1936 Bogen (376) 1936 Preiss (2986–2988) 1937 Bradford et al. (424) 1937 Pyatnitskii and Kashirin (3008) 1939 Dittmar (985, 987) 1939 Roffo (**D**) (3324, 5359) 1939 Wenusch (4202) 1939/40 de Campos (920) 1942 Hofmann (1812) 1948 Pyriki (3022) 1951 Garner (5189) 1954 Kosak (2170)	1948 Pyriki (3022)
27175-64-0	Pyridine, dimethyl- {lutidine}	1871 Vohl and Eulenberg (4064) 1932 McNally (2524) 1908 Lehmann (2342a) 1954 Kosak (2170)	1871 Vohl and Eulenberg (4064) 1928 Shmuk (5382)
108-48-5	Pyridine, 2,6-dimethyl- {2,6-lutidine}	1932 McNally (2524)	
1333-41-1	Pyridine, methyl- {picoline}	1871 Vohl and Eulenberg (4064, 4065) 1908 Lehmann (2342a) 1914 Bush (5140) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1954 Kosak (2170)	1871 Vohl and Eulenberg (4064) 1928 Shmuk (5382) 1929 Gabelya and Kipriyanov (1263)
109-06-8	Pyridine, 2-methyl- {2-picoline}	1929 Gabelya and Kipriyanov (**Dr**) (1263) 1932 McNally (2524) 1944 Woodward et al. (25A84)	1928 Shmuk (5382)
29611-84-5	Pyridine, trimethyl- {collidine}	1871 Vohl and Eulenberg (4064, 4065) 1908 Lee (5263) 1908 Lehmann (2342a) 1954 Kosak (2170)	1871 Vohl and Eulenberg (4064) 1928 Shmuk (5382)
108-75-8	Pyridine, 2,4,6-trimethyl- {2,4,6-collidine}	1932 McNally (2524)	
532-12-7	Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)- {*l*-myosmine}	1933 Wenusch and Schöller (4208) 1935 Wenusch and Schöller (4210) 1936 Wenusch and Schöller (5462) 1939 Wenusch (4202) 1954 Kosak (2170)	1934 Wenusch and Schöller (4209) 1936 Späth et al. (3762) 1944 Woodward et al. (4275a) 1946 Frankenburg (1221) 1952 Frankenburg and Gottscho (1223) 1953 Tso and Jeffrey (3983a)
525-74-6	Pyridine, 3-(3,4-dihydro-1-methyl-2*H*-pyrrol-5-yl)- {*N*-methylmyosmine}		1946 Frankenburg (1221) 1949 Swain et al. (5416) 1952 Willaman (5468)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
24380-92-5	Pyridine, 3-(1-methyl-2-piperidinyl)-, (S)- {*N*-methylanabasine}		1937 Späth and Kesztler (5407) 1946 Frankenburg (1221) 1953 Sadykov et al. (5366)
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine}	1826 Unterdorden (**Dr**) (5427) 1843 Melsens (2528) 1844 Melsens (2528) 1871 Vohl and Eulenberg (4064, 4065) 1872 Heubel (5225) 1882 Kissling (2100) 1892 Lowenthal (2401) 1898 Kissling (2103) 1899 Thoms (3909) 1900 Thoms (3910) 1901 Habermann (1466) 1902 Ludwig (2408) 1903 Pontag (2973) 1904 Bamberger (5118) 1904 Paschkis (5325) 1904 Schmidt (3517) 1905 Theodorvits (3896) 1906 Rattner (5346) 1906 Warburg (4132) 1907 Bitter (5130) 1907 Kuhles (2225) 1908 Lee (5263) 1908 Noda (2793) 1908 Biederbeck (5129) 1908 Toth (3930) 1909 Habermann and Ehrenfeld (1469) 1909 Toth (3930) 1909 Weger (5452) 1910 Toth and Krampera (3934) 1911 Fröhlich (5183) 1911 Von Frankl-Hochwart (5443) 1912 Anonymous (5099, 5100) 1914 Bush (5140) 1914 Favenger (5175) 1915 Kütt (2247) 1916 Toth and Dangelmajer (3928) 1919 Silberbauer (3670) 1919 Van Leeuwen (4039) 1920 Asherson (5104) 1920 Hahn and Langer (1484) 1920 Hirschfelder et al. (5226) 1921 Bogner (378) 1922 Popp and Contzen (2980) 1923 Baumberger (218) 1923 Heinz (5219) 1923 Rhode (5351)	1807 Cerioli (5144) 1809 Vauquelin (5430) 1822 Hermbstädt (5223) 1826 Unterdorden (5427) 1828 Posselt and Reimann (2981) 1842 Barral (5121) 1842 Ortigosa (5324) 1843 Melsens (2528) 1847 Barral (5122) 1852 Vleminckx (5439a) 1867 Huber (5229) 1868 Jullien (1990) 1969 Kopff (5247) 1873 Weidel (5453) 1877 Von Laiblin (5444) 1879 Von Laiblin (5445) 1880 Prescott (2989) 1884 Takayama (5419) 1886 Liebrecht (5267) 1892 Gautier (5198) 1893 Blau (5131) 1893 Étard (5171) 1893 Pinner (5335, 17B44) 1894 Behrens (5126) 1894 Étard (5172) 1895 Pinner (5336) 1897 Pictet and Genequand (5331) 1904 Kissling (5244) 1904 Pictet and Rotschy (17B43) 1904 Schmidt (3517) 1908 Lee (5263) 1909 Garner (1276) 1909 Weger (5452) 1912 Chuard and Mellet (5146) 1914 Bush (5140) 1922 Popp and Contzen (2980) 1923 Rhode (5351) 1927 Heiduschska and Muth (1608–1610) 1927 Pfyl and Schmitt (2938) 1927 Winterstein and Trier (5474) 1928 Harlan and Hixon (5213) 1928 Popp (2979) 1928 Shmuk (5382) 1929 Heiduschska and Muth (1611–1613) 1930 Braun (427, 428) 1930 Faitelowitz (5174)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	1927 Dixon (5166) 1927 Pfyl and Schmitt (2938) 1927 Winterstein and Aronson (5470) 1927/28 Schöller (3521) 1927/28 Wenusch (4167) 1928 Wenusch (4168) 1928 Winterstein and Aronson (5471) 1929 Bogen (375) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1929 Wenusch (4169–4172) 1929 Winterstein and Aronson (5472, 5473) 1930 Bodnár (362, 363) 1930 Bolm (388) 1930 Braun (427, 428) 1930 Heiduschka (1606) 1930 Storp (5414) 1930 Wenusch (4173, 4174) 1931 Barta and Toole (196) 1931 Ehrismann (1118) 1931 Frank (5179) 1931 Hahn and Ehrismann (1483) 1931 Herrmann (1624) 1931 Kovalenko (2181) 1931 Pyriki (3009) 1931 Van Druten (4016) 1931 Wenusch (4175, 4176, 4178) 1932 Barta and Toole (197, 198) 1932 Heiduschka and Post (1614) 1932 Kissling (2110, 2111) 1932 Margasinski (2459) 1932 McNally (2524) 1932 Michalowsky (2535) 1932 Molinari (2603) 1932 Nagy (2669, 2670) 1932 Paffgen (2880) 1932 Post (2982) 1932 Pyriki (3011, 3012, 5343) 1932 Schaarschmidt et al. (3426) 1932 Schlossmann and Schlesinger (3446) 1932 Shmuk et al. (3658) 1932 Skumburdis and Kissling (3682) 1932 Traube (3943) 1932 Van Druten (4017) 1932 Waser and Stähli (4140, 4141) 1933 Hofmann (1811) 1933 Nagy and Dickman (2673) 1933 Pfyl (2936, 2937) 1933 Pyriki (3012) 1933 Schlossmann (3445) 1933 Stähli (3784)	1930 Harlan and Hixon (5214) 1930 Heiduschka (1606) 1930 Windus and Marvel (5469) 1931 Auprecht (5106) 1931 Hukusima and Oika (1848) 1931 Tonn (3925) 1932 Post (2982) 1932 Waser (5451) 1933 Dobrin (1020) 1933 Hofmann (1811) 1933 Toole (3926) 1936 Cuvelier (5159) 1935 Koperina and Kalibab (2166) 1935 Späth and Kesztler (5405) 1935 Wenusch (4189) 1935 Wenusch and Schöller (4210) 1936 Busbey and McIndoo (21A07, 21A08) 1936 Dixon et al. (5165) 1936 Malaquin (2446) 1936 McIndoo et al. (21A40–21A42) 1937 Bailey and Petre (5112) 1937 Späth and Kainrath (5404.) 1937/38 Mulinos and Cockrill (5294) 1938 Molinari (2606) 1939 Avens and Pearce (5107) 1939 Shmuk (5389) 1939 Shmuk and Borozdina (5391) 1940 Reif (5349) 1942 Dawson (5161) 1942 Haag and Larson (17B14) 1943 Pyriki (3019) 1944 Larson and Haag (5258) 1945 Clemo and Swann (5150) 1945 Haag et al. (5209) 1945 Larson and Haag (5259) 1946 Frankenburg (1221) 1948 Brice (429e) 1948 Dawson (915b) 1948 Griffith and Jeffrey (1393) 1948 Pyriki (3022) 1948 Shmuk (5390) 1948 Wenusch (4207) 1948 Willits (4266a) 1949 Porter et al. (5339) 1949 Swain et al. (5416) 1950 Dawson (5162) 1950 Willits et al. (4267) 1951 Garner (5189) 1952 Weybrew et al. (5463) 1953 Bortner and Hamilton (5133)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-{*l*-nicotine} (cont.)	1933 Starkenstein and Stejskal (5412) 1933 Toole (3926) 1934 Graham (1341) 1934 Koperina (2164) 1934 Koperina and Shageeva (2167) 1934 Nagy and Barta (2672) 1934 Preiss (2984) 1934 Pyriki (3012, 3013, 3028) 1934 Waser and Stähli (4142) 1934 Wenusch (4179–4183) 1934 Wulfert (4291) 1935 Bastedo (5124) 1935 Bodnár et al. (364, 365) 1935 Jensen and Haley (1942) 1935 Koperina and Kalibab (2166) 1935 Preiss (2985) 1935 Pyriki (3012, 3014) 1935 Schürch and Winterstein (3562) 1935 Wenusch (4189) 1935 Wenusch and Schöller (4210) 1936 Bogen (376) 1936 Cuvelier (5159) 1936 Heiduschka (1607) 1936 Malaquin (2446) 1936 Preiss (2986) 1936 Wenusch (4190, 4191) 1936 Wenusch and Schöller (4213) 1937 Bailey and Petre (5112) 1937 Bradford et al. (424) 1937 Derr et al. (5163) 1937 Pierce (2958) 1937 Pyriki (3015) 1937 Wenusch (4194, 4197, 4198) 1938 Justin-Müller (5236) 1938 Molinari (2606) 1938 Nagy (2671) 1939 Wenusch (4202) 1939/40 Haag (1464) 1940 Haag (5207) 1940 Haag and Neale (5210) 1940 Haag et al. (5211) 1940 Wenusch (4203, 4204) 1941 Hofmann (1812) 1941 Pierce (2959) 1941 Wenusch (4205) 1942 Wenusch (4206, 5458, 5459, 5460) 1943 Pyriki (3019, 3021) 1944 Larson and Haag (5258) 1944 Woodward et al. (4275a) 1944 Woodward et al. (25A84, 25A85)	1953 Cundiff and Markunas (866) 1953 Sadykov et al. (5366) 1953 Tso and Jeffrey (3983a) 1953 Wright and Burton (5477)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	1945 Larson and Haag (5259) 1946 McCormick and Smith (2517) 1947 Finnegan et al. (1188) 1948 Pyriki (3022) 1948 Shmuk (5390) 1948 Sollmann (5401) 1949 Dabrowska (888) 1949 Ling and Wynn Parry (2371) 1949 Wenusch (5461) 1950 Rayburn (3089) 1950 Willits et al. (4267) 1951 Garner (5189) 1951 Marchand and Renard (2458) 1951 Vettors (5431) 1952 Bailey (160) 1952 Greenberg et al. (1380) 1952 Larsen (2263) 1952 Rakieten et al. (3072b) 1953 Cundiff and Markunas (866) 1953 Staub and Furrer (3790) 1953 Wahl and Heil (4082) 1953 Wolman and Stark (5475, 5476) 1954 Kosak (2170)	
2820-55-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, 1-oxide, (S)- {nicotine *N*-oxide}	1950 Rayburn et al. (5348)	1885 Pinner (5334) 1950 Rayburn et al. (5348) 1952 Frankenburg and Gottscho (1223) 1953 Tso and Jeffrey (3983a)
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, organic acid salts	1937 Wenusch (4196)	1809 Vauquelin (5430) 1822 Hermbstädt (5223) 1823 Hermbstädt (5224) 1939 Shmuk (5389)
487-19-4	Pyridine, 3-(1-methyl-1*H*-pyrrol-2-yl)- {nicotyrine}	1935 Wenusch and Schöller (4210) 1939 Wenusch (4202) 1954 Kosak (2170)	1898 Pictet and Crépieux (5330) 1928 Wibaut and Overhoff (5465) 1932 Wibaut and Hackman (5464) 1935 Wenusch (5454) 1937 Späth and Kesztler (5407) 1946 Frankenburg (1221)
494-52-0	Pyridine, 3-(2-piperidinyl)-, (S)- {*l*-anabasine}	1933 Haag (5205)	1931 Ehrenstein (1116) 1931 Smith (5397) 1932 Smith (5398) 1935 Olchansky (5321) 1935 Smith (17B53) 1937 Späth and Kesztler (5406) 1939 Shmuk and Borozdina (5391) 1942 Smith and Smith (5399) 1946 Dubinin and Chelintsev (1075a) 1946 Frankenburg (1221) 1948 Matveev (5276) 1048 Sadykov et al. (5365) 1948 Shmuk (5390) 1949 Porter et al. (5339)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
			1951 Garner (5189)
			1953 Sadykov et al. (5366)
			1953 Tso and Jeffrey (3983a)
	Pyridine, 3-(2-piperidinyl)-, 6-oxo- {6-oxoanabasine}		1939 Henry (5222)
494-97-3	Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine}	1944 Larson and Haag (5258)	1928 Shmuk (5382)
		1945 Larson and Haag (5259)	1935 Späth and Zajic (5409)
			1936 Wenusch (5455)
			1936 Späth et al. (5408)
			1937 Späth and Kesztler (5406)
			1944 Larson and Haag (5258)
			1945 Larson and Haag (5259)
			1946 Frankenburg (1221)
			1948 Brice (429e)
			1948 Dawson (915b)
			1948 Shmuk (5390)
			1949 Swain et al. (5416)
			1951 Garner (5189)
			1952 Weybrew et al. (5463)
			1953 Tso and Jeffrey (3983a)
			1953 Wright and Burton (5477)
494-98-4	Pyridine, 3-(1*H*-pyrrol-2-yl)- {nornicotyrine}		1946 Frankenburg (1221)
	Pyridine bases	1932 McNally (2524)	
		1954 Kosak (2170)	
98-92-0	3-Pyridinecarboxamide {nicotinamide}		1953 Tso and Jeffrey (3983a)
100-54-9	3-Pyridinecarbonitrile {nicotinonitrile}	1944 Woodward et al. (25A84)	
59-67-6	3-Pyridinecarboxylic acid {nicotinic acid}	1944 Woodward et al. (25A84)	1879 Von Laiblin (5445)
			1938 Chen et al. (5145)
			1952 Gottscho and Frankenburg (1222)
			1953 Tso and Jeffrey (3983a)
289-95-2	Pyrimidine {1,3-diazine}		1950 Steinberg (5413)
107-49-3	Pyrophosphoric acid, tetraethyl ester {TEPP} A metabolite of phosphorus-containing pesticides		1951 Vinzant (5439)
109-97-7	Pyrrole	1909 Lehmann (2343)	1928 Shmuk (5382)
		1929 Gabelya and Kipriyanov (**Dr**) (1263)	1937 Fromm (1244)
		1939 Roffo (**D**) (3324, 5359)	
		1939/40 de Campos (920)	
		1954 Kosak (2170)	
	Pyrroles, structure unspecified	1932 McNally (2524)	
		1937 Fromm (1244)	
		1954 Kosak (2170)	
123-75-1	Pyrrolidine	1909 Lehmann (2343)	1908 Pictet and Court (4837a)
			1928 Shmuk (5382)
120-94-5	Pyrrolidine, *N*-methyl-	1932 McNally (2524)	1905 Pictet (5329)
		1954 Kosak (2170)	1908 Pictet and Court (4837a)
			1928 Shmuk (5382)
			1939 Späth and Biniecki (5403)
91-22-5	Quinoline	1929 Gabelya and Kipriyanov (**Dr**) (1263)	
		1944 Woodward et al. (25A84)	
7440-14-4	Radium		1937 Drobkov (5167)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
10043-92-2	Radon		1937 Drobkov (5167)
	Reconstituted tobacco sheet		1857 Von der Porten (5442)
9037-80-3	Reductase		1913 Oosthuizen and Shedd (5323)
			1946 Garner (5188)
			1951 Garner (5189)
	Resin	1893 Kissling (5243)	1904 Kissling (5244)
		1932 Koperina (2163)	1914 von Degrazia (5441)
		1934 Koperina (2165)	1924 Shmuk (5381)
		1935 Wenusch (4185, 4186)	1931 Hukusima and Oika (1848)
		1937 Wenusch (4192, 5456)	1935 Shirokaya (5380)
		1949 Dabrowska (888)	1938 Gaertner (5185)
		1950 Mazzulli (2511)	1940 Pyriki (3017)
		1954 Kosak (2170)	
	Resin acids	1893 Kissling (5243)	
		1954 Kosak (2170)	
	Resinol		1924 Shmuk (5381)
3615-41-6	Rhamnose		1936 Neuberg and Kobel (2704a)
	Rhoeadin		1936 Späth and Zajic (3763)
83-88-5	Riboflavin		1952 Jensen (1941)
7440-17-7	Rubidium		1862/63 Grandeau (20A25)
			1950 Yamagata (5479)
	Saccharides	1940 Dittmar (988)	1940 Dittmar (988)
			1941 Pyriki (3018)
129990-04-1	Saponin (from tobacco)		1935 Kobel and Neuberg (2153a)
7782-49-2	Selenium		1933 Martin and Trelease (5274)
6898-95-9	Serine		1952 Frankenburg and Gottscho (1223)
			1953 Pearse and Novellie (2911c)
			1953 Zacharius and Frankenburg (4398c)
7631-86-9	Silica		1894 Behrens (5126)
7440-21-3	Silicon	1952 Bailey (160)	1925 MacIntyre et al. (5269)
			1928 Bailey and Anderson (5113)
			1951 Garner (5189)
7440-22-4	Silver		1936 Johnson (951)
	α-Socratine = {nicotyrine + 2,3′-bipyridine + nicotinic acid + nornicotine + anatabine} (2224)	1919 Kissling (2107)	1934 Wenusch and Schöller (4209)
		1933 Wenusch and Schöller (4208)	1935 Wenusch and Schöller (4210)
		1935 Wenusch and Schöller (4210)	
		1936 Wenusch and Schöller (5462)	
		1954 Kosak (2170)	
	β-Socratine = {nicotyrine + 2,3′-bipyridine + nicotinic acid + nornicotine + anatabine} (2224)	1919 Kissling (2107)	1934 Wenusch and Schöller (4209)
		1933 Wenusch and Schöller (4208)	1935 Wenusch and Schöller (4210)
		1935 Wenusch and Schöller (4210)	
		1936 Wenusch and Schöller (5462)	
		1954 Kosak (2170)	
	γ-Socratine = *l*-nornicotine (2224)	1919 Kissling (2107)	1928 Shmuk (5382)
		1933 Wenusch and Schöller (4208)	1934 Wenusch and Schöller (4209)
		1935 Wenusch and Schöller (4210)	
		1936 Wenusch and Schöller (5462)	1935 Wenusch and Schöller (4210)
		1954 Kosak (2170)	
		1952 Bailey (160)	1928 Bailey and Anderson (5113)
7440-23-5	Sodium		1938 Gaertner (5185)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	References: Tobacco
			1950 Frankenburg (5181)
			1950 Yamagata (5479)
			1951 Garner (5189)
			1953 Wolff et al. (4273)
9005-25-8	Starch		1885 Müller-Thurgen (5298)
			1894 Behrens (5126)
			1914 Garner et al. (5194)
			1934 Pyriki (5344)
			1935 Koenig (2154)
			1942 Ward (5449)
			1951 Bacon et al. (5108)
			1951 Garner (5189)
			1952 Bacon et al. (5109)
			1952 Willaman (5468)
			1953 Phillips and Bacot (2947c)
7440-24-6	Strontium	1952 Bailey (160)	1897 Trimble (5424)
			1921 Headden (5218)
57-50-1	Sugar		1885 Müller-Thurgen (5298)
			1914 Garner et al. (5194)
			1934 Pyriki (5344)
			1935 Koenig (2154)
			1936 Dixon et al. (5165)
			1951 Garner (5189)
8013-17-0	Sugar, invert		1951 Garner (5189)
14808-79-8	Sulfate		1923 Garner et al. (5195)
			1935 Koenig (2154)
			1951 Garner (5189)
7704-34-9	Sulfur		1914 Shedd (5378)
			1928 Bailey and Anderson (5113)
			1934 Heiserich (5220)
			1937 McMurtrey (5282)
			1941 Ward (5448)
			1951 Garner (5189)
71010-48-5	α-Tabacenic acid {α-tobacco acid}		1914 von Degrazia (5441)
			1924 Shmuk (5381)
			1934 Shmuk and Shirokaya (3660)
			1951 Garner (5189)
71010-46-3	β-Tabacenic acid {β-tobacco acid}		1914 von Degrazia (5441)
			1924 Shmuk (5381)
			1934 Shmuk and Shirokaya (3660)
			1951 Garner (5189)
71010-47-4	γ-Tabacenic acid {γ-tobacco acid}		1914 von Degrazia (5441)
			1924 Shmuk (5381)
			1934 Shmuk and Shirokaya (3660)
			1951 Garner (5189)
1401-55-4	Tannins {tannic acid}		1894 Behrens (5126)
			1924 Shmuk (5381)
			1935 Koenig (2154)
			1953 Phillips and Bacot (2947c)

(*continued*)

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
494-04-2	3,2′:4′,3′′-Terpyridine {nicotelline}		1901 Pictet and Rotschy (5332) 1914 Noga (5312) 1928 Shmuk (5382)
544-63-8	Tetradecanoic acid {myristic acid}		1944 Venkatarao et al. (4042c)
7440-28-0	Thallium		1932 McMurtrey (5280) 1934 Heffer et al. (20A26) 1938 Van Der Veen (5428) 1940 Shear and Ussery (5377)
59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride {thiamine}		1952 Jensen (1941)
463-56-9	Thiocyanic acid	1938 Schöller (3525) 1954 Kosak (2170)	1938 Schöller (3525) 1950 Molinari (2607)
505-14-6	Thiocyanogen	1909 Toth (3931)	
72-19-5	Threonine		1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
7440-31-5	Tin		1934 Heffer et al. (20A26) 1941 Ward (5448)
7440-32-6	Titanium	1952 Bailey (160)	1913 Traetta-Mosca (5422) 1921 Headden (5218) 1941 Ward (5448)
	Tobacco, combustion products		1898 Cavalli (637)
	Tobacco, general		1793 Murray (5299) 1895 Carpenter (5143) 1905 Kissling (2104) 1907 Lehmann (2342) 1908 Kissling (2105) 1910 Kissling (2106) 1913 Traetta-Mosca (3942b) 1919 Kissling (2107) 1930 Ehrenstein (1116) 1930 Gabelya and Kipriyanov (5184) 1931 Shmuk (5386) 1934 Garner et al. (5192) 1935 Waser (4139) 1935 Wenusch (4188) 1936 Brückner (451) 1937 Schöller and Molinari (3526) 1938 Brandt (425, 426) 1939 Gaertner (5186) 1940 Bodnár and Votisky (366) 1940 Smirnov et al. (3A19) 1941 Palfray et al. (2890) 1943 Pyriki (3020) 1950 Pyriki (3023)
	Tobacco smoke, general	1923 Baumberger (219) 1930 Gabelya and Kipriyanov (5184) 1931 Koperina (2162) 1933 Kurilo (2241) 1934 Tschebull (3968) 1937 Pyriki (3016) 1937 Rohrbach (3333)	

TABLE 0.4 (continued)
Chronology from 1800 to Late 1953 of Identified Items in Tobacco, Tobacco Smoke, and Tobacco Distillate

		References	
CAS No.	Name (per CA Collective Index)	Tobacco Smoke and/or Tobacco Distillate [Dry (Dr), Destructive (D)]	Tobacco
		1937 Wenusch (4193, 4196) 1938 Brandt (425, 426) 1939 Smirnov and Sirotenko (3710) 1939 Wenusch (4201) 1940 Bodnár and Votisky (386) 1941 Hillsman (1655) 1941 Matthews (2499) 1946 Fromm (1245) 1948 Matthews (2500) 1951 Laskowski (2267) 1953 Warner and Hobbs (4134)	
638-68-6	Triacontane		1937 Shmuk (5388)
	17-Tritriacontanone	1935 Schürch and Winterstein (3562) 1954 Kosak (2170)	
	Triglycerides		1944 Venkatarao et al. (4042c)
73-22-3	Tryptophan		1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
	Tyrosinase		1953 Barrett et al. (5123)
60-18-4	Tyrosine		1952 Frankenburg and Gottscho (1223) 1953 Pearse and Novellie (2911c) 1953 Zacharius and Frankenburg (4398c)
112-37-8	Undecanoic acid	1952 James and Martin (1917)	
7440-61-1	Uranium		1937 Drobkov (5167) 1949 Drobkov (5168)
97-59-6	Urea, (2,5-dioxo-4-imidazolidinyl)- {allantoin}		1933 Vickery et al. (5436) 1935 Vickery et al. (5435) 1946 Garner (5188) 1951 Garner (5189)
9002-13-5	Urease		1953 Barrett et al. (5123)
	Uronic acids		1935 Kobel and Neuberg (2153a) 1953 Phillips and Bacot (5328)
7004-03-7	Valine		1952 Frankenburg and Gottscho (1223) 1953 Zacharius and Frankenburg (4398c)
7440-62-2	Vanadium		1941 Ward (5448)
7732-18-5	Water	1857 Vogel (4060) 1929 Gabelya and Kipriyanov (**Dr**) (1263) 1930 Braun (427, 428) 1932 McNally (2524) 1940 Haag (5207)	1884 Takayama (5419) 1936 Dixon et al. (5165) 1948 Barnhardt (194a)
7440-66-6	Zinc		1926 Sommer and Lipman (5402) 1934 Heffer et al. (20A26) 1938 McMurtrey and Robinson (5285) 1941 Ward (5448) 1951 Garner (5189) 1952 Nicholas (5308)

for numerous additional studies of this type are listed by Rodgman and Perfetti [see Chapter 20 in (5078)]. Among the metals and nonmetals in tobacco smoke, the one much studied pre-1954 was of course arsenic. Between 1917 and 1951, the As level in tobacco rose from about 12 to 57 μg/g (1459). As, usually considered as As_2O_3 in tobacco, was removed from tobacco agronomy in 1952.

While our Bibliography contains numerous references on the isolation, identification, and quantitation of many of the tobacco components listed in Table 0.4, also available are literally hundreds of pre-1954 references on studies that dealt with the effect of several components in tobacco smoke, e.g., nicotine and carbon monoxide, or in chewing tobacco, e.g., nicotine and related alkaloids, on a host of human biological activities. Many such studies are cataloged in the 1961 Larson et al.'s book on experimental and clinical studies on tobacco (2264).

In Table 0.4 are listed two dozen enzymes identified in tobacco prior to 1954. This early research was done primarily to obtain an insight into the mechanism of tobacco curing, fermentation, and aging. With the subsequent escalation of technologies pertinent to the isolation and characterization of enzymes, their number in plants, including the various types of tobacco, has increased dramatically. The number of completely identified tobacco enzymes listed by Rodgman and Perfetti approximated 500, but many thousands of enzymes present in the tobaccos have been cataloged [see Chapter 22 in (5078)].

Paralleling the increase in identified chemical components in tobacco smoke from the fewer than 100 in 1954 (2170) to more than 5300 recently cataloged (5078) and to more than 6000 in this version of our book has been the increase in identified chemical components of tobacco from 325 (see Table 0.4) to the nearly 5000 recently cataloged (5078) and to almost 5600 herein cataloged.

OTHER COMPOUNDS APPLIED TO TOBACCO BUT NOT SPECIFICALLY IDENTIFIED IN TOBACCO OR TOBACCO SMOKE PRIOR TO 1954

In reviewing the tobacco and smoke literature prior to 1953, two additional sets of compounds are provided for historical purposes. These include either (1) compounds applied on tobacco prior to 1953 for the treatment of disease (molds, spores, fungi, viruses, etc.) and pests or (2) compounds applied on tobacco as flavorants, casings, and/or humectants. The listings are not complete as farmers did not always reliably report such usage for their crops and tobacco manufacturers rarely reported the composition of flavor additives, casings, and humectants used on tobacco prior to 1953. Tables 0.5 and 0.6 are primarily of historical value as the chemicals applied to tobacco for disease control and the types of additives applied to tobacco have markedly changed over time. Most of the chemicals in Tables 0.5 and 0.6 are not listed in Table 0.4 because they were not isolated and confirmed to be present on tobacco samples that were analyzed in the articles reviewed. Nonetheless, these compounds were applied to tobacco and may have been present as residues in the case of the fungicides and pesticides or at larger levels in the case of flavorants and humectants. These compounds are listed in Tables 0.5 and 0.6.

IDENTIFIED COMPONENTS OF TOBACCO AND TOBACCO SMOKE IN THE MASTER CATALOG

Many of the components identified in tobacco have also been identified in its smoke because they transfer in part from tobacco to its smoke during the smoking process. Many other identified tobacco components are not found in smoke because they decompose during the smoking process. The level of many tobacco components considered to contribute to the acceptable taste of its smoke is augmented by inclusion in various additive formulations used in the U.S. tobacco industry (1053, 3263).

Figure 0.3 illustrates the increase in number of identified components in tobacco and its smoke. Green and Rodgman (1373) discussed the contribution of improved analytical technologies to the periodic escalation in the number of identified components in each.

An enormous number of references exist pertinent to the isolation, identification, and biological studies of the great number of components in tobacco and tobacco smoke. To avoid considerable repetition, these are presented as a unified References section which contains the references cited not only in this Introduction but also in each chapter. Together with this Introduction, the References section has been issued prior to the beginning of the components catalog. It is obvious that some references have been omitted, but we assure the reader that any omission was not by design but was done unwittingly.

The references cited for a particular tobacco and/or tobacco smoke component may deal simply with its identification or with a variety of topics pertinent to the particular component. Such topics may include the following:

1. The isolation and identification of the component.
2. The characterization of the component by classical chemical means, e.g., the definition of the structure of solanesol isolated from flue-cured tobacco by Rowland et al. (3359), the characterization of a component by spectrographic means such as UV, IR, NMR, MS, and chromatographic retention time, e.g., the identification by Snook et al. of numerous PAHs (3756–3758) and aza-arenes (3750) in cigarette MSS.
3. The search for the precursor in tobacco of a particular component in cigarette MSS (3616).
4. The quantitation of the component on a per gram of tobacco basis or on its per cigarette MSS yield.
5. Improvements/developments in the analytical technology to determine the per cigarette MSS and/or SSS yield of the component, e.g., see Table 6 in (3306b).

TABLE 0.5
Some Compounds Applied to Tobacco for Treatment of Diseases and Pests Prior to 1953

CAS No.	Name	Reference
Fungicides:		
50-00-0	Formaldehyde	1945 Clayton (5149)
7761-88-8	Silver nitrate	1951 Garner (5190)
7487-94-7	Corrosive sublimate {mercuric chloride} $HgCl_2$	1951 Garner (5190)
71-43-2	Benzol {benzene}	1951 Garner (5190)
106-46-7	*p*-Dichlorobenzene	1951 Garner (5190)
1317-39-1	Copper oxide {yellow cuprocide}	1951 Garner (5190)
577-11-7	Sulfosuccinate	1951 Garner (5190)
14882-18-9	Bismuth subsalicylate	1951 Garner (5190)
14484-64-1	Ferric dimethyldithiocarbamate {fermate}	1951 Garner (5190)
7758-98-7	Copper sulfate, anhydrous {Bordeaux mixture}	1951 Garner (5190)
Pesticides:		
12002-03-8	Copper acetoarsenite {Paris Green}	1951 Garner (5190)
592-01-8	Calcium cyanide	1951 Garner (5190)
98-95-3	Nitrobenzene	1951 Garner (5190)
7784-40-9	Lead arsenate {diplumbic lead arsenate}	1901 Marlatt (5272)
		1908 Marlatt (5272)
		1951 Garner (5190)
15096-52-3	Sodium aluminofluoride = sodium fluoaluminate {cryolite}	1951 Garner (5190)
83-79-4	Rotenone	1951 Garner (5190)
16893-85-9	Sodium fluosilicate	1951 Garner (5190)
107-49-3	Tetraethyl pyrophosphate	1951 Garner (5190)
56-38-2	Parathion dust	1951 Garner (5190)
8003-34-7	Pyrethrum	1936 LaForge and Haller (21A33)
		1944 LaForge and Barthel (21A32)
		1951 Garner (5190)
74-90-8	Hydrogen cyanide	1951 Garner (5190)
75-21-8	Ethylene oxide	1951 Garner (5190)
124-38-9	Carbon dioxide	1951 Garner (5190)
75-15-0	Carbon disulfide	1951 Garner (5190)
65-30-5	Nicotine sulfate	1917 Moore and Graham 5290
		1936 Busbey and McIndoo (21A07, 21A08)
		1951 Garner (5190)
68038-71-1	*Bacillus thuringiensis* {B.t.} {Dipel®}	1924 Staudinger and Ruzicka (21A54)

6. Studies on the biological activity of a particular component.
7. Discussions and/or assertions of the toxicity and/or tumorigenicity of a component in MSS, SSS, or ETS.
8. Studies on the inhibition of adverse biological activity of a tobacco smoke component by another component of the smoke, e.g., the inhibition of the mouse-skin tumorigenicity of B[*a*]P by *n*-hentriacontane and *n*-pentatriacontane (4314, 4336), the inhibition of the mouse-skin tumorigenicity of DB[*a,h*]A by B[*a*]A (3814), the inhibition of the mutagenicity of *N*-nitrosodimethylamine (NDMA) by nicotine (2327a, 2327b).
9. Controversies over the extrapolation of the biological effect of a specific component administered individually *vs*. its biological effect when the component in a highly complex mixture such as MSS is administered to a different species, by a different route, and at dose level far in excess of its level in the complex mixture (1318a, 3300, 3627).
10. Description of the design technologies to control the per cigarette MSS yield of FTC "tar" and a particular component, e.g., see Table 16 in (3300).

In many instances, the references cited for a particular component may also contain additional references pertinent to the component.

The categories of chemical components in tobacco and tobacco smoke derived from our Master Catalog will be presented in the sequence shown in Table 0.7:

Each component chapter contains a major Alphabetical Component Index section. As information for the reader, Table 0.8 depicts the first page of the catalog for the alkanes (Table 0.10). A similar component catalog is present in the chapter for each component class.

TABLE 0.6
Some Flavorants, Casings, and Humectants Applied to Tobacco Prior to 1953

CAS No.	Name	Reference
	Liquidambar {sap of the sweet gum tree}	1632 Diaz del Castillo (5164)
8008-94-4	Licorice	1951 Garner (5191)
68916-91-6		
57-50-1	Sugar	1951 Garner (5191)
50-99-7	Glucose	1951 Garner (5191)
8013-17-0	Invert sugar	1951 Garner (5191)
8028-66-8	Honey	1951 Garner (5191)
9000-40-2	St. John's bread	1951 Garner (5191)
68476-78-8	Molasses	1951 Garner (5191)
8024-04-2	Tonka bean	1951 Garner (5191)
	Deer's tongue	1951 Garner (5191)
91-64-5	Coumarin	1951 Garner (5191)
90604-31-1	Rum	1951 Garner (5191)
91450-09-8		
56-81-5	Glycerol	1951 Garner (5191)
111-46-6	Diethylene glycol	1951 Garner (5191)

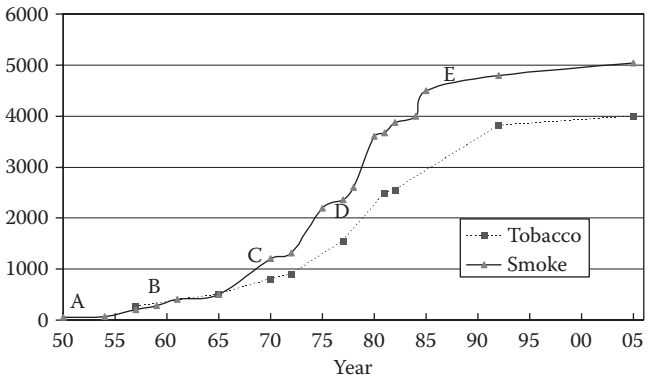


FIGURE 0.3 Number of identified tobacco and tobacco smoke components reported since 1954: accumulative by year: A, prior to 1953: "classical" chemical techniques; B, 1953–1960: column chromatography; C, 1960–1970: gas chromatography; D, 1970 to mid-1970s: glass capillary gas chromatography coupled with mass spectrometry; E, mid-1970s to date: derivatives for HRGC, HPLC, mass spectrometry.

Tobacco smoke, particularly cigarette smoke, is an aerosol comprising literally millions of liquid droplets suspended in a gaseous system [see Ingrebrethsen (1860)]. The liquid droplet portion of this smoke is defined as the particulate phase (PP), the gaseous portion as the vapor phase (VP). The PP is also described alternatively in several ways depending upon the context of the discussion; e.g., the PP collected by a variety of collection techniques such as the Cambridge filter pad, electrostatic precipitation, and jet impaction [cf. review by Dube and Green (1067)] is termed wet total particulate matter (WTPM). Correction for the water content yields total particulate matter (TPM). Subtraction of the nicotine level from TPM gives the Federal Trade Commission (FTC)-defined "tar." The reasons

TABLE 0.7
Sequence of Chemical Component Categories

Chapter 1	*Hydrocarbons*
1.1	Alkanes
1.2	Alkenes and Alkynes
1.3	Alicyclic Hydrocarbons
1.4	Monocyclic Aromatic Hydrocarbons
1.5	Polycyclic Aromatic Hydrocarbons
Oxygen-Containing Components	
Chapter 2	*Alcohols and Phytosterols*
2.1	Alcohols
2.2	Phytosterols
Chapter 3	*Aldehydes and Ketones*
Chapter 4	*Acids*
4.1	Carboxylic Acids
4.2	Amino Acids
Chapter 5	*Esters*
Chapter 6	*Lactones*
Chapter 7	*Anhydrides*
Chapter 8	*Carbohydrates*
Chapter 9	*Phenols and Quinones*
9.1	Phenols
9.2	Quinones
Chapter 10	*Ethers*
Nitrogen-Containing Components	
Chapter 11	*Nitriles*
Chapter 12	*Amines*
Chapter 13	*Amides*
Chapter 14	*Imides*
Chapter 15	*N-Nitrosamines*
Chapter 16	*Nitroalkanes, Nitroarenes, and Nitrophenols*
Chapter 17	*Nitrogen Heterocyclic Components*
17.1	Monocyclic Four and Five-Membered *N*-Containing Ring Compounds
17.2	Monocyclic Six-Membered *N*-Containing Ring Compounds
17.3	Lactams
17.4	Oxazoles and Oxazines
17.5	Aza-Arenes
17.6	*N*-Heterocyclic Amines
Chapter 18	*Miscellaneous Components*
18.1	Sulfur-containing Components
18.2	Halogenated Components
Chapter 19	*Fixed Gases*
Chapter 20	*Metallic and Nonmetallic Elements, Isotopes, and Ions*
Chapter 21	*Pesticides and Growth Regulators*
Chapter 22	*Genes, Nucleotides, and Enzymes*
Chapter 23	*"Hoffmann Analytes"*
Chapter 24	*Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients*
Chapter 25	*Pyrolysis*
Chapter 26	*Carcinogens, Tumorigens, and Mutagens vs. Inhibitors, Anticarcinogens, and Antimutagens*
Chapter 27	*Free Radicals*
Chapter 28	*Summary*

TABLE 0.8
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	106-97-8	Butane $H_3C\text{-}(CH_2)_2\text{-}CH_3$	85, 112, 151, 199, 238, 239, 544–546, 604, 605, 620, 621, 966, 1140, 1153, 1154, 1243, 1284, 1420, 1634, 1966, 2060, 2079, 2270, 2293, 2310, 2634, 2781, 2782, 2799a, 2804, 2857, 2909, 2939, 2940, 2942, 2946, 3059, 3308, 3583, 3584, 3769, 3797, 3876, 3882, 3901, 3939, 3940, 3950, 3973, 4052, 4056, 4162, 4249, 4319, 5811b		3901, 4052, 4056
20.	75-83-2	Butane, 2,2-dimethyl- $(H_3C)_3{\equiv}C\text{-}CH_2\text{-}CH_3$	348, 966, 1140, 2939, 3302, 3876, 4249, 5777, 5811, 5811b		
21.	78-78-4 102056-77-9	Butane, 2-methyl- {methylbutane} $(H_3C)_2{=}CH\text{-}CH_2\text{-}CH_3$	85, 112, 199, 348, 604, 605, 1140, 1153, 1154, 2060, 2767, 2781, 2782, 2804, 2946, 3226, 3308, 3557, 3769, 3797, 4249, 5811b	3973	
2.	124-18-5	Decane $H_3C\text{-}(CH_2)_8\text{-}CH_3$	142, 151, 222–224, 568b, 1445, 1634, 2387, 2543, 2570, 3308, 3365, 4570a, 5770, 5811b	151, 182, 568b, 3797, 4249, 5811b	2387
3.	61193-21-3	Decane, methyl- $C_{10}H_{21}\text{-}CH_3$	1822, 4249		
4.	6975-98-0	Decane, 2-methyl- $H_3C\text{-}CH(CH_3)\text{-}(CH_2)_7\text{-}CH_3$	3557, 4249	925	
5.	13151-34-3	Decane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_6\text{-}CH_3$	1827, 1884, 3557, 4249		
6.	13151-35-4	Decane, 5-methyl- $H_3C\text{-}(CH_2)_4\text{-}CH(CH_3)\text{-}(CH_2)_3\text{-}CH_3$	1884, 4249		
7.	629-97-0	Docosane $H_3C\text{-}(CH_2)_{20}\text{-}CH_3$	568b, 619, 625, 727, 1360, 1375a, 1378, 1427, 1488, 1586, 2176, 2387, 2570, 2761, 2762, 2767, 2777, 2875, 3308, 3557, 3768, 3797, 4249, 5811b	182, 248, 404, 568b, 727, 840, 1488, 1978, 2339a, 3469, 3547, 3604, 3703, 3797,, 4249, 4337, 5811b	1360, 1375a, 1378, 2387
22.	1560-81-2	Docosane, 2-methyl- $(H_3C){=}CH\text{-}(CH_2)_{19}\text{-}CH_3$	1195, 1375, 4249	840, 4337, 5811b	
8.	72227-00-0	Docosane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{18}\text{-}CH_3$	1195, 1375, 4249	840	
9.	112-40-3	Dodecane $H_3C\text{-}(CH_2)_{10}\text{-}CH_3$	568b, 619, 1371, 1425, 1427, 1445, 1488, 1586, 2570, 2767, 3308, 3410, 3557, 3768, 3797, 4248, 4249, 4570a, 5811b	182, 404, 568b, 1488, 2339a, 2753, 2917a, 3186, 3188, 3547, 3797, 4249, 5657, 5811b	
10.	1560-97-0	Dodecane, 2-methyl- $H_3C\text{-}(CH_2)_9\text{-}CH{=}(CH_3)_2$		925	

for exclusion of nicotine and water to give the FTC "tar" value were the long-recognized nontoxicity of water plus the low toxicity of cigarette smoke nicotine as described in the 1964 report of the Advisory Committee to the U.S. Surgeon General (3999). Thus, we have the following relationships among these entities:

$$\text{WTPM} = \text{TPM} + H_2O = \text{FTC "tar"} + \text{nicotine} + H_2O.$$

The equation most frequently used in the United States since the late 1960s is the following:

$$\text{FTC "tar"} = \text{WTPM} - \text{nicotine} - H_2O$$

In many instances, collected cigarette smoke PP is called CSC.

In many countries, cigarette "tar" is determined by use of the International Organization of Standardization (ISO) method. The "tar" yield in the ISO method ISO 4387:1991 is calculated in the same manner as in the FTC method [Pillsbury et al. (2962)], i.e., by subtraction of the water and nicotine from the WTPM collected (ISO 1991). The ISO cigarette equilibration and smoking procedure differ slightly from those in the FTC procedure [see Table 1, p. 496 in Rustemeier and Piadé (3369a)]. These differences typically result in slightly lower measured yields for the ISO method *vs*. the FTC method. The measured values between FTC and

ISO methods are within the detection limits of the test. They differ by no more than 0.4 mg for "tar" and no more than 0.04 mg for nicotine for cigarettes that yield over about 10 mg of "tar." As described by Dixon and Borgerding (988a), under standard smoking regimes, the ISO and FTC methods give very similar results.

The physical nature of cigarette smoke is discussed in the following.

Periodically during the past five decades, various reviews and catalogs on the composition of tobacco smoke, with particular emphasis on cigarette MSS, have been published. These have dealt with the components of total MSS (the VP and the PP components) [Kosak (2170), Bentley and Berry (282, 283), Berry (296), Johnstone and Plimmer (1971), Izawa (1900), Philip Morris, Inc. (2939), Stedman, (3797), Ishiguro and Sugawara (1884), IARC (1871)], with MSS PP components only or with MSS VP components only [Elmenhorst and Schultz (1140)], with both MSS and SSS components [Sakuma et al. (3394, 3397, 3398), RJRT (3190), Klus (2133), Klus and Kuhn (2142)], with MSS, SSS, and ETS components [Brunnemann et al. (462), Eatough et al. (1099, 1100)], and with particular classes of smoke components, e.g., nitrogen-containing components [Neurath (2724), Schmeltz and Hoffmann (3491)] or PAHs [Elmenhorst and Reckzeh (1139)].

The majority of these reviews described the composition of smoke from cigarettes with a filler that was primarily tobacco. Although not published in the readily available scientific literature, substantial data are available from studies conducted on the smoke from cigarettes whose filler was not primarily tobacco but a "tobacco substitute" or a tobacco: "tobacco substitute" mixture. Inclusion of tobacco in the filler mixture ensures that the smoke will include the components usually found in an all-tobacco cigarette. Such data appear not only in documents from Celanese describing the composition of MSS from cigarettes containing only its Cytrel® product or in documents by Imperial Tobacco and Imperial Chemical Industries describing the MSS composition from cigarettes containing only their New Smoking Material® (NSM®) product but also in RJRT R&D reports which outline its studies on the composition of smoke from cigarettes made with Cytrel® only, NSM® only, the Sutton Smoking Material (SSM) only, or J-10 only (a tobacco substitute, comprising a puffed grain, developed in-house at RJRT). Recently, an article by Green et al. (1375a) on the effect of several tobacco substitutes on cigarette MSS composition has been published.

At RJRT, all available data on the composition of MSS from cigarettes made with various tobacco types, tobacco blends, various "tobacco substitutes," and/or celluloses have been routinely cataloged by R&D personnel, including one of the present authors (A.R.), for over five decades (2270, 2292a, 3224, 3245, 3252, 3253, 3301–3304, 3308).

Until the early 1980s, the majority of the studies on tobacco smoke composition dealt with the composition of cigarette MSS. PP composition was the major research topic throughout the 1950s with studies on VP composition receiving increased emphasis in the early 1960s when the biological response in laboratory animals could not be explained by nature and/or the level of any of the PP components acting individually or in concert.

TOBACCO SMOKE AND THE EXAMINATION OF ITS TUMORIGENICITY IN LABORATORY ANIMALS

The initial research efforts were directed at attempts to identify the components in the CSC that could be responsible for the observed biological response in the CSC-painted animals. Immediately, the class of compounds selected for intense investigation was the PAHs. Why was this class of compounds selected? Primarily, it was because of the 20 years of research effort since the initial findings in the early 1930s (194, 2078) that had shown that many PAHs were tumorigenic to mouse skin (1544), with several being classified as highly potent carcinogens to mouse skin (3306b).

After more than a century of research during which investigators attempted to induce malignant tumors in laboratory animals by administration of a variety of industrial tars, soots, oils, etc., success was finally achieved by Yamagiwa and Ichikawa (4361) who reported the first induction of tumors in laboratory animals skin-painted with coal tar solutions. Their findings, which subsequently led to extensive research on the induction of malignant tumors by skin painting of laboratory animals with various tars and oils, also led to the definition in 1923 of the terms carcinogen, carcinogenesis, and carcinogenicity: carcinogenesis was defined as the induction of a carcinoma by the treatment. In 1930, a synthetic pentacyclic PAH, dibenz[*a,h*]anthracene (DB[*a,h*]A) {I} (760, 1184), was reported to be highly carcinogenic to mouse skin by Kennaway and Hieger (2078). In the early 1930s, Cook et al. (796a, 797) isolated several PAHs from two tons of coal tar. One of the PAHs, initially unknown, was demonstrated by characterization and synthesis to be benzo[*a*]pyrene (B[*a*]P) {II}, another pentacyclic PAH structurally similar to DB[*a,h*]A (see Figure 0.4). Subsequently, it was demonstrated by Barry et al. (194) that B[*a*]P was also a potent carcinogen for the skin of susceptible mouse strains. The finding of the carcinogenicity of these two individual compounds, DB[*a,h*]A and B[*a*]P, was the stimulus for the synthesis and bioassay of literally hundreds of PAHs (and structurally similar nitrogen analogs) and their alkyl derivatives. Many of the PAHs with four or more fused rings were reported to be carcinogenic to mouse skin. A wealth of data was generated from research on attempts to correlate carcinogenic potency with PAH structure [Coulson (829), Pullman and Pullman (3003), Lacassagne et al. (2247a)]. The carcinogenic potency to mouse skin is dependent on the PAH structure and its substituents; e.g., benz[*a*]anthracene (B[*a*]A) {III} is a relatively weak carcinogen to mouse skin, whereas its 7,12-dimethyl homolog (DMBA) {IV} is an extremely potent one (983). The tricyclic PAH phenanthrene {V} is noncarcinogenic to mouse skin, but its 1,2,3,4-tetramethyl homolog {VI} is slightly carcinogenic (983).

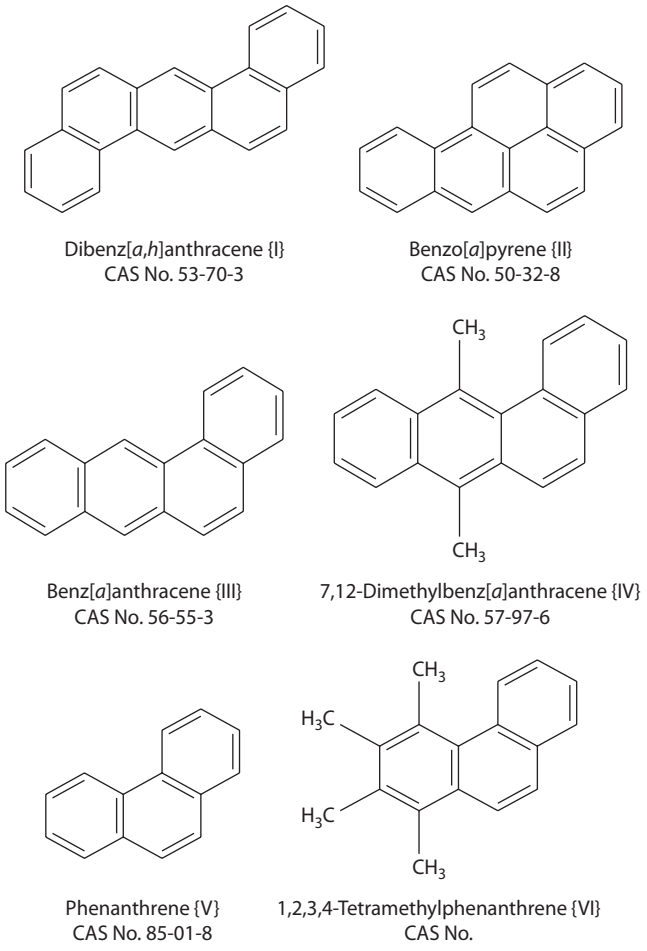


FIGURE 0.4 Polycyclic aromatic hydrocarbons.

Kennaway (2073–2076) reported that pyrolysis of a variety of organic compounds (methane, acetylene, isoprene, cholesterol) or mixtures containing organic compounds yielded pyrolysates which were tumorigenic to mouse skin. Subsequently, it was reported that a variety of carcinogenic PAHs, including B[*a*]P, were components of similar pyrolysates, e.g., the pyrolysates from the tobacco smoke components methane [Burrows and Lindsey (529a)] and isoprene [Oró et al. (2864b)], as well as the pyrolysate from the tobacco phytosterols structurally similar to cholesterol [Wynder et al. (4355), Van Duuren (4022), Schmeltz et al. (3511), Severson et al. (3616)].

For several years in the early 1950s, whether PAHs were present in tobacco smoke was a highly controversial subject. The early claims of the presence of B[*a*]P in cigarette smoke were criticized by Kosak et al. (2177) in 1956 and by Fieser (1181) in 1957 because of the failure to duplicate the reported findings when similar analytical techniques were used. Logic dictated that the PAHs, including B[*a*]P, would indeed be present since they arise pyrogenetically from organic compounds under a variety of conditions. Several of the demonstrated PAH precursors are known to be components of tobacco used in a cigarette, cigar, or pipe. The smoking process involves pyrolysis and/or combustion. The differences between the effect of pyrolysis of an individual compound *vs*. the effect of the cigarette smoking process on the same compound in the complex tobacco mixture were discussed by Rodgman et al. (3307), and their discussion will be summarized in a later chapter. However, even as late as 1957, Fieser, one of the eminent American authorities on tumorigenic PAHs, was not convinced that the presence of B[*a*]P in cigarette smoke had been demonstrated. Fieser (1181) discussed the available published data from various laboratories as follows:

> British [Cooper and Lindsey (820)] and American groups [Lefemine et al. (2335), Alvord and Cardon (55), Cardon and Alvord (593)] have claimed identification of benzpyrene following extensive chromatography of tars from cigarette smoke, but in each case the evidence of identity is correspondence of the smoke factor with the synthetic carcinogen in fluorescence spectrum, coupled with the correspondence of the two materials in one region of the ultraviolet absorption spectrum… In the absence of complete ultraviolet correspondence, the smoke-factor reported by the two groups of investigators can be described as nothing more than a benzpyrene-like substance, which may or may not be carcinogenic…
>
> Kuratsune (2237) [examined] the smoke from cigarettes of two Japanese brands and detected no benzpyrene… In my laboratory 20 g of cigarette smoke tar (from 500 cigarettes) to which 9.7 μg/g of benzpyrene was added was chromatographed… and rechromatographed… the recovery [of benzpyrene] was 7.8 μg/g of tar (80%)… In a parallel experiment with 20 g of the same tar and no additive, fractions corresponding to the positive fractions of the control were all negative… Our estimate was that benzpyrene could be present in amounts no greater than 1 part in 5 million parts of tar.
>
> Present evidence thus indicates that benzpyrene is formed in trace amounts on pyrolysis of constituents of tobacco (probably cellulosic), but that no appreciable amount passes into the smoke, and hence that this hydrocarbon is not the agent responsible for the observed carcinogenicity to mice of cigarette smoke tar [Wynder et al. (4306a)].

Fieser also reported that his colleagues Huang and Johnston failed to detect B[*a*]P in the MSS from American cigarettes even though they determined its level (80% recovery) in CSC "spiked" with B[*a*]P (1181). In Japan, Kuratsune, unable to demonstrate the presence of B[*a*]P in the CSC from Japanese cigarettes, was able to demonstrate its presence in roasted coffee beans and various other pyrolysates [Kuratsune (2237), Kuratsune and Hueper (2238)]. After subsequent studies by Orris et al. (2865) and Kiryu and Kuratsune (2099) or assessment of more complete laboratory data, Fieser (1182) and other critics reversed their earlier positions and eventually accepted that B[*a*]P was indeed present in tobacco smoke. The ultimate confirmation of the presence of B[*a*]P in cigarette smoke was its isolation in crystalline form and characterization by chemical means rather than reliance solely on the correspondence of the ultraviolet spectrum of the isolate with that of an authentic sample. Isolation of crystalline B[a]P from the MSS of a 70 mm nonfiltered cigarette was reported in 1956 by Rodgman (3240) and by Hoffmann [see Wynder and Hoffmann (4307)] in 1959 and from a filtered cigarette in 1960 by Rodgman and Cook (3273). Fieser, the

major architect of the chapter on smoke composition in the 1964 report of the Advisory Committee to the U.S. Surgeon General (3999), had access to the published data by Wynder and Hoffmann (4307) on the isolation of crystalline B[*a*]P from cigarette smoke. However, numerous proponents of the adverse effect of cigarette smoke, e.g., Wynder and Wright (4282a, 4354) and Wynder and Hoffmann (4307, 4312), asserted that the level of B[*a*]P in CSC or the levels of several tumorigenic PAHs including B[*a*]P could only account for a few percent of the biological response observed in mouse-skin-painting studies with CSC.

Since much of the post-1950 effort on MSS composition was directed to the definition of the cancer-causing agents in MSS possibly responsible for the association between lung cancer and cigarette smoke in smokers, it is a requisite that the various terms used in laboratory studies of tumor generation be understood.

In their 1990 list, Hoffmann and Hecht (1727) cataloged the tobacco and/or tobacco smoke components classified as "tumorigenic agents" and the range of the per cigarette MSS yields of each. Prior to examining the individual components on the list, an important distinction between "tumorigenicity" and "carcinogenicity" should be noted. In the 27th edition (1988) of Dorland's medical dictionary (1051b), the definition of carcinogenesis, first enunciated in 1923, is the same as that listed in the 13th edition issued in 1927 (1051b). Some investigators incorrectly use the term "carcinogenesis" for the production of any tumor type, not just for a carcinoma. The correct term, if used in this manner, is "tumorigenesis." The term "carcinogen" is often applied, again often incorrectly, to any factor that induces any type of tumor. Common in the past, but seldom used now, was the term "sarcogenesis" used to describe the production of sarcoma, the endpoint obtained in many investigations in which the mode of administration of the compound under test, e.g., a PAH, was by subcutaneous injection.

Additionally, terms such as *carcinogen*, *carcinogenicity*, and/or *carcinogenesis* or *sarcogen*, *sarcogenicity*, and/or *sarcogenesis* should not be considered as fixed properties of compounds. It should be noted that in several of their early publications, Wynder and Hoffmann (4342, 4343a, 4346) and Hoffmann and Wynder (1801) carefully differentiated among the terms *carcinogenesis*, *sarcogenesis*, and *tumorigenesis* but eventually discontinued this practice. Other investigators have done the same.

Because of the successful induction of cancer in a laboratory animal by Yamagiwa and Ichikawa (4361) and the discovery that several PAHs were tumorigenic when painted on the skin of laboratory animals (194, 797, 2078), the tumorigenicity of literally hundreds of PAHs (and structurally similar nitrogen analogs) and their alkyl derivatives was studied from 1922 to 1941. Many of the assertions made about the correlation between the laboratory findings and human experience were extremely farfetched and caused much confusion. This led to the request for Shear of the U.S. National Cancer Institute to attempt to return order to the field of carcinogenicity. The result was the classical description by Shear and Leiter (3627), a description which is still valid today.

Carcinogenicity is a variable property, depending on a number of factors. It differs from other properties of a compound that are fixed, e.g., melting point, boiling point, refractive index, specific gravity, crystalline form. As noted by Shear and Leiter (3627), by Hartwell (1544), and by many others, a substance or factor can show a range of effects from carcinogenicity to noncarcinogenicity to anticarcinogenicity, and the response will differ in the laboratory depending on the animal used (species, strain, sex, age), dose, route of administration (inhalation, ingestion, injection [subcutaneous, intravenous, intraperitoneal], skin painting, douching), mode of administration (single *vs*. multiple doses, neat, in solution, as an aerosol, as a vapor), diet supplied to the animals, and cage care.

SMOKE-FORMATION PROCESSES, DISTRIBUTION (MSS, SSS, ETS), CHEMICAL COMPOSITION, AND ANALYTICAL METHODS FOR IDENTIFICATION

Cigarette smoke composition is dependent on two major processes occurring during the smoking of tobacco: the direct transfer by vaporization of volatile tobacco components directly to the smoke and the pyrogenesis of smoke components from tobacco components. The pyrogenesis involves a variety of reactions including oxidation, reduction, aromatization, hydration, dehydration, condensation, cyclization, polymerization, depolymerization, etc.

Table 0.9, adapted from Kosak (2170), lists the fewer than 100 tobacco smoke components reported in the scientific literature to that date. Examination of his compilation reveals the following:

1. Of the approximate 80 entries, the identities of 33 (over 40%) of the components were questioned by Kosak because he did not "consider the evidence cited in the literature to be definitive proof" of their identities.
2. Two of the listed items (B[*a*]P, "condensed aromatics") were reported by Roffo (3323, 3324) whose research did *not* involve the study of tobacco smoke but involved a study of material obtained by the "destructive distillation" of tobacco.
3. Several of the alkaloid-related components (α-, β-, and γ-socratine, obelin, lohitam, anodmin, lathraein, poikiline, and gudham) first reported by Wenusch and Schöller (4210, 4211) and listed under *Alkaloids* were subsequently demonstrated to be mixtures or a component listed elsewhere in Table 0.9. For example, Kuffner et al. (2224) demonstrated that obelin was a salt of ammonia, α- and β-socratine were mixtures of nicotyrine and 2,3′-bipyridine, and γ-socratine was *l*-nornicotine. Poikiline was characterized as 4-amino-1-(3-pyridyl)-butanone. Many of these characterization corrections are described in Johnstone and Plimmer (1971).
4. Kosak listed references to phenol (1857, 4202), catechol (2107, 4202), and "phenolic acids" (3324) as tobacco smoke components. However, he failed to report the

1952 presentation by Rayburn (3089) of the unequivocal identification of phenol, guaiacol (2-methoxyphenol), *o*-cresol (2-methylphenol), and *m*-cresol (3-methylphenol) in the smokes from the four major tobacco types (flue-cured, burley, MD, Oriental).

5. Azulene, a bicyclic $C_{10}H_8$ hydrocarbon isomeric with naphthalene, was first reported as a tobacco smoke component by Ikeda (1857) and subsequently by Gilbert and Lindsey (1287, 1288), Lindsey (2365), and Lyons (2426). Despite improved analytical technology and hundreds of studies on the identification of PAHs in tobacco smoke, very few reports of its identification have appeared since those in the 1950s. This suggests the possibility that the azulene reported in tobacco smoke condensate in the 1940s and 1950s may have been formed artifactually.

In summary, Kosak's 1954 list, shown in Table 0.9, included only about 50 components, the identities of which were certain.

TABLE 0.9
Tobacco Smoke Components Listed by Kosak (2170)

Class	Component	Class	Component	Class	Component
Hydrocarbons	Hentriacontane (?)	*Ketones*	3-Pentanone	*Acids*	Formic acid
	Acetylene		4-Heptanone		Acetic acid
	"Unsaturated hydrocarbons"		17-Tritriacontanone (?)		Butyric acid
			2,3-Butanedione		Valeric acid
	Azulene phenanthrene (?)		"Higher" ketones (?)		Caproic acid
	Anthracene (?)				C_7 and C_8 aliphatic acids (?)
	Benzopyrene (?)				Succinic acid (?)
	"Condensed aromatics" (?)				Fumaric acid (?)
					Citric acid (?)
					Benzoic acid (?)
					Phenolic acids (?)
Alcohols and phenols	Methanol	*Alkaloids*	Nicotine	*Miscellaneous components*	Levoglucosan[c]
	Glycerol		Pyridyl ethyl ketone		"Phytosterol" (?)
	Diethylene glycol[a]		Myosmine		$C_{10}H_{14}O$ (a furan ?)
	Ethylene glycol[a]		Nicotyrine		"Resins" (?)
	Phenol (?)		α-Socratine[b]		"Resin acids" (?)
	Catechol (?)		β-Socratine[b]		
			γ-Socratine[b]		
			Obelin[b]		
			Lohitam[b]		
			Anodmin[b]		
			Lathraein[b]		
			Poikiline[b]		
			Gudham[b]		
Aldehydes	Formaldehyde	*Other* N-*containing components*	Pyrrole (?)	*Inorganic components*	Ammonia
	Acetaldehyde		"Pyrroles" (?)		Carbon monoxide
	Butyraldehyde acrolein (?)		"*N*-Methyl-pyrrolidines" (?)		Carbon dioxide
	Benzaldehyde				Hydrogen cyanide
	2-Furaldehyde (?)[d]		Pyridine		Hydrogen sulfide
			"Picoline" (?)		Thiocyanic acid (?)
			"Lutidine" (?)		Oxygen
			"Collidine" (?)		Arsenic[e]
			"Pyridine bases" (?)		"Acetates" (?)
			Methylamine (?)		"Chlorides" (?)
			"Chlorophyll degradation products" (?)		"Cyanides" (?)
					"Nitrates" (?)
			"Uric acids" (?)		

[a] In smoke because of transfer of an humectant added to tobacco.

[b] Subsequent study demonstrated this component was not a well-defined compound but an artifact, a mixture, or an ammonium salt [see discussion by Johnstone and Plimmer (1971)].

[c] 1,6-Anhydro-β-*D*-glucopyranose.

[d] The question mark indicates that Kosak did not consider the evidence in the literature to be definitive proof of the identity of the component.

[e] Probably present as As_2O_3.

The number of identified components in cigarette tobacco smoke has increased almost 100-fold from the 50 definitively identified tobacco smoke components listed by Kosak (2170) to the more than 5000 components identified to date and cataloged by RJRT personnel. Components were originally included in the RJRT catalog only if their identification criteria satisfy the identification criteria of classical organic chemistry. Later, identification criteria from modern analytical chemistry were employed. From 1950 to 1955—the early years of the great escalation of interest in the composition of cigarette smoke—"isolations" were often accomplished with no regard to the possibility of artifact formation. Also, "identifications" of tobacco smoke components were often based on less than complete spectral data, e.g., the PAHs and their ultraviolet spectra, R_f values, color tests, and the like. Because of the state of the art of the isolation techniques available in the early 1950s, the level in smoke of a component under investigation often precluded its isolation in quantities sufficient for application of the classical chemical techniques (melting point and mixture melting point determinations, derivative preparation, elemental analysis, etc.) used for identification.

The authors of some of the early reviews and catalogs on tobacco smoke composition listed the smoke components reported in the literature without regard to the analytical validity of their identification. This problem has progressively decreased over the years as analytical technology has increased in sophistication.

Few, if any, commercial products have experienced the analytical scrutiny that has been applied to tobacco smoke or tobacco. The composition of coffee has been examined, but the number of components identified is less than 25% of the number identified in tobacco smoke. Despite the identification of over 4700 additional smoke components since the 1954 listing by Kosak, various investigators have estimated from gas chromatographic scans that for each component identified in tobacco smoke, there are 5–20 components present at extremely low per cigarette yields that have not yet been identified. Thus, as noted by Wakeham (4103), when the identified tobacco smoke components numbered about 1350, "Gas chromatographic scans indicate there are many more, probably over ten thousand, possibly even a hundred thousand [tobacco smoke components]."

Grob (1422), one of the pioneers of the use of glass capillary gas chromatography in tobacco smoke composition studies, as well as other tobacco smoke investigators also noted that the number of peaks, each of which represented at least one component, in the chromatographic scans far exceeded the number of identified components.

In addition to the advancement in knowledge of the chemical composition of cigarette smoke was the advancement in the knowledge of its physical properties, that of an aerosol. An aerosol is defined as a colloidal system of dispersed liquid or solid material in a gaseous medium: cigarette smoke is an aerosol comprising liquid droplets in a gas.

For nearly two decades, investigators have accumulated knowledge on the conditions involved in the formation of MSS and SSS aerosols during the smoking of a cigarette and the factors contributing to or modifying their yields and composition. Theories on smoke formation in vogue in the late 1950s and early 1960s were demonstrated to be incorrect; e.g., many investigators thought that all smoke components not originally present in tobacco and thus appearing in the MSS by pyrogenesis from the tobacco were formed at or near the fire cone at temperatures in excess of 900°C. New and more nearly correct theories replaced the old ones. Advances in our knowledge of smoke formation and transport were possible because of improved technologies developed to accomplish the following tasks [cf. Townsend (3941a)]:

1. Accurately measure temperatures during puffs and during the smolder period between puffs at various sites within the burning cigarette and its fire cone.
2. Follow the formation of specific components and their subsequent passage and transport, in the case of MSS components, through the tobacco rod by puff-driven volatilization, repetitive condensations and revolatilizations, filtration by tobacco rod and filter-tip material, etc.
3. Follow the formation of specific components and their subsequent emission, in the case of SSS components, to the atmosphere.

Baker (163a, 166) has written at length on his original research and that of others on MSS and SSS aerosols and the conditions involved in the cigarette in their formation and transport. He has also periodically authored or coauthored several excellent and detailed reviews (167, 169, 170a, 171a, 171b, 174d) on this subject.

It is now known that the fire cone temperature of 900+°C measured during the puff primarily generates gaseous components such as the carbon oxides, water, ammonia, and nitric oxide. During the puff, pyrogenesis of most MSS components occurs in a 3–4 mm cylinder of the tobacco rod a few millimeters behind the fire cone–tobacco rod interface where the temperature ranges from 500°C to 650°C. During the smolder period, the fire cone temperature is 500°C–600°C, and it is at this temperature range that SSS is generated from the tobacco.

Just as profound quantitative differences exist among the chemical compositions of fresh and aged MSS, fresh and aged SSS, and ETS, there are several differences in the physical properties of these smokes. One physical property important in these various types of cigarette smoke, their inhalation, and their retention is their particle size. There are several ways to describe particle size. A frequently used one is mean mass aerodynamic diameter (MMAD).

In his review of the aerosol studies on cigarette smoke, Ingebrethsen (1860) points out that two factors are extremely important with respect to the measured particle size of an aerosol: (1) the time between aerosol generation and particle size measurement and (2) the concentration of the aerosol.

High aerosol concentration and extended time between generation and measurement result in increased coagulation

of particles and increased particle size. Freshly generated MSS and SSS have the major fraction of particle sizes, expressed as MMAD, in the range 0.3–0.4 μm [Ingebrethsen (1860c)]. Since SSS—both intra- and interpuff generated—is the major contributor, estimated at 85%–90%, to ETS, it is important to realize that its physical properties are constantly and progressively changing. These changes begin the moment it is generated and continue during its extensive dilution as it disperses through the room until it is eventually perceived as ETS. Depending on the proximity of the measuring device to the source of the SSS, it is obvious that a range of particle sizes could be found, ranging from that measured in freshly generated SSS to that found in essentially equilibrated ETS. The behavior of particles in SSS under carefully controlled conditions has been studied in detail by Ingebrethsen and Sears (1860e).

Another problem of determining the contribution of ETS to a given air space (home, office, restaurant, aircraft, etc.) is that other non-ETS contributors to VP and PP are measured at the same time as the contribution of ETS to VP and PP is measured. These include contributions from cooking oils and foods in homes and restaurants, cleaning preparations and furniture polishes, personal products (perfumes, after-shave lotions, hair sprays, deodorants, etc.), and vehicular exhausts where the air space is adjacent to much-traveled roads. Chromatographic scans of samples collected in a conference room before and after a 2 h meeting during which smoking was permitted revealed that chromatographic peaks, some representing compounds from nontobacco sources, were much larger than those known to be due to ETS (1352a). Similar findings were reported by Bayer and Black (223) who compared volatile organic contaminants (VOCs) in the offices of smokers and nonsmokers. The authors noted:

> Building materials and furnishings are the most common source of these VOCs. [The] VOC building background makes it difficult to distinguish ETS contamination from the VOCs out-gassing from other sources.

A major distinction between MSS and SSS that affects particle size is that MSS is acidic,* with a pH ranging from 6.0 to 6.6; whereas, the pH of SSS ranges from 6.7 to 7.5. The SSS from most cigarettes is alkaline with pH above 7.0. Under acidic conditions (pH < 7.0), smoke amines such as nicotine are considered to be protonated and have relatively low volatility. Under alkaline conditions (pH > 7.0), such amines are considered to be nonprotonated, i.e., "free," and are relatively more volatile.

The differences and similarities in the physical properties among MSS, SSS, and ETS are summarized in Table 0.10.

When freshly generated, MSS is inhaled during smoking; the aerosol particles in the smoke are exposed in the respiratory tract to an atmosphere whose temperature is 37°C and whose relative humidity exceeds 95%. As a result, the inhaled particles absorb water and increase in size. Those particles that are exhaled are, on average, 20%–25% larger than the inhaled particles (273, 1860b, 1860d, 1860e). When these water-saturated exhaled MSS particles (temperature at 37°C) are released into the atmosphere (temperature generally below 30°C and relative humidity below 50%), they cool and immediately undergo several evaporative processes which are completed in a few milliseconds. These processes include the following:

1. Components, usually gaseous under ambient conditions, evaporate from the particle.
2. Components with modest vapor pressures evaporate from the particle.
3. Water, incorporated into the particle either during the smoke-formation process in the tobacco rod or during its residence time in the highly humid confines of the respiratory tract, evaporates.

SSS particles behave much differently than MSS particles. Although little research has been conducted on fresh, undiluted SSS, it is reasonable to expect that the particles are physically similar to those in MSS. However, the high dilution which occurs almost immediately upon generation has the effect of preventing coagulation and promoting evaporative losses. Also, because of the alkalinity of SSS, basic components are nonprotonated and readily evaporate from the particle. Studies in 1985 by Eudy et al. (1169) on SSS and ETS, both generally alkaline (pH > 7.0), indicated that little (<5%) of the nicotine remains in the ETS particle, the bulk of it (>95%) evaporates from the particle and appears in the VP.

As a result of these various processes, the SSS and exhaled MSS particles, on their way to contribute to ETS, decrease both in particle mass and in particle size to an MMAD ranging from 0.15 to 0.20 μm for the major fraction of the particles. Experimental data for the decrease in SSS particles size were presented by Ingebrethsen and Sears (1860e, 1860f). Ten minutes after smoke generation, a major fraction of the SSS particles showed a particle size with an average MMAD of 0.198 μm.

It should be noted that these various evaporative processes involve relatively volatile smoke components. The particle size is not diminished to any appreciable degree by evaporation of nonvolatile and high-molecular-weight components such as the PAHs (B[*a*]P, DB[*a,h*]A, indeno[1,2,3-*cd*]pyrene, dibenz[*a,i*]pyrene) listed by Hoffmann and Hecht (1727) and Hoffmann and Hoffmann (1740, 1741) and other components such as solanesol, the phytosterols, α-tocopherol, and the saturated aliphatic hydrocarbons. These components remain in the particles.

In addition to the dilution that occurs when the ETS particles disperse through the room space, an additional dilution occurs by the deposition of ETS particles on the surfaces present. These processes—evaporation, dispersion, deposition—decrease the concentration of ETS particles. Ventilation, air exchanges per unit time, nature of the surfaces (fabric, plastic, wood, etc.), temperature, relative humidity, number

* The MSS from cigarettes fabricated from dark air-cured tobacco or air-cured cigar-type tobacco shows a slightly alkaline pH.

TABLE 0.10
Physical Properties[a] of MSS, SSS, and ETS

Properties	MSS	SSS	ETS
Number of identified components	Over 4300 in PP; about 1000 in VP. Some components are present in both the PP and VP, e.g., HCN, simple phenols, volatile *N*-nitrosamines	Composition assumed to be qualitatively similar to that of MSS; i.e., the number and identity of the SSS and ETS components are the same as those in MSS. Quantitative differences in component levels are substantial. The distribution of a component between PP and VP depends on the nature (acid, base, neutral) and the physical properties (vapor pressure, etc.) of the particular component. The decay (decrease) of an individual ETS component is also dependent on numerous factors such as its nature, its physical properties, and the temperature, relative humidity (RH), ventilation, and nature of surfaces (carpets, drapes, upholstered furnishings, etc.) in the smoke space	
Approximate temperature of			
• Fire cone	850°C–950°C	500°C–650°C	
• Smoke formation	500°C–600°C	500°C–600°C	
Approximate % of tobacco rod consumed[b]	30–40	50–60	
Particle size, μm	Fresh whole MSS particles have MMAD = 0.3–0.4 μm[c] and contain volatile components which readily vaporize from the particles. Because of coagulation, hydration, evaporative transfer, and other physical processes, e.g., the cloud effect, MSS particles behave as though they have a MMAD in the micron range[c]	Fresh SSS particles are about the same size as MSS particles; within a short time (<10 min) after generation, the MMAD ≫ 0.2 μm[c] for SSS particles	During dilution to ETS, exhaled MSS particles lose H2O and other volatile PP components; particle size decreases to an MMAD = 0.15–0.20 μm[c] SSS particles lose H_2O and other volatile PP components such as nicotine and amines. Thus, particle size decreases to an MMAD = 0.15–0.20 μm[c]
Particle concentration, number/cm^3	10^9–10^{10}		~1–5 × 10^5
Retention of particulate matter in respiratory tract	50%–90% Percentage retention as measured by weight loss between time of inhalation and exhalation due to mechanical trapping plus loss of volatiles from inhaled particles		10%–11% Low percentage retention as measured by weight loss is due to virtual absence of coagulation and other physical phenomenon, e.g., cloud effects, and lack of water and other volatile components which may be lost by inhaled ETS particles
Smoke pH	6.0–6.6 for cigarette MSS[d]	6.7–7.5 for cigarette SSS. Some investigators have reported SSS pH values as high as 8.0	Neutral (pH 7.0) to slightly alkaline
Inhalability of smoke into lungs	MSS inhalability favored by pH less than 7.0	Inhalability of smoke (whether cigarette SSS, pipe MSS, or cigar MSS) is progressively diminished as smoke pH increases above pH 7.0	Because of extreme dilution by air and near neutrality (pH close to 7.0), the inhalability of ETS is nearly the same as that of air
Nicotine behavior	99+% of nicotine in cigarette MSS is in the PP; because the MSS pH is much less than 7.0, amines such as nicotine are protonated; nicotine in MSS PP is presumed to be protonated by the low-molecular-weight acids present in MSS[e]	Because of alkalinity of SSS and the high concentration of SSS particles near the burning cone, nicotine (and other volatile smoke components) is distributed between the SSS PP and SSS VP; PP–VP equilibrium for these compounds is not attained adjacent to the cigarette burning cone	Because of the extremely high dilution of ETS and its pH at or slightly above 7.0, little nicotine (or other amines) is found in ETS PP; more than 95% of the nicotine in ETS is in the nonprotonated form and is found in ETS VP

TABLE 0.10 (continued)
Physical Properties[a] of MSS, SSS, and ETS

Properties	MSS	SSS	ETS
Relationship of smoke yield to cigarette design	MSS controllable by • Tobacco rod length and circumference • Filter type and dimensions • Tilter-tip additives • Tobacco blend and weight • Processed tobacco (reconstitution, expansion) • Paper and paper additives • Air dilution (paper porosity and filter perforation)	Interpuff SSS, the major contributor to total SSS, is primarily controlled by cigarette tobacco blend and weight and to a lesser degree by paper properties and additives	Since ETS comprises 85%–90% diluted and aged SSS plus 10%–15% exhaled MSS, the control of ETS resides primarily with those factors which control intrapuff SSS generation

[a] Properties listed are those for unaged and undiluted smoke.
[b] Tobacco rod not consumed during smoking estimated at 5%–8% for filtered cigarettes and 20%–25% for nonfiltered cigarettes.
[c] MMAD value listed is that for a major fraction of the smoke.
[d] The MSS from cigarettes fabricated from dark air-cured tobacco or air-cured cigar-type tobacco shows a slightly alkaline pH.
[e] Protonation of nicotine in tobacco due to long-chained acids (palmitic acid, stearic acid, etc.) and polycarboxylic acids (oxalic acid, malic acid, citric acid).

of cigarettes smoked per unit time, and number of persons present are some of the known variables that will also influence the concentration of ETS particles.

Questions are frequently raised about the particle size of MSS, SSS, and ETS and the relationship between particle size and retention in the respiratory tract of the inhaled smoke. Usually, particle size plays an important role in determining mainstream particulate retention in the lungs. Based on a comparison of particle size, one might expect ETS and MSS to be retained similarly in human lungs on a percentage basis. Empirical data demonstrate that this is not the case. In the case of MSS, other factors come into play. These drastically alter the amount of MSS particulate matter that is retained. Weight-loss measurements give values ranging from 50% to 90% for the percentage retention of inhaled MSS (1860c). The percentage retention is a characteristic of the individual smoker. The retention of inhaled MSS is much higher than would be predicted by the measured MMAD of fresh smoke, 0.3–0.4 µm. Ingebrethsen (1860c) reviewed the literature on the retention of MSS and identified five factors which might be responsible for increased MSS particle retention. These include coagulation, electrical charge, growth by water condensation, evaporative transfer, and cloud effects. Evaporative transfer and cloud effects were deemed to be the most significant factors. Recently, Moldoveanu et al. (2601b) and Moldoveanu and St. Charles (2601a) reported on the different degrees of retention by humans of 160 cigarette MSS components by comparison of their levels in smoking-machine-generated MSS *vs*. their levels in smoker-exhaled MSS.

ETS particles behave quite differently from MSS particles in terms of human retention. Unlike MSS, the retention of ETS in the lung is not affected by evaporative transfer and cloud effects. Instead, ETS retention is mainly influenced by particle size. Theoretical calculations indicate that the percentage retention of particles equivalent in size to ETS particles should vary between 10% and 20%. A value within the theoretical range was obtained: Hiller et al. from studies with human mouth-breathing volunteer nonsmokers who inhaled orally polystyrene latex spheres of particle sizes similar to those of diluted SSS (1654a) and five volunteers who inhaled a tobacco smoke defined as "sidestream smoke at a concentration similar to that encountered indoors with smokers present" (1654b), estimated the percentage retention of the smoke to be 11%.

The difference in particle retention between MSS and ETS is due largely to the high dilution which SSS particles experience almost upon formation. This dilution causes ETS particles to behave as model, nonvolatile, inert particles by preventing coagulation, obviating cloud effects, and promoting evaporation prior to inhalation.

As noted earlier (Table 0.10), numerous technologies introduced sequentially from the mid-1950s to the late 1960s were incorporated into cigarette design to control MSS yield and composition, what some have characterized as a "less hazardous" cigarette when included in cigarette design [Gori and Bock (1334b), NCI (2683), USPHS (4005, 4009)]. These technologies include

1. Tobacco blend and weight
2. Tobacco rod length and circumference
3. Filter tips (material type and additives)
4. Processed tobaccos (reconstituted tobacco sheet, expanded tobacco)
5. Paper (type and additives)
6. Air dilution (increased paper porosity, filter-tip perforations)

The chronology of introduction of these technologies in U.S. cigarette products is noted in Figure 0.5. Over the years,

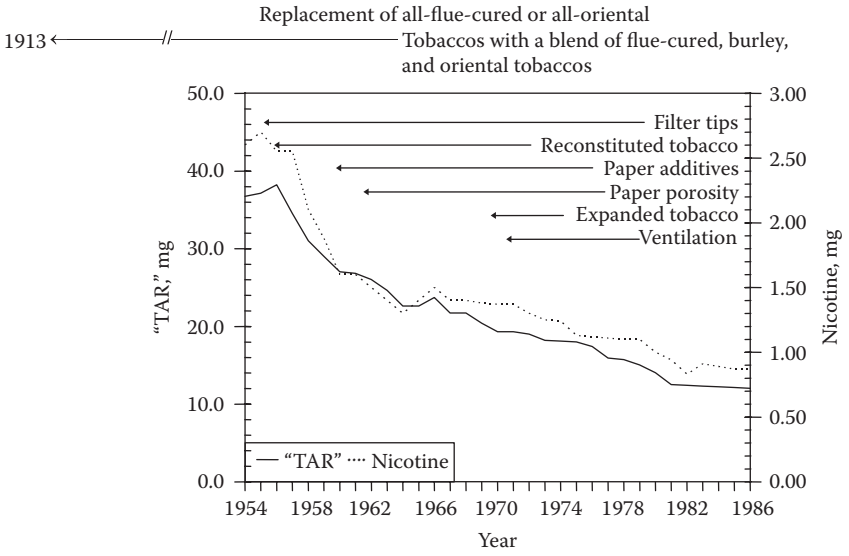


FIGURE 0.5 "Tar" and nicotine yields, sales-weighted average basis, U.S. cigarette products.

use of these technologies in concert and to various degrees in cigarette design has provided the consumer with a great variety of products whose number has increased from about a dozen in the mid-1950s to nearly 1250 in 1995 (1177c). It should be remembered that the cigarette is a system: All of these technologies used in cigarette design are interactive. That is, inclusion of or change in the level of use of any particular technology may require other adjustments in the cigarette design to maintain certain attributes acceptable to the consumer. In contrast, by current technology, SSS yield is controlled almost totally by tobacco blend and weight. The SSS is not subjected to filtration, the effect of filter-tip additives which specifically remove certain MSS components from MSS (phenols, volatile *N*-nitrosamines) or air dilution effects.

Adams et al. (31) reported data on MSS and SSS yields of 14 components in the smokes from four U.S. commercial cigarettes of different design: a nonfilter cigarette, two filtered cigarettes, and a perforated-filter cigarette. MSS and SSS yield data for TPM, nicotine, a PAH–(B[*a*]P), a phenol–catechol, a volatile *N*-nitrosamine–*N*-nitrosodimethylamine (NDMA), and a tobacco-specific *N*-nitrosamine–*N*-nitrosonornicotine (NNN) are summarized in Table 0.11.

The SSS TPM yields shown in Table 0.11 for the nonfiltered and two filter-tipped cigarettes are, on average, about 58% higher than the SSS TPM yield from the perforated-filter cigarette. Most perforated-filter cigarettes, such as Perforated Filter-D in Table 0.11, not only incorporate a perforated filter with a high percentage air dilution to reduce MSS TPM but also incorporate substantial levels (30%–50%) of expanded tobacco in the cigarette design. The inclusion of such a large percentage of expanded tobacco in the blend substantially reduces the weight of tobacco in the tobacco rod and the weight of tobacco consumed during the SS-generating smolder periods. Thus, these data show the SSS TPM yield from the perforated-filter cigarette is substantially less (37%) than the average of the SSS TPM from the other three cigarettes.

In a more recent study on the MSS and SSS yields from cigarettes classified as low tar, Chortyk and Schlotzhauer (723, 724a) provided data which differ substantially from the Adams et al.'s (31) data in Table 0.11 and from other data (3190) reported for comparable "tar"-yield cigarettes. The differences in the data for comparable FTC "tar"-yield cigarettes were found for cigarettes delivering approximately 23, 10, and 7 mg. In their MSS and SSS collection and analysis, Chortyk and Schlotzhauer (724a) used their previously reported SSS collection procedure (723) in the generation of their data. Green (1353) commented on several deficiencies in the procedures used and interpretations made by Chortyk and Schlotzhauer (724a) from their data. Examination of their data and comparison of them with the Adams et al. (31) and RJRT (3190) data (see Table 0.12) reveal an additional problem: For the three cigarette categories (23, 10, and 7 mg FTC "tar" yields), the SSS/MSS ratios for the TPMs in the Chortyk–Schlotzhauer study were between two and seven times greater than those reported in the other studies. Similarly for nicotine, the Chortyk–Schlotzhauer SSS/MSS ratios were from about 1.5 to over 7 times greater than those reported in the other studies. This strongly suggested a problem with their SSS collection procedure.

The escalation of the number of identified tobacco and tobacco smoke components is depicted in Figure 0.3. This tremendous increase in the number of identified tobacco smoke (and tobacco) components was made possible by successive advances in analytical technology, particularly the technology pertinent to the separation of components in complex mixtures.

It is realized that investigators who pioneered an emerging analytical technology were often involved with the development and/or use of the technology prior to the period indicated in Figure 0.5. No slight of their noteworthy contributions is intended. The periods indicated in Figure 0.5 are those when the analytical technology in question was sufficiently advanced and used by almost all investigators

TABLE 0.11
MSS/SSS Distribution of Selected Components Delivered by Four U.S. Commercial Cigarettes

Smoke Component, Yield/Cig	Nonfiltered A		Filtered B		Filtered C		Perforated Filter D	
	MSS	SSS	MSS	SSS	MSS	SSS	MSS	SSS
TPM, mg	20.1	22.6	15.6	24.4	6.8	20.0	0.9	14.1
Nicotine, mg	2.04	4.62	1.50	4.14	0.81	3.54	0.15	3.16
Catechol, mg	41.9	58.2	71.2	89.9	26.9	69.5	9.1	117
B[*a*]P, ng	26.2	67.0	17.8	45.7	12.2	51.7	2.2	44.8
NDMA, ng	31.1	735	4.3	597	12.1	611	4.1	685
NNN, ng	1007	857	88	307	273	185	66.3	338

TABLE 0.12
Comparison of SSS/MSS Ratios for Different Cigarette Types

	Adams et al. (31)			Chortyk and Schlotzhauer					
	20 mg Cigarette			23 mg Cigarette (724a)			23 mg Cigarette (723)		
Analyte[a]	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS
TPM	20.1	22.6	1.12	21.8	56	2.57	22.9	54.9	2.40
Nicotine	2.04	4.62	2.26	1.68	9.08	5.40	1.30	5.29	4.07
	R.J. Reynolds (3190)			Chortyk and Schlotzhauer (724a)					
	1R4F			10 mg Cigarette			10 mg Cigarette		
Analyte[a]	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS
TPM	11.5	16.9	1.47	10.4	60	5.77	9.5	53	5.58
Nicotine	0.79	5.60	7.09	0.90	9.10	10.11	1.05	10.46	9.96
	Adams et al. (31)			Chortyk and Schlotzhauer (724a)								
	7 mg Cigarette			7 mg Cigarette			6 mg Cigarette			6 mg Cigarette		
Analyte[a]	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS	MSS	SSS	SSS/MSS
TPM	6.8	20.0	2.94	6.7	59	8.81	5.4	60	11.11	6.0	50	8.33
Nicotine	0.81	3.54	4.37	0.58	8.95	15.43	0.22	7.04	32.00	0.55	8.06	20.77

[a] mg/cig.

involved in the analysis of tobacco smoke and/or definition of its composition.

Prior to the early 1950s, the major part of tobacco smoke component isolation effort involved so-called classical chemical techniques, i.e., separation of the smoke condensate into neutral, acidic (acids and phenols), and basic fractions by partitioning between water-immiscible organic solvents and water, aqueous basic solutions, and/or aqueous acidic solutions, followed by crystallizations and/or distillations of the subfractions.

In the early 1950s, liquid column chromatography on column packings such as alumina, silicic acid, or Fluorosil® of the neutral, acidic, or basic fractions, as appropriate, permitted further separation of the components prior to application of the classical chemical techniques. UV and IR spectrometry was also available and used not only to combine chromatographic fractions rich in a specific component but also to assist in the identification of the component. UV absorption and fluorescence spectrophotometry were extremely useful in identification of the PAHs in tobacco smoke.

In the late 1950s/early 1960s, commercial equipment for gas chromatography became available. This technique, coupled with those mentioned previously, augmented the investigator's ability to separate, isolate, and identify smoke components. Mass spectrometry and nuclear magnetic resonance equipment and techniques were also more readily available and became additional tools that facilitated component identification. In the early days of gas chromatography, there were fewer than a dozen chromatographic column packings commercially available, and most of these did not permit satisfactory separations above 200°C. By the late

1960s, the number of available column packings increased, and the properties of newly designed column packing materials permitted separations at temperatures of approaching 350°C.

In the early 1960s, investigators such as Grob (1413) began the study on capillary gas chromatography and subsequently glass capillary gas chromatography. A major contribution by Grob was his development of methods to prepare and coat the inner wall of a capillary tube to increase its effectiveness and efficiency in separations. By the late 1960s/early 1970s, this emerging technology—glass capillary gas chromatography—had become an extremely powerful analytical tool and was used to great advantage in the study of the complex mixtures tobacco smoke [cf. Grob (1416–1419, 1422) and Grob and Völlmin (1426, 1427)] and tobacco extracts [Lloyd et al. (2389)]. The glass capillary column was usually a small-diameter (about 1 mm or so) glass or quartz tube, extremely long (50 to 300–400 m) whose interior was not packed with a solid adsorbent or an inert material mixed with a liquid adsorbent as in the previously used gas chromatographic columns. The inner wall of the narrow-bore capillary was coated with a thin layer of a liquid adsorbent. This technology not only enhanced separation capability but permitted separations to be made with extremely small samples. These advances in analytical technology were usually accompanied by a break and an increased slope in the plot of number of identified tobacco smoke components *vs.* time (see Figure 0.3). The next break in the plot and increased slope occurred in the mid-1970s when more and more investigators enhanced the effectiveness of glass capillary gas chromatography by coupling the gas chromatograph to a mass spectrometer. This permitted separation of the components of the particular tobacco smoke fraction under study and determination of the molecular weight and/or fracture pattern of each component as it exited the chromatograph and was analyzed in the mass spectrometer. Interpretation of the data thus obtained, usually in concert with findings from UV, IR, and/or NMR spectra, permitted very rapid and unequivocal identification of the components from the smoke fraction (1426, 1427). An outstanding example of the use of gas chromatography–mass spectrometry in the definition of tobacco smoke composition is the study by Snook et al. (3756–3759) on the PAHs in cigarette MSS. Over 500 individual PAHs and their homologs were detected, and many were identified unequivocally. The early to mid-1970s also saw the emergence of high-performance liquid chromatography (HPLC) (830a, 1361), a highly efficient and effective variation of liquid column chromatography.

The traditional method used to examine CSC (or a tobacco extract) usually involved its initial partition between an aqueous alcohol solution and a water-immiscible organic solvent such as hexane, cyclohexane, or diethyl ether. The organic solvent-soluble material was then separated into several neutral, acidic, and basic fractions. These, in turn, were then subjected to the various analytical techniques available at the time. Considerable success was attained in isolation and identification of the organic solvent-soluble smoke components. For many years, however, there was no satisfactory technique available to separate, isolate, and identify the many components in the aqueous alcohol fraction from the aqueous alcohol–water-immiscible organic solvent partition. Many of the aqueous alcohol-soluble components are highly polar, highly oxygenated compounds, and no chromatographic system was available to effect clean separations. In addition, many of these components—because of their structures—were highly labile at the temperatures used in gas chromatographic separation. By use of the technology known as silylation, these sometime heat-sensitive, highly polar components were converted to chromatographable stable silyl derivatives which can be readily separated by glass capillary gas chromatography and identified by mass and other spectral techniques.

By use of the latest analytical technology available at the time, the mainstream CSC from a typical cigarette was reexamined with particular emphasis on the composition of the aqueous alcohol-soluble material. The separation and identification of 1125 previously unidentified tobacco smoke components were described by Schumacher et al. (3553), Newell et al. (2769), and Heckman and Best (1587) (see Table 0.13). A striking example of the effectiveness of the improved analytical technology on tobacco smoke component identification is the following: In 1977, Schmeltz and Hoffmann (3491) cataloged about 420 nitrogen-containing components identified in MSS. They indicated that the number of identified nitrogen-containing tobacco smoke components had increased by about 200 since a previous review of nitrogen-containing tobacco smoke components by Neurath (2724). In a presentation and publication, Heckman and Best (1587) described the separation and identification of nearly 270 new nitrogen-containing smoke components, an increase of more than 60% over the number described by Schmeltz and Hoffmann (3491) in their review article.

TABLE 0.13
Number of Tobacco Smoke Components Reported (1587, 2769, 3553)

Investigators	Total Identified	Newly Identified	Confirmed Previous Identification
Heckman and Best (1587)	368	268	100
Newell et al. (2769)	643	470	173
Schumacher et al. (3553)	479	387	92
Totals	1490	1125	365

The following is another example of the impact the improved analytical technologies had on the ability to further define the composition of tobacco smoke: In the late 1950s/early 1960s, the composition of an aliphatic ester fraction isolated from flue-cured tobacco by Rowland and Latimer (3358) and from cigarette MSS by Rodgman et al. (3294) was partially defined in both cases by Rodgman et al. (3294). By saponification of the aliphatic ester fraction, followed by separation of the alcohol and acid moieties, Rodgman et al. showed that the tobacco- and tobacco-smoke-derived aliphatic ester fractions were qualitatively the same and theoretically comprised at least 272 esters formed from at least 17 aliphatic acids [myristic (C_{14}) to octacosanoic (C_{28}), oleic, linoleic, and linolenic] and 16 normal long-chained, primary aliphatic alcohols [1-dodecanol (C_{12}) to 1-heptacosanol (C_{27})]. In 1984, with improved chromatographic capability and a mass spectrometric system capable of detecting much higher molecular weights than those used by Rodgman et al. in 1961, Arrendale et al. (103) reexamined the aliphatic ester fraction from tobacco. The saponification and subsequent separation of acids and alcohols were no longer required. Arrendale et al. were able to identify unequivocally many of the individual esters by glass capillary gas chromatography and mass spectroscopic examination of the aliphatic ester fraction isolated from the tobacco. The alcohol moiety of the esters identified ranged from 1-tetradecanol (C_{14}) to 1-dotriacontanol (C_{32}); the acid moiety ranged from lauric acid (C_{12}) to *n*-dotriacontanoic acid (C_{32}) plus numerous *iso*- (from C_{13} to C_{28}) and *anteiso*- (C_{13}–C_{18} plus C_{20}) isomers of several saturated aliphatic acids. Since each ester reported by Rodgman et al. was found in tobacco and smoke (3294), logic dictates that each new tobacco ester found by Arrendale et al. is also present in smoke (103). Thus, the Arrendale et al. findings substantially increased both the number of components in tobacco and tobacco smoke.

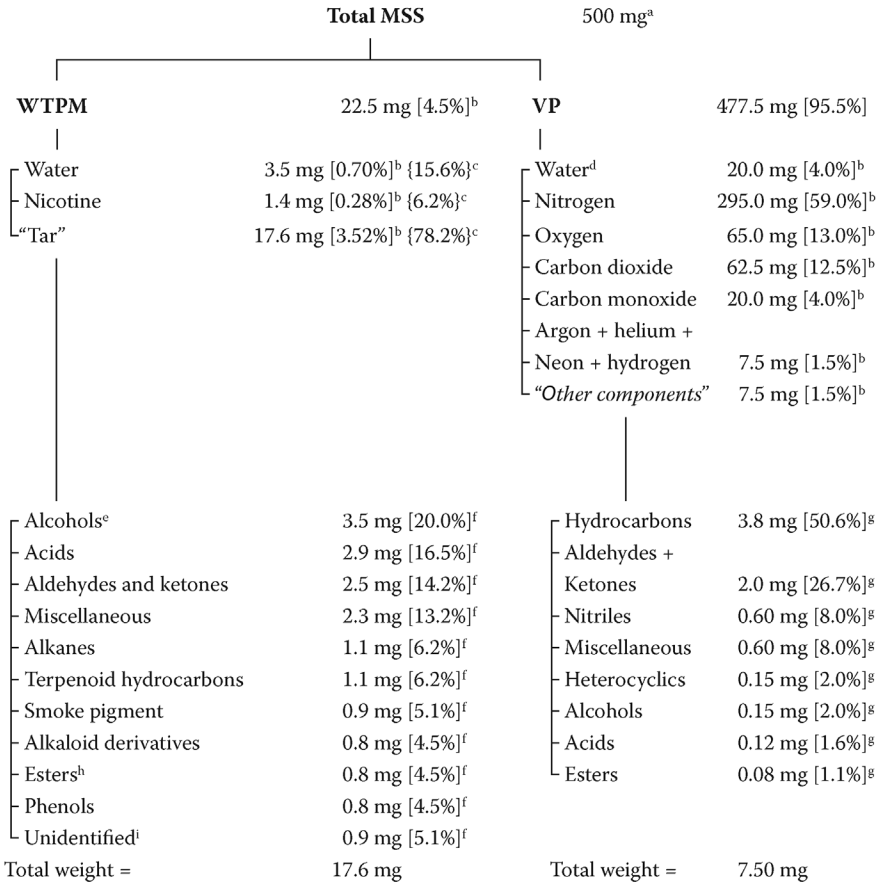
Most of the studies reported in the literature from the mid-1950s to the late 1970s/early 1980s on tobacco smoke composition dealt with the composition of the MSS from the cigarette. Gradually during the late 1970s, more and more studies were reported describing the composition of cigarette SSS [cf. Klus and Kuhn (2142)]. Presently, the major emphasis on tobacco smoke composition involves the composition of ETS, health problems reportedly associated with passive smoking, i.e., exposure to ETS, and the levels of specific components reported to be associated with these health problems [Ecobichon and Wu (1108a), Environmental Protection Agency (EPA) (1148, 1148a, 1148b), Guerin et al. (1445)]. SSS and ETS are discussed in later sections. Because of the relative efforts expended on cigarette MSS, cigarette SSS, and ETS, the numbers of identified components in each of these smokes were reported as approximately 4800, 500, and 100, respectively (3255). Given sufficient time and effort, any component identified in MSS could eventually be identified in SSS and ETS.

The approximate (and general) composition of cigarette MSS is well defined. An 85 mm cellulose acetate filter-tipped commercial cigarette (65 mm tobacco rod, 20 mm filter tip) whose filler, a typical American blend of tobaccos, weighed approximately 1000 mg was machine smoked with the FTC-prescribed smoking parameters (35 mL puff volume, 2 s puff duration, 1 puff/min, 25°C, 60% relative humidity, FTC-specified butt length) (1177b). This cigarette gave approximately 500 mg of total MSS. To separate the tobacco smoke aerosol into its two major phases—the PP and the VP—the smoke was passed through a Cambridge filter pad which retains more than 99.9% of the PP, defined as total WTPM. The VP is that portion of the smoke aerosol which passes through the Cambridge filter pad, and the major portion of its weight is due to the components of air drawn through the cigarette during the smoking process (nitrogen, oxygen, argon, etc.).

The distribution and approximate composition of the total MSS emerging from this cigarette are summarized in Figure 0.6. The data in Figure 0.6 represent a consolidation of composition data from several sources including data from RJRT R&D [Laurene (2299a)] plus data from Keith and Tesh (2068), Norman (2799a), and Browne et al. (445). To simplify the calculations throughout Figure 0.6, one value was deliberately adjusted slightly for convenience: The total MSS collected actually weighed slightly in excess of 497 mg, but the value 500 mg was used to calculate the percentages shown throughout Figure 0.6. In addition, no attempt was made with these data to define the degree of partition of some components between the PP and the VP. Because of their vapor pressure properties, significant quantities of some smoke components are found in both the PP and VP of cigarette MSS. These include hydrogen cyanide, several of the simple phenols (phenol, *o*-cresol, *m*-cresol, *p*-cresol), and several of the volatile *N*-nitrosamines.

It is obvious from the data in Figure 0.6 that the particulate matter, whether described as WTPM, TPM, or FTC "tar," comprises less than 5% (100 × 22.5/500 = 4.5%) of the total MSS emerging from the cigarette. This is true of nearly all commercial U.S. cigarettes no matter what the FTC "tar" yield. The composition of the MSS VP has been almost completely defined. It is estimated that components representing less than 1 mg of the PP (5.1% of the FTC "tar," less than 0.2% of the total MSS) remain unidentified. If the number of unidentified components is as high (as many as 100,000) as some investigators estimate (1422, 4103), then the level of each unidentified component must average in the low-nanogram range.

The extremely wide variations in the yields of components delivered in the MSS during the smoking of a cigarette have presented unique challenges to those involved in not only the identification of smoke components but also in their quantitation. Table 0.14 is a minor modification of the initial version presented in 1996 by Green and Rodgman (1373). In it, the logarithmic presentation is a more concise depiction of this wide variation in the levels of selected smoke components. For most of the components shown in Table 0.14, there obviously is a range of values, and the extent of the range for each component is dependent on the cigarette type under study (filtered, nonfiltered) and the



Note: The properties of the cigarette studied were as follows: 85 mm filtered cigarette, 68 mm, tobacco rod, 17 mm triacetin-plasticized cellulose acetate filter tip, cased commercial American blend.

[a] It is now estimated that over 5000 components have been identified in MSS from tobacco cigarettes. Some components such as water, the simple phenols, hydrogen cyanide, and the volatile *N*-nitrosamines are found in both the VP and PP of cigarette MSS. Hence, the total of the number in the two phases appears to exceed the number in the whole.

[b] Value in brackets represents percent of Total MSS weight, 500 mg.

[c] Value in parentheses represents percent of WTPM, 22.5 mg.

[d] Much of this water is contributed by the air drawn through the cigarette during puffing (35 mL puff, 1 s duration, 1 puff/min, total puffs = 10) in a laboratory whose atmosphere is controlled to the specifications proposed by the FTC, namely, temperature = 25°C, relative humidity (RH) = 60%.

[e] This class of compounds includes added humectants (glycerol, propylene glycol) transferred from the tobacco rod to the MSS. The transferred humectants constitute about 10%–12% of the FTC "tar."

[f] Value in brackets represents percent of FTC "tar" weight, 17.6 mg.

[g] Value in brackets represents percent of "Other Components" weight, 7.5 mg.

[h] This class of compounds includes transfer to smoke of some triacetin added to the filter tip plus its degradation products mono- and diacetin.

[i] There have been various estimates of the number of unidentified components present in extremely small amounts in the FTC "tar." Several investigators have estimated the number of unidentified components to range from 5 to 20 times the number of identified components, i.e., from about 20,000 to 100,000.

FIGURE 0.6 Approximate composition of cigarette MSS.

TABLE 0.14
Cigarette MSS Components: Logarithmic Listing of per Cigarette Yields

VP	Yield/Cig			PP	
	-400 mg				
Nitrogen	-				
	-				
	-200				
	-				
	-				
	-100 mg				
	-80				
Oxygen, carbon dioxide	-				
	-				
	-40				
	-				
	-				
Water, carbon monoxide	-20	⎡			
	-	⎨ FTC "tar"			
	-	⎣			
	-10 mg				
	-8				
	-				
	-				
	-4	Water			
	-				
	-				
	-2				
	-	Humectants (glycerol, propylene glycol)			
	-				
Acetaldehyde[a]	**-1000 mg = 1 mg**			Nicotine	
	-800				
Isoprene[b]	-	Total alkanes	The five acids: palmitic, stearic, oleic, linoleic, and linolenic		
	-				
Limonene	-400				
	-	Saturated aliphatic esters			
	-				
Nitric oxide	-				
	-200				Catechol
	-				
HCN	-				
	-100 mg	Solanesol		Total alkyl pyridines	Phenol
	-80	Phytosterols			
Acrolein	-				
1,3-Butadiene[b]	-				
	-40	Solanesyl esters			*
	-				
Formaldehyde[a] ⎤	-				
2-Furaldehyde ⎬	-20				*o*-Cresol
Crotonaldehyde[a] ⎥	-				
Benzene[a] ⎦	-	Phytyl esters			
	-10 mg				
Acrylonitrile[a]	-8			Indole	
	-		a-Tocopherol	Indole, 3-methyl-	
	-		Solanesyl acetate		

(*continued*)

TABLE 0.14 (continued)
Cigarette MSS Components: Logarithmic Listing of per Cigarette Yields

VP	Yield/Cig			PP	
	-4			Anabasine	
	-				
	-				
	-2			NAB[a]; indole, 3-ethyl-	
	-			NNN[a]; quinoline[a]	
	-				
	-1 mg = 1000 ng				
	-1000 ng = 1 mg				
Propane, 2-nitro-[a]	-800			Nornicotine	
	-				
	-				
	-400			Indole, dimethyl-	
	-	α- and β-Duvanediols		NNK[a]	
	-			A*a*C[b]	
NDMA[a]	-200	α-Levantenolide			
	-			Indole, trimethyl-,	
	-			Carbazole	Anthracene
NPYR[a]	**-100 ng**				Pyrene, chrysene[a]
	-80				
	-				Fluoranthene
	-	Lead[a], cadmium[a]			B[*a*]A[a]
	-40	b-Levantenolide			
	-			MeA*a*C[b], PhIP[b]	
NDEA[a]	-			Carbazole, 2,9-dimethyl-	
Hydrazine[a]	-20	Arsenic[a]	1-Naphthylamine	Carbazole, 3,9-dimethyl-	
Ethyl carbamate[a]	-	Chromium[a]	2-Naphthylamine[a]		Benz[*e*] acephenanthrylene[a,c]
	-				Indeno[1,2,3-*cd*] pyrene-NEMA[a]
	-				
	-10 ng				Pyrene[a], benzo[*a*]pyrene[a]
Vinyl chloride[a]	-8				Benzo[*j*]fluoranthene[a]
	-			Carbazole, 1,9-dimethyl-	
	-				
	-4				
	-			Carbazole, 9-ethyl-	
	-			Carbazole, 4,9-dimethyl-	
	-2		Biphenyl, 4-amino-[a]		Dibenz[*a,h*]anthracene[a]
	-				Dibenzo[*rst*]pentaphene[a,d]
	-				
	-1000 pg = 1 ng			Dibenz[*a,j*]acridine[a]	
	-800			Glu-P-1[b] and P-2[b]	
	-			Trp-P-2[b]	
	-			MeIQ	
	-400			Dibenzo[*c,g*]carbazole[a]	Chrysene, 5-methyl-[a]
	-				
	-			IQ[b]	
	-200			Trp-P-1[b]	
	-				
	-				

TABLE 0.14 (continued)
Cigarette MSS Components: Logarithmic Listing of per Cigarette Yields

VP	Yield/Cig	PP
	100 pg	
	80	Dibenz[*a,h*]acridine[a]

Trp-P-1, 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole; Trp-P-2, 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole; Glu-P-1, 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole; Glu-P-2, 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole; A*a*C, 2-amino-9*H*-pyrido[2,3-*b*]indole; MeA*a*C, 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole; IQ, 2-amino-3-methylimidazo[4,5-*b*]quinoline; PhIP, 2-amino-1-methyl-6-phenylimidazo[4,5-*b*]pyridine; NDEA, *N*-nitrosodiethylamine; NDMA, *N*-nitrosodimethylamine; NEMA, *N*-nitrosoethylmethylamine; NPYR, *N*-nitrosopyrrolidine; NAB, *N*′-nitrosoanabasine; NNK, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone; NNN, *N*′-nitrosonornicotine.

[a] This tobacco smoke component was included in a list published by Hoffmann and Hecht (1727) in which the component was one of 43 components defined as a "tumorigenic agent in tobacco and tobacco smoke."

[b] In a modified list of "tumorigenic agent in tobacco and tobacco smoke," Hoffmann and Hoffmann (1740) increased the number of components from 43 to 60 and included several of the "cooked food" mutagens as well as several other MSS components (1,3-butadiene, isoprene, etc.).

[c] Benz[*e*]acephenanthrylene is the currently accepted name for benzo[*b*]fluoranthene.

[d] Benzo[*rst*]pentaphene is the currently accepted name for dibenzo[*a,i*]pyrene.

weight of tobacco consumed during the smoking of the cigarette for the analysis. In general, the locations of the various components on the logarithmic plot have been adjusted for a cigarette yielding about 18–20 mg/cig of FTC "tar." If the design of the cigarette has been modified to reduce FTC "tar" yield, diminution of the yields of the other components will occur but not necessarily to the same extent as the decrease in FTC "tar" yield. Cigarette design parameters [tobacco rod length and dimensions, filter type and dimensions, filter-tip additives, tobacco blend and weight, processed tobaccos (reconstituted tobacco sheet, expanded tobacco), paper and paper additives, and air dilution (paper porosity and filter perforation)] have profound effects on cigarette MSS yield and composition. Also shown in Table 0.14 are those components listed by Hoffmann et al. (1727, 1740, 1741, 1743, 1744) as "tumorigenic components of tobacco and tobacco smoke" and cited as such by the U.S. Surgeon General (4012), the U.S. EPA (1148a), and the U.S. Occupational Safety and Health Administration (OSHA) (2825). The validity and meaning of their classification of specific tobacco smoke components as tumorigenic were recently discussed by Rodgman (3265).

Yields for the VP components range from a high of 50–60 mg/cig for carbon dioxide to lows in the nanogram range for vinyl chloride and the volatile nitrosamines such as *N*-nitrosoethylmethylamine. The major portion of the nitrogen (≫300 mg/cig) and oxygen (≫65 mg/cig) in MSS is derived from the air drawn through the cigarette during the smoking process.

The number of components identified in various tobacco types also increased substantially during the 1950s, 1960s, and 1970s both within and outside the tobacco industry. The purpose of such studies was essentially twofold: to define the tobacco components that (1) provided taste and aroma to the smoke to render it acceptable to the consumer and (2) were precursors of the smoke components asserted to be responsible for the health problems induced by tobacco smoke. Participating investigators over the years included USDA personnel initially under the leadership of Stedman in Philadelphia and subsequently by Chortyk after the move of the USDA tobacco research group from Philadelphia, PA, to Athens, GA.

The precursor research will be discussed in much greater detail in subsequent chapters dealing with those precursors in tobacco of MSS components considered adverse to the smoker, e.g., the precursors in tobacco of the PAHs, the phenols, the aldehydes and ketones, the *N*-nitrosamines, the *N*-heterocyclic amines. It is interesting to note that even the precursor studies led to differences of opinion among the scientists with views on the health problems associated with components in cigarette MSS. In 1942, Roffo (3327) proposed that the precursors of PAHs in the destructive distillate of tobacco were the tobacco phytosterols. In 1957, Fieser commented that the major precursor in tobacco of PAHs in MSS was probably cellulose (1181). Coauthors of several presentations and publications, Wynder, Wright, and Lam differed in their views on the major precursors in tobacco of PAHs in tobacco smoke. Because of his research findings from 1955 to 1959, Lam was a proponent of the concept that the long-chained aliphatic hydrocarbons were the major precursors in tobacco of the PAHs, including B[*a*]P, in MSS (2255–2258). Wynder was a proponent of the concept that the major precursors in tobacco of PAHs in MSS were the long-chained aliphatic hydrocarbons and the phytosterols (4354).* Wright, a colleague of Wynder from the early to the late 1950s, held a different view from that of Wynder and that of Lam. Wright considered the major precursors of PAHs in MSS to be the phytosterols and long-chained terpenoids

* Even though this article was coauthored by Wynder and Wright, the view held by Wright on the major precursors in tobacco of PAHs in smoke was omitted from the manuscript by Wynder.

such as solanesol (4282). Eventually, precursor studies by Rodgman and Cook (3269) in 1958 indicated that the view held by Wright was the correct one. The Rodgman and Cook 1958 findings were subsequently confirmed in the late 1970s at the USDA by Severson et al. (3616).

There were significant contributions by Rowland et al. in the early 1950s from their studies on the composition of flue-cured tobacco, studies which resulted in the isolation and identification by classical chemical means of the 45-carbon terpenoid alcohol solanesol (3359), its acetate and several other of its esters (3294, 3296, 3358), neophytadiene (3345), α-tocopherol and solanachromene (3347), the four isomeric 4-(2-butenylidene)-3,5,5-trimethyl-2-cyclohexen-1-ones (the megastigmatrienones) (3355), and several cyclotetradecanediols (3220, 3221, 3351, 3360) plus their oxabicyclo derivatives (3361). Over a decade later, with more advanced analytical technology, Lloyd et al. (2389) identified several hundred previously unidentified flue-cured tobacco components. From their early composition studies, similar to those of Rowland on flue-cured tobacco, Schumacher and Vestal isolated and identified numerous previously unidentified Oriental tobacco components (3561), including sclareolide (3533) and the first glucose tetraester (3535). Schumacher also defined numerous components in Maryland tobacco (3550). Roberts and Rohde in their study of the composition of burley tobacco identified numerous previously unidentified tobacco burley components, including several cyclotetradecanediols (3219).

As analytical methodology advanced after the 1950s, the number of identified tobacco and tobacco smoke components escalated dramatically. In addition to its study of tobacco smoke by Arnap (91–94) and Enzell et al. (1153, 1154), the R&D staff at the Swedish Tobacco Company published nearly 100 articles on the composition of tobacco, primarily Oriental tobacco. The many Swedish Tobacco Company investigators included Aasen, Almqvist, Behr, Enzell, Hlubucek, Kimland, Nishida, and Wahlberg, all of whom coauthored many tobacco composition articles (1–13, 52, 53, 84, 91–94, 227, 229–236, 1149–1157a, 1205a, 1660–1662, 2092–2095, 3315, 4083–4102). Excellent detailed summaries of their identification of hundreds of tobacco components and the generation of them from various terpenoid structures such as the noncyclic and cyclic carotenoids and the cyclotetradecane derivatives were presented and published in the late 1970s and early 1980s by Enzell (1149, 1150), Enzell and Wahlberg (1156), and Wahlberg and Enzell (4089, 4090).

In the 1960s and 1970s, the Demoles and their colleagues at Firmenich SA in Switzerland also studied the composition of flue-cured, burley, and Oriental tobaccos and characterized many previously unreported compounds in each, e.g., the studies by Demole et al. on burley tobacco composition (936–944), on flue-cured tobacco composition (945, 946, 948), and on Oriental tobacco composition (947).

As noted previously, it was estimated by Wakeham (4103) and Grob (1422) from their examination of gas chromatograms that the number of components in tobacco smoke far exceeded the number of identified components. A similar situation exists with the composition of tobaccos. As early as the mid-1970s, Dejong and Lam (922d) commented that the estimated number of enzymes in green leaves, including tobacco, ranged from 1,000 to 10,000. Our Master Catalog from which the various lists of component classes are derived comprises over 8000 components. The chapter on enzymes will list many of the tobacco enzymes but obviously will not include all of the great number of enzymes reported in tobacco.

The MSS yields for components of the PP range from that of FTC "tar" itself, shown as a yield of about 20 mg/cig in Table 0.14 (1373), to that of dibenz[*a,h*]acridine at an MSS yield of 0.1 ng/cig (100 pg/cig).* The magnitude of the range of yields for cigarette MSS components is demonstrated by the following: The ratio of the per cigarette yield of nitrogen (the most plentiful MSS component shown in Table 0.14) to that of dibenz[*a,h*]acridine (the lowest yield shown) is $\gg 3 \times 10^9$, i.e., ≫300 mg *vs.* 0.1 ng. The need for analytical methodology to determine smoke components from the high-milligram- to the low-picogram yield was one of the driving forces behind many of the developments and improvements in analytical technology for the study of complex mixtures.

ALPHABETICAL INDEX TO COMPONENTS IDENTIFIED IN TOBACCO, TOBACCO SMOKE, AND TOBACCO SUBSTITUTE SMOKE

The Index was created for two purposes. The first was to capture in one site all the basic information on the identified tobacco and tobacco smoke components discussed in the chapters of this book. The components in the Index are listed alphabetically. Secondly, the Index may permit the reader to easily retrieve or search for information on a specific tobacco and/or smoke component or class of components so that further study will be facilitated. To achieve these goals, the Index was constructed to include the following: (1) The CAS No. for many of the components; (2) an indication of the component identification in tobacco, tobacco smoke, or both; (3) the structure of many of the components; (4) the table number and chapter in which the component is not only referenced but its properties are described, particularly if they are considered adverse; and (5) for multifunctional components, several chapters and table numbers are cited. Additionally, the publishers of this book, Taylor & Francis/CRC Press of Boca Raton, Florida, have provided the Index in compact disc (read-only memory) (CD-ROM) format. Hopefully, the searchable format of the CD-ROM will aid the reader in retrieving any desired information.

The Index comprises almost 9600 components completely or partially identified in tobacco, tobacco smoke, and tobacco substitute smoke. It includes not only over 9600 identified components but also several hundred compounds

* Several new entries concerning *N*-heterocyclic amine data that were not available in 1996 for inclusion by Green and Rodgman (1373) are included in Table 5.

not identified in tobacco or tobacco smoke but reported by Doull et al. (1053) as tobacco ingredients used in the United States and by Baker et al. (172a, 174b) as tobacco ingredients used outside the United States and in a summary by Rodgman (3266) and in our Chapter 24. Because the transfer from a tobacco product to smoke of very few of the added ingredients has been examined, they primarily are listed as tobacco components. Exceptions include several humectants used in tobacco products for many years. However, it should be noted that the detailed pyrolysis study by Baker and Bishop (172a) indicated that many such added ingredients would transfer in part to MSS during the tobacco smoking process.

In some instances, the reader may wonder about the peculiar nature of the component listing. For example, a tobacco smoke component initially reported as 2-butene was later shown to be present in the smoke as *cis*- and *trans*-2-butene. Thus, three items are listed in the Index for 2-butene, namely, 2-butene (CAS No. 107-10-7), 2-butene, (*Z*)- (CAS No. 590-18-1), and 2-butene, (*E*)- (CAS No. 624-64-6). In the appropriate chapter and table, Chapter 1 and Table 1.11, references to the identification of each are provided. 2-Butenedioic acid is similarly listed in Chapter 4, Table 4.3 as 2-butenedioic acid (CAS No. 6915-18-0), 2-butenedioic acid, (*Z*)-(maleic acid) (CAS No. 110-16-7), 2-butenedioic acid, (*E*)-(fumaric acid) (CAS No. 110-17-8).

The reader will also find in the Index certain broad classifications of components, like oxidases and free radicals. These and similar examples in the Index are not there to confuse the reader, as many of the individual components in the broad classifications have specific CAS numbers. Generally, the references associated with these classes of components (found within the chapters noted in the Index) will provide the reader with information of a common nature. In nearly all cases, individual components such as ascorbate oxidase, choline oxidase, cytochrome oxidase, and glycolate oxidase follow after the broadly classified component, oxidase. Likewise, specific free radicals such as methyl-acyl radical, ethyl-acyl radical, and propyl-acyl radical {two isomers} may be found in the Index. For some components in the Index, several partially identified isomers exist, their number noted, and included in the total number of components identified in tobacco and/or smoke.

Although the number of enzymes, genes, and nucleotides listed in the Index is fewer than 500, their known number, as noted in Chapter 22, exceeds many thousands. The paltry number of enzymes, genes, and nucleotides listed in Chapter 22, Table 22.2 was never intended to represent the total biological agents operating in the plant. Those selected for inclusion were from texts, research manuscripts, and patents where active research was conducted in the past in attempts to better understand the physiology and biochemistry of tobacco. As future genetic research develops, it is envisioned that the identity and function of hundreds of thousands of additional chemicals will be published.

The authors hope that the format of the Index and accompanying CD-ROM will help the reader to reach a better understanding of the components of tobacco and tobacco smoke.

1 Hydrocarbons

1.1 ALKANES

In his catalog of tobacco smoke components reported in early 1954, Kosak (2170) listed hentriacontane as the only alkane identified in tobacco smoke. Subsequently, numerous investigations resulted in the identification of a great number of alkanes in tobacco and tobacco smoke.

Over 120 alkanes—ranging from the C_1 hydrocarbon methane to the C_{36} hydrocarbon hexatriacontane—have been identified in tobacco and tobacco smoke. Many of the higher molecular weight alkanes have been reported to be present in three isomeric forms, i.e., the *normal*, the *iso* (2-methyl), and the *anteiso* (3-methyl) isomer:

	$H_3C\text{-}CH(CH_3)\text{-}(CH_2)_{n-1}$	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{n-2}$
$H_3C\text{-}(CH_2)_n\text{-}CH_3$	$\text{-}CH_3$	$\text{-}CH_3$
n-alkane	*iso*-alkane	*anteiso*-alkane

In 1958, Barbezat-Debreuil (181), using column chromatography and x-ray analysis to examine the alkanes in tobacco and tobacco smoke, reported her identification of branched isomers in the alkane fraction from both sources. The next year, Carruthers and Johnstone (613) reported the results of their study on the long-chained alkanes in tobacco and the smoke from cigarettes containing it. Their analyses involved gas–liquid chromatography and mass spectroscopy. They also noted that the minor differences between the mass spectroscopic data for tobacco and smoke were not significant because, at that time, the precision of such an analysis was not high. Their findings are summarized in Tables 1.1 and 1.2.

Cuzin et al. (883) in their study of *Gauloise* cigarette mainstream smoke (MSS) reported that 1.2% of the total particulate matter (TPM) consisted of *n*-C_{25}, *n*-C_{26}, *n*-C_{28}, *n*-C_{29}, *n*-C_{30}, *n*-C_{31}, and *n*-C_{32} alkanes and 75% of this weight involved the C_{30}, C_{31}, and C_{32} compounds. They reported that their evidence indicated no *n*-alkane higher than the *n*-C_{32} alkane was present. However, in 1960, Kosak and Swinehart (2176) reported the presence in cigarette MSS of the *n*-alkanes from C_{22} to C_{36} and branched alkanes from C_{21} to C_{32}. Table 1.3 summarizes their findings. Possibly due to the status of analytical methodology at the time, Dymicky and Stedman (1081) had earlier suggested the possible presence of *n*-tetracontane ($C_{40}H_{82}$) in tobacco, but their finding has never been confirmed. In 1967, Ivanov and Ognyanov (1893b) reported the isolation of a crystalline alkane mixture, m.p. 62°C–64°C, which they proposed might contain a series of alkanes from C_{25} to C_{40}.

Carugno (619) reported the C_{31} alkanes to be the most abundant in tobacco but also noted that the C_{27}, C_{29}, C_{30}, C_{32}, and C_{33} homologs were present in appreciable amounts. Only a small portion of the alkanes in the alkane fraction from the MSS from four tobacco types and a commercial tobacco blend was found with carbon chain lengths equal to or less than C_{24}; only trace amounts of alkanes at or below *n*-hexadecane were found by Spears et al. (3768). Spears et al. also reported that nearly 48% of an alkene-free alkane fraction (0.75 mg/cig) from MSS consisted of *n*-hentriacontane (0.182 mg/cig), *n*-dotriacontane (0.108 mg/cig), and *n*-tritriacontane (0.069 mg/cig).

In their article on the pyrolysis of tobacco constituents, Badger et al. (142) reproduced a gas chromatogram provided by Reid on the alkanes in a tobacco sample. The peaks for the alkanes from C_{23} to C_{33} are readily discernible in the chromatogram. Badger et al. estimated that the tobacco alkane fraction amounted to 0.32% of the tobacco weight. Based on their pyrolysis studies, Badger et al. also proposed an elaborate mechanism for the formation of the polycyclic aromatic hydrocarbons (PAHs). It involved the degradation of the alkane to smaller fragments, followed by recombination of the fragments into substituted cyclic entities and their aromatization.

As listed in Table 1.4 adapted from Mold et al. (2595), about 25%–50% of the total alkanes in tobacco comprise nearly equal amounts of the *iso* and *anteiso* isomers of the alkanes. In the series of *normal*- and *iso*-alkanes, the homologs with odd-numbered carbons predominate with the C_{31} and C_{33} homologs being present in the largest amounts. In the *anteiso*-alkanes, the alkanes with even-numbered carbons predominate with the C_{32} homolog being present in the largest amount. The data provided by Mold et al. (2595) were reproduced by Tso in his 1990 book (3973).

As Stedman (3797) noted in his 1968 review of the composition of tobacco and smoke, it was thought at one time that *anteiso*-alkanes comprised only those homologs with even-numbered carbons, but eventually homologs with odd-numbered carbons were reported by Carugno and Rossi (625) and Chortyk et al. (727). Carugno and Rossi (625) reported the presence of both normal and branched C_{21}–C_{34} alkanes in cigarette smoke condensate (CSC).

In a later comparison of the composition of the alkane fraction in a reference tobacco (University of Kentucky 1R1) and its cigarette MSS, Chortyk et al. (727) reported that "the ratio among the constituents in leaf paraffins is almost identical [with] the ratio among the smoke paraffins." It is possible, however, that changes in agronomic practices over the years since the 1970s may have resulted in tobaccos whose contents of alkanes and distribution among the alkane homologs are substantially different from those of the tobaccos studied in the 1960s and 1970s. This, of course, would also affect the content and distribution among the alkane homologs in the tobacco smoke.

Table 1.5 summarizes the tobacco smoke alkane isomers described by Stedman (3797) and those known to be present in 1992. The number of identified alkanes in these three isomeric forms was almost doubled during the period 1968–1992.

TABLE 1.1
Relative Percentage Composition of Tobacco Alkanes in Tobacco and Cigarette Smoke, Based on Mass Spectroscopic Analysis (613)

	Tobacco			Cigarette Smoke		
No. of Carbons	*n*-	*iso*-	Total	*n*-	*iso*-	Total
25	0.9	0	0.9	0	0	0
26	0.6	0	0.6	0.5	0	0.5
27	3.0	0.9	3.9	5.2	0.8	6.0
28	0.1	0	0.1	0.5	0	0.5
29	6.6	15.9	22.5	5.2	15.3	20.5
30	0.9	2.5	3.4	1.0	1.5	2.5
31	24.1	24.4	48.5	25.7	20.2	45.9
32	3.9	2.4	6.3	4.3	1.9	6.2
33	10.8	3.3	14.1	14.3	3.5	17.8
Total	50.9	49.3	100.3	56.7	43.2	99.9

TABLE 1.2
Relative Percentage Composition of *n*-Alkanes in Tobacco and Cigarette Smoke, Based on Gas–Liquid Chromatographic Analysis (613)

No. of Carbons	Tobacco	Cigarette Smoke
n-24	—	0.1
n-25	0.5	0.6
n-26	0.3	0.4
n-27	7.5	6.3
n-28	0.6	1.1
n-29	8.8	7.4
n-30	3.9	3.8
n-31	47.0	48.4
n-32	12.5	13.0
n-33	18.9	22.8
n-34	—	1.1

Many of the isomeric C_8 through C_{36} alkanes have been identified in the organic solvent-soluble extracts from one or more of the major tobacco types (flue-cured, burley, Oriental, Maryland). Their presence in tobacco smoke is the result of their volatilization during the puff and smolder phases of the smoking process and subsequent direct transfer from the tobacco to its MSS and sidestream smoke (SSS). The bulk of these higher alkanes are found in the particulate phase of the smoke aerosol with traces of the lower ones (C_8–C_{12}) in the vapor phase.

The lower molecular weight alkanes (C_1 through C_7) are found predominately in the vapor phase of the MSS and SSS aerosols, and are readily separated and identified by a variety of analytical techniques.

In general, the *n*-alkanes from C_1 to C_4 are gases, those from C_5 to C_{16} are liquids, and those above C_{17} are solids. The melting points and boiling points of some of the solid alkanes in tobacco and smoke are summarized in Table 1.6.

As a result of the successful induction in the mid-1950s of carcinomas on the skin of mice painted repeatedly with concentrated

TABLE 1.3
Alkane Content of Cigarette MSS (2176)

No. of Carbons	Normal	Branched
21	—	0.16
22	0.11	0.21
23	0.49	0.21
24	0.92	0.21
25	2.50	0.16
26	1.40	1.63
27	6.60	0.87
28	1.80	13.90
29	6.30	2.31
30	3.30	15.33
31	22.90	0.90
32	4.80	1.13
33	9.70	—
34	1.20	—
35	0.97	—
36	0.05	—
% of Total	63.0	37.0

solutions of CSC (4306a), the search for the causative agent in the condensate began. The demonstration in the early 1930s of the tumorigenicity of dibenz[*a,h*]anthracene (DB[*a,h*]A) (2078) and benzo[*a*]pyrene (B[*a*]P) (796a, 797) to mouse skin triggered an enormous research effort between 1932 and 1953, excluding the World War II years, which involved the synthesis of hundreds of PAHs and their testing for tumorigenicity. Because many of them were found to be tumorigenic to mouse skin, particularly those tetracyclic and higher, the PAHs were proposed in the mid-1950s by many investigators as possible causative agents for the lung cancer type (squamous cell carcinoma) observed in cigarette smokers. This proposal led to the demonstration of the presence of numerous PAHs in CSC, determination of their levels, and studies to elucidate their precursors in the tobacco.

Despite the fact that in 1942 the phytosterols in tobacco had been proposed by Roffo (3327) as the precursors in tobacco of PAHs in a "destructive distillate" of tobacco, the tobacco phytosterols were essentially ignored in the early 1950s. Because of the research results described by Lam (2255–2258) on the pyrogenesis of PAHs from alkanes, the high-molecular-weight alkanes in tobacco were proposed as the precursors of the PAHs in tobacco smoke. Roffo's suggestion on phytosterols was discounted by Wynder and Hoffmann (4320, 4322) because his research did not involve tobacco smoke but involved the composition and specific tumorigenicity of "destructive distillates" from control and organic solvent-extracted tobacco.

Although Zeise (4406) and Kissling (2100, 2102) reported the isolation of alkane-like components from tobacco and tobacco smoke, Kosak (2170) in his catalog of smoke components classified their data as inconclusive. However, the evidence provided by Thorpe and Holmes (3914) left little doubt as to the presence of the alkanes in tobacco leaf. The Thorpe–Holmes report was followed by numerous descriptions of the isolation of alkanes from tobacco and tobacco

TABLE 1.4
Relative Percentage Composition of Tobacco Alkanes Based on Gas–Liquid Chromatographic Data

	Commercial Tobacco Blend			Flue-Cured Tobacco			Burley Tobacco			Oriental Tobacco		
No. of Carbons	*n-*	*iso-*	*ante-*	*n-*	*iso-*	*ante-*	*n-*	*iso-*	*ante-*	*n-*	*iso-*	*ante-*
25	1.7	—	—	2.0	—	—	1.15	—	—	1.4	—	—
26	0.8	—	—	1.0	—	—	0.5	—	—	0.7	—	—
27	7.7	—	—	5.7	—	—	4.8	—	—	8.6	—	—
28	0.9	—	0.1	1.4	—	0.4	1.1	—	0.4	1.8	—	0.2
29	6.7	1.2	—	5.9	3.1	—	5.4	2.5	—	7.9	1.8	—
30	3.2	—	5.6	3.1	—	6.7	2.9	—	6.8	5.5	—	5.3
31	26.3	10.9	—	24.5	14.3	—	27.5	12.6	—	23.2	6.7	—
32	4.9	—	13.0	4.2	—	11.3	5.6	—	11.7	7.4	—	8.9
33	10.8	5.6	—	7.2	6.4	—	8.1	6.5	—	12.8	4.9	—
34	—	—	1.2	—	—	2.9	—	—	2.6	—	—	2.3

Figures rounded from those provided by Mold et al. (2595).

TABLE 1.5
Alkane Isomers Identified in Cigarette Mainstream Tobacco Smoke, 1968 versus 1992

1968[a]			1992		
Carbon Number			Carbon Number		
normal	*iso*	*anteiso*	*normal*	*iso*	*anteiso*
C_1–C_9	C_4–C_6	C_6	C_1–C_{36}	C_4–C_6	C_6–C_8
C_{12}–C_{36}	C_{27}–C_{33}	…	…	C_8–C_9	C_{11}–C_{12}
…	…	…	…	C_{11}–C_{13}	C_{16}–C_{18}
…	…	…	…	C_{16}–C_{18}	C_{21}–C_{36}
…	…	…	…	C_{21}–C_{36}	…

[a] From Stedman (3797).

smoke (see Table 1.7 for a cross section of some of the published reports, particularly those issued prior to the 1980s). Also included in Table 1.7 are references to some of the studies in which the alkanes were investigated as PAH precursors by pyrolysis or by "spiking" of the tobacco filler in a cigarette.

In 1934, Chibnall et al. (701) were among the first investigators to report that the alkane fraction, comprising a mixture of several individual alkanes, melted sharply over a narrow temperature range (63.3°C–63.8°C), a melting point behavior for a mixture that was contrary to the organic chemistry teachings of the day.

From the results of studies on the pyrolysis of the "tobacco paraffins," which comprise the *n-*, *iso-*, and *anteiso*-alkanes, it was suggested by Lam (2255–2258), Wynder et al. (4356), Wynder and Hoffmann (4319, 4332), and Hoffmann and Wynder (1798) that these components were the major precursors in tobacco of the PAHs in tobacco smoke. However, in 1958, Rayburn and his colleagues (3091, 3092) challenged the proposal that the tobacco alkanes were the major precursors of the smoke PAHs, but their experimental data were not overly conclusive in support of their challenge. Nevertheless, it should be realized that in one sense Rayburn et al. were partly correct: As PAH precursors, the tobacco alkanes do contribute to the PAHs in tobacco smoke, but their contribution is much less significant than other precursors (the phytosterols and terpenoids such as solanesol) in tobacco [cf. Wright (4282), Rodgman and Cook, (3269, 3286), Severson et al. (3616)].

TABLE 1.6
Melting Point and Boiling Point Data for *n*-Alkanes

n-Alkane	Formula	m.p., °C	b.p., °C	*n*-Alkane	Formula	m.p., °C	b.p., °C
Undecane	$C_{11}H_{24}$	–25.6	196	Heneicosane	$C_{21}H_{44}$	40.4	357
Dodecane	$C_{12}H_{26}$	–9.6	216	Docosane	$C_{22}H_{46}$	44.4	369
Tridecane	$C_{13}H_{26}$	–6	230	Tricosane	$C_{23}H_{48}$	47.4	380
Tetradecane	$C_{14}H_{30}$	5.5	251	Tetracosane	$C_{24}H_{50}$	51.1	391
Pentadecane	$C_{15}H_{32}$	10	268	Pentacosane	$C_{25}H_{52}$	53.3	402
Hexadecane	$C_{16}H_{34}$	18.1	280	Triacontane	$C_{30}H_{62}$	66.0	450
Heptadecane	$C_{17}H_{36}$	22.0	303	Pentatriacontane	$C_{35}H_{72}$	74.6	
Octadecane	$C_{18}H_{38}$	28.0	308	Hexatriacontane	$C_{36}H_{74}$	75	
Nonadecane	$C_{19}H_{40}$	32.0	330	Tetracontane	$C_{40}H_{82}$	81.0	
Eicosane	$C_{20}H_{42}$	36.4	343	Pentacontane	$C_{50}H_{102}$	92	

TABLE 1.7
Chronology of Studies on Alkanes in Tobacco and Tobacco Smoke

	Selected Studies of		
Year	**Alkanes[a] in Tobacco**	**Alkanes in Tobacco Smoke**	**Alkanes as Polycyclic Aromatic Hydrocarbon Precursors**
1901	Thorpe and Holmes (3914)		
1930	Kurilo (2239, 2240)		
1934	Chibnall et al. (701)		
1934, 1937		Wenusch (4184, 4192, 4194)	
1935	Schürch and Winterstein (3562)	Schürch and Winterstein (3562)	
1936	Brückner (450)		
1941	Palfray et al. (2890)		
1942	Hukusima and Oike (1848)		
1954		Kosak (2170)	
1954		Kosak (2170)	
1955, 1956	Lam (2255–2257)		Lam (2255–2257)
1956		Dickey and Touey (966)	
1956	Onishi and Yamasaki (2863)	Kosak (2172)	
1956	Wright and Wynder (4354)	Kosak et al. (2177)	
1956, 1957		Wright and Wynder (4284)	
		Wynder and Wright (4354)	
1956, 1957		Rodgman (3240, 3242)	
1957	Rowland (3345)		
1957		Izawa et al. (1905)	
1958	Clemo (767)	Clemo (765)	
1958	Cuzin et al. (876)	Cuzin et al. (876)	
1958	Rayburn and Wartman (3091)	Trillat and Cuzin (3964)	Rayburn and Wartman (3091)
1958	Rayburn et al. (3092)	Van Duuren and Kosak (4030)	Rayburn et al. (3092)
1958	Rodgman and Cook (3269)		Rodgman and Cook (3269)
1958, 1959			Wynder et al. (4355, 4356)
1959	Dymicky and Stedman (1081)	Carruthers and Johnstone (613)	
1959	Gladding and Wright (1308)	Cuzin (877)	
1959, 1960	Stedman and Rusaniwskyj (3807, 3808)		
1960		Schepartz (3431)	Schepartz (3431)
		Kosak and Swinehart (2176)	
1961		Izawa (1900)	
1962	Carugno (619)	Carugno (619)	
1962, 1963		Spears et al. (3768)	
1964, 1967	Wynder and Hoffmann (4319, 4332)	Wynder and Hoffmann (4319, 4332)	Wynder and Hoffmann (4319, 4332)
1965, 1966	Ivanov and Ognyanov (1893, 1893a)	Osman et al. (2875).	Badger et al. 142
1966, 1967	Carugno and Rossi (625)	Carugno and Rossi (625)	
1967	Mokhnachev et al. (2583)		Mokhnachev et al. 2583
1968	Hoffmann and Wynder (1798)	Hoffmann and Wynder (1798)	Hoffmann and Wynder 1798
1968			Schlotzhauer and Schmeltz (3465)
1970		Jenkins et al. (1935)	
1974, 1975	Chortyk et al. (727)	Chortyk et al. (727)	
1978		Severson et al. (3608)	
1979	Severson et al. (3616)		
1989		Bass et al. (208)	
2003		Coleman and Gordon (776)	

[a] Most of the studies dealt with alkanes C_{10} and greater.

TABLE 1.8
Polycyclic Aromatic Hydrocarbons from Tobacco Aliphatic Hydrocarbons Pyrolyzed in Air at Various Temperatures

	Quantity (µg) of PAH Formed on Pyrolysis (in Air) of Aliphatic Tobacco Hydrocarbons (1.0 g)				
	At 800°C		At 700°C		At 600°C
Polycyclic Aromatic Hydrocarbon	PAH, µg/g	PAH/B[*a*]P[a]	PAH, µg/g	PAH/B[*a*]P[a]	PAH, µg/g
Naphthalene	14,260	41.94 [2/5][b]	4,760	158.7	0
Acenaphthene	0	0 [3/5][c]	0	0	0
Acenaphthylene	3,520	10.35 [3/5][c]	480	16.00	0
Phenanthrene	3,840	11.29 [3/5][c]	580	19.33	0
Anthracene	580	1.71 [3/5][c]	110	3.67	0
Pyrene	960	2.82 [4/5][d]	320	10.67	0
Fluoranthene	1,700	5.00 [4/5][d]	24	0.80	0
Chrysene	400	1.18 [4/5][d]	86	2.87	0
Perylene	34	0.10 [5/5][e]	4	0.13	0
Benzo[*a*]pyrene	**340**	**1.00**	**30**	**1.00**	0
Benzo[*e*]pyrene	400	1.18 [5/5][e]	80	2.67	0
Dibenzo[*def,mno*]chrysene	42	0.12 [6/5][f]	<1	<0.03	0
Totals	26,076	86.87	6,474	21.47	0

[a] B[*a*]P, benzo[*a*]pyrene.
[b] [2/5], bicyclic/pentacyclic B*a*P.
[c] [3/5], tricyclic/pentacyclic B*a*P.
[d] [4/5], tetracyclic/pentacyclic B*a*P.
[e] [5/5], pentacyclic/pentacyclic B*a*P.
[f] [6/6], hexacyclic/pentacyclic B*a*P.

Table 1.8, adapted from Lam (2257), demonstrates the relationship between PAH generation and pyrolysis temperature for aliphatic tobacco hydrocarbons (the alkanes) pyrolyzed in air at several temperatures. Calculation of the yield ratios [PAH µg/g–B[*a*]P µg/g] of the other PAHs versus B[*a*]P reveals significant information: In this simple case of pyrolysis, there is little consistency between the change in ratios of PAH/B[*a*]P as the temperature is increased from 700°C to 800°C. For example, in the case of the tetracyclic hydrocarbons, the PAH/B[*a*]P ratio decreases for pyrene and chrysene but increases for fluoranthene. For the pentacyclic hydrocarbons, the ratio decreases for both perylene and benzo[*e*]pyrene. For the hexacyclic hydrocarbon dibenzo[*def,mno*]chrysene, the ratio increases. These same trends exist whether the PAH/B[*a*]P ratios are calculated in terms of molar yields or, as in Table 1.8, in terms of the absolute quantities (µg of PAH generated per gram of aliphatic tobacco hydrocarbons pyrolyzed). The significance of these data and calculations is their demonstration in 1956 that in even the simplest pyrolysis situation*, B[*a*]P is not a valid "indicator" or "marker" for the PAHs with four or more rings and/or their supposed relationship to tumorigenic activity as suggested by Wynder and Hoffmann (4317, 4320, 4332). In addition to these data by Lam, other contrary data which demonstrated the invalidity of the concept of B[*a*]P as an "indicator" or "marker" for PAHs with four or more rings and the tumorigenicity of the substrate (CSC, pyrolysate, etc.) containing them were generated not only in studies by Wynder et al. (4355, 4356) but also in studies by Campbell and Lindsey (583), Rodgman (3240), Rodgman and Cook (3269, 3286), Gori (1329, 1330, 1332, 1333), NCI (2683), and Severson et al. (3616).

When used as a solvent for B[*a*]P in mouse skin-painting tests, the C_{10}, C_{12}, or C_{16} *n*-alkanes—although noncarcinogenic per se in this bioassay—were reported by Horton et al. (1835) to accelerate the tumor-producing capability of B[*a*]P and 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene). Horton et al. reported that *n*-octane, the C_8 alkane, did not exhibit this property. The acceleration finding of the C_{10}, C_{12}, or C_{16} *n*-alkanes was incorporated by Carruthers and Johnstone (613) into an explanation of why the % tumor-bearing animals (% TBAs) was much greater in mice painted with CSC than could be predicted by the levels of tumorigenic polycyclic hydrocarbons in the CSC: They extrapolated the finding of this property of the C_{10}, C_{12}, and C_{16} *n*-alkanes to the longer chained homologs in cigarette smoke.

In contrast, however, to the findings of Horton et al. (1835), Wynder and Hoffmann (4314, 4319, 4332) reported that the specific tumorigenicity of B[*a*]P in mouse skin-painting

* For several decades, Wynder, Hoffmann, and some other investigators asserted that the fate of a given tobacco component during inert atmosphere pyrolysis was equivalent to its fate in the oxygen-deficient (but not oxygen-free) atmosphere in the tobacco rod during the cigarette smoking process (cf. Wynder and Hoffmann (4320, 4332), Hoffmann and Wynder (1798)). At the same time, many other investigators maintained that the two processes were *not* equivalent. Hoffmann and colleagues demonstrated in 1979 with radiolabeled nicotine that the two processes were *not* equivalent, and they suggested that this nonequivalence observed for the fate of nicotine was applicable to the fate of other tobacco components (3512).

experiments was significantly "inhibited" when it was administered with the individual alkanes *n*-hentriacontane ($C_{31}H_{64}$) or *n*-pentatriacontane ($C_{35}H_{72}$) and the ratio of the alkane–B[*a*]P was either 200:1 or 100:1. These ratios are much less than those encountered in CSC. Wynder and Hoffmann also reported that increasing the level of the alkane fraction in the applied CSC from 3% to 4% (a 33% increase) resulted in a decrease (from 40% to 24%) in the % TBAs after 19 months and a decrease (from 24% to 18%) of % TBAs with malignant tumors. Surprisingly, Wynder and Hoffmann did not consider these decreases significant! These alkane–B[*a*]P data, originally presented at an AACR meeting (4314), did not appear in any journal but were included in the Wynder–Hoffmann review (4319) and book (4332) on tobacco smoke carcinogenesis.

Although they did not catalog their bioassay findings from the alkane–B[*a*]P experiments in their extensive tabulation of the induction of carcinoma in skin-painting studies with tobacco products [see pp. 330–331 in (4319) and pp. 370–371 in (4332)], Wynder and Hoffmann offered the following explanation for the result observed:

> The effect of alkanes may not be inhibitory to tumorigenicity but rather a consequence of having influenced resorption. The tumor response data of these experiments clearly express a delay of tumor appearance, a result that we believe to be due to the retarding effect of the *n*-alkanes.

Earlier, Wynder and Wright (4354) had reported that the slight tumorigenicity observed with an alkane fraction of tobacco smoke condensate in a mouse skin-painting bioassay was due not to the alkanes per se but to trace amounts of PAHs in the alkane fraction.

In later experiments with gasoline engine exhaust "tar" versus CSC, the observed tumorigenicities observed by Wynder and Hoffmann (4315) did not parallel the levels of the PAHs considered to be the major contributors to the observed skin tumors. To explain the difference (and the less than anticipated tumorigenicity of the exhaust "tar"), the authors attributed the depressed tumorigenicity of the exhaust "tar" not only to alkanes but also to nontumorigenic PAHs present in engine exhaust "tar" at levels far in excess of those of the tumorigenic PAHs such as B[*a*]P and DB[*a,h*]A (see Table 1.9). Although the ratios are not as great for CSC as for exhaust "tar," it should be noted that the levels of nontumorigenic (and antitumorigenic) PAHs in CSC far exceed those of the tumorigenic PAHs. Wynder and Hoffmann (4315) summarized their findings as follows:

> It was anticipated that the…exhaust gas "tar" and nicotine would be many times more active than tobacco smoke condensate. However,…it is only approximately twice as active. This relatively small increase in biological activity of exhaust gas "tar" raises the question of possible anticarcinogenic factors that may be more prevalent in engine exhaust "tar" … one may theorize that some of the noncarcinogenic polynuclear hydrocarbons that are present in engine exhaust gas "tar" in far greater concentrations than in tobacco smoke condensate may interfere with the resorption of the "tar." Some of the oily materials in gasoline engine exhaust "tar" and the paraffins in tobacco smoke condensate may also act as anticarcinogens.

In their comparison of the composition of the alkane fraction in a reference tobacco (University of Kentucky 1R1) and its cigarette MSS, Chortyk et al. (727) reported that "the ratio among the constituents in leaf paraffins is almost identical [with] the ratio among the smoke paraffins." They interpreted this finding as suggesting the paraffins undergo little pyrolytic degradation during the smoking process. Although octatriacontane has not been identified in either tobacco or tobacco smoke, Bass et al. (208) employed [18-^{14}C]octatriacontane to study its transfer to cigarette smoke. Their findings with this alkane agreed with those of Chortyk et al. (727) on the series of alkanes in tobacco and their transfer to smoke and with those of Jenkins et al. (1935) on the transfer of [16,17-^{14}C]dotriacontane from tobacco to smoke.

Table 1.10 lists the alkanes identified in tobacco and mainstream tobacco smoke. The citations do not necessarily include every reference to the identification or discussion

TABLE 1.9
Ratios for Individual Polycyclic Aromatic Hydrocarbons in Gasoline EET and CSC

Polycyclic Aromatic Hydrocarbon	Ratio PAH_{EET}:PAH_{CSC}	Polycyclic Aromatic Hydrocarbon	Ratio PAH_{EET}:PAH_{CSC}
Benz[*a*]anthracene	600:1	Dibenzo[*def,mno*]chrysene[a]	>440:1
Benz[*a*]anthracene, alkyl	>10:1	Benzo[*a*]pyrene	45:1
Benz[e]acephenanthrylene[b]	640:1	Benzo[*a*]pyrene, alkyl	>10:1
Benzo[*ghi*]fluoranthene	1500:1	Benzo[*e*]pyrene	4200:1
Benzo[*j*]fluoranthene	85–110:1	Fluoranthene	275–390:1
Benzo[*k*]fluoranthene	200–360:1	Fluoranthene, alkyl-	230–275:1
11*H*-Benzo[*b*]fluorene	100:1	Indeno[1,2,3-*cd*]pyrene	>80:1
Benzo[*ghi*]perylene	255–340:1	Indeno[1,2,3-*cd*]fluoranthene	>30:1
Chrysene	87–115:1	Pyrene	500–700:1
Chrysene, alkyl-[c]	33–45:1	Pyrene, alkyl-	3–4:1
Dibenz[*a,h*]anthracene	17–25:1	Triphenylene	4400:1

[a] Formerly known as anthanthrene.
[b] Formerly known as benzo[*b*]fluoranthene.
[c] Similar to 5-methylchrysene.

TABLE 1.10
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	106-97-8	Butane $H_3C\text{-}(CH_2)_2\text{-}CH_3$	85, 112, 151, 199, 238, 239, 544–546, 604, 605, 620, 621, 966, 1140, 1153, 1154, 1243, 1284, 1420, 1634, 1966, 2060, 2079, 2270, 2293, 2310, 2634, 2781, 2782, 2799a, 2804, 2857, 2909, 2939, 2940, 2942, 2946, 3059, 3308, 3583, 3584, 3769, 3797, 3876, 3882, 3901, 3939, 3940, 3950, 3973, 4052, 4056, 4162, 4249, 4319, 5811b		3901, 4052, 4056
2.	75-83-2	Butane, 2,2-dimethyl- $(H_3C)_3{\equiv}C\text{-}CH_2\text{-}CH_3$	348, 966, 1140, 2939, 3302, 3876, 4249, 5777, 5811, 5811b		
3.	78-78-4 102056-77-9	Butane, 2-methyl-{methylbutane} $(H_3C)_2{=}CH\text{-}CH_2\text{-}CH_3$	85, 112, 199, 348, 604, 605, 1140, 1153, 1154, 2060, 2767, 2781, 2782, 2804, 2946, 3226, 3308, 3557, 3769, 3797, 4249, 5811b	3973	
4.	124-18-5	Decane $H_3C\text{-}(CH_2)_8\text{-}CH_3$	142, 151, 222–224, 568b, 1445, 1634, 2387, 2543, 2570, 3308, 3365, 4570a, 5770, 5811b	151, 182, 568b, 3797, 4249, 5811b	2387
5.	61193-21-3	Decane, methyl- $C_{10}H_{21}\text{-}CH_3$	1822, 4249		
6.	6975-98-0	Decane, 2-methyl- $H_3C\text{-}CH(CH_3)\text{-}(CH_2)_7\text{-}CH_3$	3557, 4249	925, 5657, 5811b	
7.	13151-34-3	Decane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_6\text{-}CH_3$	1827, 1884, 3557, 4249		
8.	13151-35-4	Decane, 5-methyl- $H_3C\text{-}(CH_2)_4$ $\text{-}CH(CH_3)\text{-}(CH_2)_3\text{-}CH_3$	1884, 4249		
9.	629-97-0	Docosane $H_3C\text{-}(CH_2)_{20}\text{-}CH_3$	568b, 619, 625, 727, 1360, 1375a, 1378, 1427, 1488, 1586, 2176, 2387, 2570, 2761, 2762, 2767, 2777, 2875, 3308, 3557, 3768, 3797, 4249, 5811b	182, 248, 404, 568b, 727, 840, 1488, 1978, 2339a, 3469, 3547, 3604, 3703, 3797, 4249, 4337, 5811b	1360, 1375a, 1378, 2387
10.	1560-81-2	Docosane, 2-methyl- $(H_3C){=}CH\text{-}(CH_2)_{19}\text{-}CH_3$	1195, 1375, 4249	840, 4337, 5811b	
11.	72227-00-0	Docosane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{18}\text{-}CH_3$	1195, 1375, 4249	840	
12.	112-40-3	Dodecane $H_3C\text{-}(CH_2)_{10}\text{-}CH_3$	568b, 619, 1371, 1425, 1427, 1445, 1488, 1586, 2570, 2767, 3308, 3410, 3557, 3768, 3797, 4248,, 4249, 4570a, 5811b	182, 404, 568b, 1488, 2339a, 2753, 2917a, 3186, 3188, 3547, 3797, 4249, 5657, 5811b	
13.	1560-97-0	Dodecane, 2-methyl- $H_3C\text{-}(CH_2)_9\text{-}CH{=}(CH_3)_2$		925, 5657	
14.	17312-57-1	Dodecane, 3-methyl- $H_3C\text{-}(CH_2)_8\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	3768, 4249	925, 5657	
15.	3891-98-3	Dodecane, 2,6,10-trimethyl-{farnesane}	1282, 4249, 5811b	404, 2917a	
16.	544-85-4	Dotriacontane $H_3C\text{-}(CH_2)_{30}\text{-}CH_3$	172, 568b, 613, 619, 625, 636, 727, 883, 907, 1375, 1445, 1586, 1651, 1935, 1937, 1979, 2176, 2524a, 2570, 2601a, 2761, 2762, 2767, 2939, 3308, 3557, 3608, 3768, 3797, 4103, 4249, 5811b	142, 182, 568b, 722, 727, 832, 883, 907, 1591, 1651, 1893b, 1933, 1935, 1937, 1978, 1979, 2595, 2939, 3469, 3476, 3604, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4103, 4249, 4337, 5811b	

(*continued*)

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
17.	1720-11-2	Dotriacontane, 2-methyl- H_3C-$(CH_2)_{29}$-CH═$(CH_3)_2$	613, 727, 1375, 1586, 2570, 2761, 2762, 2767, 3557, 4249, 5811b	727, 832, 908, 1591, 2595, 3607, 3609, 3613a, 3616, 3679, 3755, 4249, 4337, 5811b	
18.	20129-49-1	Dotriacontane, 3-methyl- H_3C-$(CH_2)_{28}$-CH(CH_3)-CH_2-CH_3	2570, 3768, 4249, 5811b	832, 1591, 3607, 3609, 3613a, 3616, 3679	
19.	16753-27-8	Dotriacontane-16,17-$^{14}C_2$	907, 1933, 1935, 1937, 4249	907, 1933, 1933a, 1935, 1937	
20.	112-95-8	Eicosane H_3C-$(CH_2)_{18}$-CH_3	613, 619, 727, 1360, 1375a, 1378, 1427, 1488, 1586, 2387, 2570, 2601a, 2761, 2762, 2765–2767, 2873, 3308, 3557, 3768, 3797, 4249, 5811b	182, 404, 619, 1488, 1978, 2339a, 2917a, 3547, 3797, 4249, 5657	1360, 1375a, 1378, 2387
21.		Eicosane, methyl-	3226, 4249		
22.	1560-84-5 52845-08-6	Eicosane, 2-methyl- {isoheneicosane} H_3C-$(CH_2)_{17}$-CH═$(CH_3)_2$	1900	5811, 5811b	
23.	6418-46-8	Eicosane, 3-methyl- H_3C-$(CH_2)_{16}$-CH(CH_3)-CH_2-CH_3		925, 5657	
24.	74-84-0	Ethane H_3C-CH_3	85, 173a, 199, 238, 239, 298, 544–546, 604, 605, 621, 722, 966, 1140, 1243, 1365, 1375a, 1377, 1420, 1472, 1478, 1664, 2060, 2079, 2252, 2270, 2310, 2582, 2583, 2634, 2782, 2799a, 2804, 2857, 2866, 2909, 2939, 2942, 2946, 3059, 3105, 3255, 3308, 3493, 3583, 3584, 3692, 3797, 3876, 3880, 3882, 3883, 3388, 3897, 3901, 3939, 4005–4007, 4052, 4056, 4135, 4162, 4249, 4319, 4360, 4393, 5811b		1375a, 1377, 3901, 4052, 4056
25.	629-94-7	Heneicosane H_3C-$(CH_2)_{19}$-CH_3	568b, 619, 625, 727, 1378, 1444, 1488, 2176, 2387, 2570, 2761, 2762, 2765–2767, 2777, 2875, 3308, 3557, 3768, 3797, 4249, 5811b	182, 404, 568b, 619, 1488, 1978, 2339a, 3547, 3797, 4249, 5657, 5811b	1378, 2387
26.	1560-82-3	Heneicosane, 2-methyl- H_3C-CH(CH_3)-$(CH_2)_{18}$-CH_3	1900	5811b	
27.	6418-47-9	Heneicosane, 3-methyl- H_3C-CH_2-CH(CH_3)-$(CH_2)_{17}$-CH_3	4249		
28.		Hentetracontane H_3C-$(CH_2)_{39}$-CH_3	625, 1659		
29.	630-04-6	Hentriacontane H_3C-$(CH_2)_{29}$-CH_3	14, 18, 239, 613, 619, 625, 727, 765, 767, 776, 883, 966, 1099, 1100, 1360, 1375, 1375a, 1375b, 1437, 1444, 1445, 1586, 1651, 1744, 1842, 2079, 2100, 2102, 2170, 2172, 2176, 2177, 2570, 2601a, 2761, 2762, 2765–2767, 2777, 2799a, 2857, 2939, 3240, 3247, 3251, 3255, 3265, 3308, 3431, 3457, 3557, 3562, 3608, 3768, 3797, 3876, 3966, 4184, 4193, 4194, 4249, 4284, 4320, 4333, 4354, 4406, 5079, 5512, 5811b	120, 181, 182, 480, 613, 619, 647, 701, 727, 832, 840, 876, 877, 883, 908, 1308, 1480, 1591, 1651, 1848, 1893b, 1978, 2079, 2101, 2270, 2283, 2595, 2939, 3194, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4249, 4337, 5079, 5189, 5345, 5657, 5682, 5811b	1360, 1375a
30.	1720-12-3	Hentriacontane, 2-methyl- $(H_3C)_2$═CH-$(CH_2)_{28}$-CH_3	613, 2570, 2767, 3797, 4249, 5811b	613, 619, 832, 840, 1591, 3607, 3609, 3613a, 3616, 3679, 3797, 4249	

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	4981-99-1	Hentriacontane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{27}$-CH_3	727, 1360, 1375, 1375a, 1375b, 2387, 2570, 2761, 2762, 2765–2767, 2777, 3557, 4249, 5811b	727, 832, 840, 1591, 2595, 3607, 3609, 3613a, 3616, 3679, 3755, 4249, 4337, 5811b	1360, 1375a, 2387
32.	7719-93-9	Heptacontane H_3C-$(CH_2)_{35}$-CH_3	4249	328, 4249	
33.	593-49-7	Heptacosane H_3C-$(CH_2)_{25}$-CH_3	613, 619, 625, 727, 776, 883, 1360, 1375, 1375a, 1375b, 1378, 1444, 1445, 1586, 1651, 2176, 2387, 2570, 2761, 2762, 2765–2767, 2777, 2939, 3247, 3251, 3308, 3557, 3608, 3768, 3797, 4249, 5811b	120, 182, 404, 613, 619, 647, 701, 727, 832, 840, 883, 1308, 1591, 1651, 1848, 1893b, 1978, 2079, 2270, 2283, 2339a, 2595, 2939, 3194, 3547, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4249, 4337, 5079, 5081, 5189, 5345, 5380, 5388, 5811b	1360, 1375a, 1378, 2387
34.	1561-00-8	Heptacosane, 2-methyl- $(H_3C)_2$═CH-$(CH_2)_{24}$-CH_3	613, 727, 2387, 2570, 3797, 4249, 4444, 5811b	613, 619, 727, 832, 840, 3607, 3609, 3613a, 3616, 3679, 3797, 4249	2387
35.	14167-66-9	Heptacosane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{23}$-CH_3	1375, 1375b, 2387, 2570, 3557, 3797, 4249	832, 840, 2595, 3607, 3609, 3613a, 3616, 3679, 3797, 4249, 4337, 4347	2387
36.	629-78-7	Heptadecane H_3C-$(CH_2)_{15}$-CH_3	568b, 619, 727, 1360, 1375a, 1378, 1427, 1488, 1586, 2387, 2543, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2875, 3308, 3557, 3768, 3797, 4249, 5811b	182, 404, 568b, 619, 727, 1488, 1978, 2339a, 3547, 3797, 4249, 5657, 5811b	1360, 1375a, 1378, 2387
37.	1560-89-0	Heptadecane, 2-methyl- H_3C-$(CH_2)_{14}$-CH═$(CH_3)_2$	1168	925, 5657	
38.	6418-44-6	Heptadecane, 3-methyl- H_3C-$(CH_2)_{13}$-$CH(CH_3)$-CH_2-CH_3		925, 5657	
39.	13287-23-5	Heptadecane, 8-methyl- H_3C-$(CH_2)_6$-$CH(CH_3)$- $(CH_2)_8$-CH_3	2731, 2735, 4249, 5811b		
40.	142-82-5	Heptane H_3C-$(CH_2)_5$-CH_3	112, 348, 568b, 1140, 1419, 1420, 1634, 1822, 2545, 2601a, 2634, 2857, 3797, 4249, 5811b	568b, 3841, 4249, 5811b	
41.		Heptane, dimethyl-	222–224		
42.	2213-23-2	Heptane, 2,4-dimethyl-		2917a	
43.	592-27-8	Heptane, 2-methyl- H_3C-$(CH_2)_4$-CH═$(CH_3)_2$	348, 1822, 1884, 4249, 5811b		
44.	15869-80-4	Heptane, 3-ethyl- H_3C-$(CH_2)_3$-CH═$(C_2H_5)_2$	348, 1182, 4249		
45.	589-81-1	Heptane, 3-methyl- H_3C-$(CH_2)_3$-$CH(CH_3)$-CH_2-CH_3	119, 1140, 1822, 4249, 5811b		
46.	7194-84-5	Heptatriacontane H_3C-$(CH_2)_{35}$-CH_3	625	1893b	
47.	630-01-3	Hexacosane H_3C-$(CH_2)_{24}$-CH_3	613, 619, 625, 727, 883, 1360, 1375, 1375a, 1375b, 1378, 1586, 1651, 2176, 2387, 2570, 2761, 2762, 2765–2767, 2777, 2939, 3308, 3608, 3768, 3797, 4249, 5811b	182, 404, 619, 727, 832, 840, 1591, 1651, 1893b, 1978, 2339a, 2595, 2939, 3547, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 4249, 4337, 4347	1360, 1375a, 1378, 2387

(*continued*)

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
48.	1561-02-0	Hexacosane, 2-methyl- $(H_3C)_2$═CH-$(CH_2)_{23}$-CH_3	2570, 3797, 4249	619, 3613a, 3797, 4249, 5811b	
49.	65820-56-6	Hexacosane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{22}$-CH_3		3607, 3609, 4249, 4803	
50.	544-76-3	Hexadecane H_3C-$(CH_2)_{14}$-CH_3	619, 727, 1371, 1378, 1427, 1488, 1586, 1979, 2387, 2524a, 2570, 2731, 2735, 2767, 2773, 2875, 3308, 3557, 3768, 3797, 4249, 5811b	182, 404, 619, 727, 1488, 1978, 1979, 2339a, 3547, 3797, 4249, 5657	1378, 2387
51.	1560-92-5	Hexadecane, 2-methyl- H_3C-$(CH_2)_{13}$-CH═$(CH_3)_2$	3768, 4249	925, 5657	
52.	6418-43-5	Hexadecane, 3-methyl- H_3C-$(CH_2)_{12}$-$CH(CH_3)$-CH_2-CH_3		925, 5657	
53.	638-36-8	Hexadecane, 2,6,10,14-tetramethyl-{phytane}	1282, 4249, 5811b	3609	
54.	60922-91-0	Hexadecane, mixture with pentane	4249		
55.	110-54-3	Hexane H_3C-$(CH_2)_4$-CH_3	85, 142, 151, 222–224, 238, 239, 568b, 604, 605, 1140, 1153, 1154, 1284, 1348–1350, 1354, 1375, 1375a, 1375b, 1420, 1481, 1586, 1589, 1634, 2060, 2543, 2545, 2570, 2634, 2777, 2782, 2799a, 2804, 2946, 3254, 3308, 3692, 3797, 3901, 4005–4007, 4052, 4056, 4249, 5811b, 5869a	568b, 1481, 1596, 3841, 4249, 4807, 5811b	1354, 1375a, 4052, 4056
56.	28777-67-5	Hexane, dimethyl- C_6H_{12}═$(CH_3)_2$	1153, 1154, 1637, 4249		
57.	589-43-5 116502-44-4	Hexane, 2,4-dimethyl- H_3C-$CH(CH_3)$-CH_2-$CH(CH_3)$-CH_2-CH_3	1822, 5811b		
58.	592-13-2	Hexane, 2,5-dimethyl- $[H_3C$-$CH(CH_3)$-$CH_2]_2$	1153, 1154, 5811b	5811b	
59.	591-76-4	Hexane, 2-methyl-	5811, 5811a, 5811b		
60.	589-34-4	Hexane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_2$-CH_3	1140, 1419, 2601a, 4249, 5811b	4249, 4807, 5811b	
61.	1071-81-4	Hexane, 2,2,5,5-tetramethyl- $(H_3C)_3$≡C-$(CH_2)_2$-C≡$(CH_3)_3$	4249		
62.	630-06-8	Hexatriacontane H_3C-$(CH_2)_{34}$-CH_3	625, 1586, 2176, 2939, 3797, 4249	1893b, 2939, 3607, 3616, 3679, 3755, 4249	
63.	52845-07-5	Isoeicosane	4249		
64.	54365-40-1	Isoheptacosane	4249	4249	
65.	52701-70-9	Isopentacosane		4249	
66.	34425-19-9	Isotriacontane	3327a		
67.	74-82-8	Methane CH_4	199, 141–143, 151, 172, 216, 237–239, 241, 298, 544–546, 604, 605, 621, 722, 966, 1067, 1140, 1242, 1284, 1365, 1375a, 1377, 1420, 1437, 1477, 1478, 1485, 1664, 1668, 1821, 1842, 1966, 2059, 2060, 2066, 2068, 2142, 2171, 2252, 2270, 2293, 2310, 2343, 2548, 2549, 2582, 2662, 2780, 2781, 2782, 2804, 2857, 2866, 2878, 2939, 2942, 2946, 3059, 3105, 3106, 3121, 3255, 3257, 3308, 3493, 3583, 3584, 3692, 3729, 3797, 3876, 3880–3883, 3901, 3939, 4005–4007, 4052, 4056, 4064, 4065, 4135, 4151, 4162, 4249, 4319, 5079, 5512, 5811b		1228, 1375a, 1377, 3901, 4052, 4056

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
68.	630-03-5	Nonacosane $H_3C\text{-}(CH_2)_{27}\text{-}CH_3$	613, 619, 625, 727, 776, 883, 1360, 1375, 1375a, 1375b, 1378, 1444, 1445, 1586, 1651, 2176, 2387, 2570, 2601a, 2761, 2762, 2765–2767, 2777, 2939, 2962, 3247, 3308, 3557, 3608, 3768, 3797, 4249, 5811b	120, 182, 404, 613, 619, 701, 727, 832, 840, 883, 1591, 1651, 1893b, 1978, 2270, 2339a, 2595, 2939, 3547, 3555, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4249, 4337, 5079, 5682, 5811b	1360, 1375a, 1378, 2387
69.	1560-75-4	Nonacosane, 2-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{26}\text{-}CH_3$	613, 2387, 2570, 3797, 4249, 5811b	619, 832, 840, 3607, 3609, 3613a, 3616, 3679, 3797, 4249, 5811b	2387
70.	14167-67-0	Nonacosane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{25}\text{-}CH_3$	727, 1360, 1375, 1375a, 1375b, 1586, 2387, 2570, 2761, 2762, 2765–2767, 2777, 3557, 4249, 5811b	727, 832, 840, 1591, 2595, 3607, 3609, 3613a, 3616, 3679, 3755, 3797, 4249, 4337, 5811b	1360, 1375a, 2387
71.	629-92-5	Nonadecane $H_3C\text{-}(CH_2)_{17}\text{-}CH_3$	568b, 619, 727, 1371, 1378, 1427, 1444, 1488, 1586, 2387, 2543, 2570, 2761, 2762, 2765, 2766, 2773, 2777, 3308, 3557, 3768, 3797, 4249, 5811b	182, 568b, 619, 1488, 1978, 2339a, 3797, 4249, 5657, 5811b	1378, 2387
72.		Nonadecane, methyl-	3226, 4249		
73.	6418-45-7	Nonadecane, 3-methyl- $H_3C\text{-}(CH_2)_{15}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$		925, 5657	
74.	111-84-2	Nonane $H_3C\text{-}(CH_2)_7\text{-}CH_3$	222–224, 568b, 1140, 1419, 1634, 1637, 3797, 4249, 5770, 5811b	182, 568b, 619, 3797, 4249, 5811b	
75.	871-83-0	Nonane, 2-methyl-	4570a		
76.	7194-86-7	Nonatriacontane $H_3C\text{-}(CH_2)_{37}\text{-}CH_3$	625	1893b	
77.	630-02-4	Octacosane $H_3C\text{-}(CH_2)_{26}\text{-}CH_3$	568b, 613, 619, 625, 727, 883, 1360, 1375, 1375a, 1375b, 1378, 1444, 1445, 1651, 1586, 2176, 2387, 2570, 2761, 2762, 2765–2767, 2777, 2939, 3308, 3557, 3608, 3768, 3797, 4249, 5811b	182, 404, 568b, 727, 613, 619, 832, 840, 883, 1591, 1651, 1893b, 1978, 2339a, 2595, 2939, 3547, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4249, 4337, 5811b	1360, 1375a, 1378, 2387
78.	1560-98-1	Octacosane, 2-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{25}\text{-}CH_3$	613, 727, 1360, 1375, 1375a, 1375b, 1586, 2387, 2570, 2761, 2762, 2765–2767, 2777, 3557, 4249, 5811b	613, 619, 727, 832, 840, 1591, 2595, 3607, 3609, 3613a, 3616, 3679, 4249, 4337, 5811b	1360, 1375a, 2387
79.	65820-58-8	Octacosane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{24}\text{-}CH_3$	2387, 2570, 4249	832, 840, 3607, 3609, 3613a, 3616, 3679, 4249, 4337	2387
80.	593-45-3	Octadecane $CH_3\text{-}(CH_2)_{16}\text{-}CH_3$	568b, 619, 727, 1378, 1427, 1444, 1488, 1586, 2543, 2570, 2761, 2762, 2765–2767, 2777, 2875, 3308, 3557, 3768, 3797, 4248, 4249, 5811b	182, 404, 568b, 619, 727, 1488, 1978, 2339a, 2917a, 3469, 3797, 4249, 5657, 5811b	1378
81.	1560-88-9	Octadecane, 2-methyl- $H_3C\text{-}(CH_2)_{15}\text{-}CH{=}(CH_3)_2$		925, 5657	
82.	6561-44-0	Octadecane, 3-methyl- $H_3C\text{-}(CH_2)_{14}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$		925, 5657	
83.	111-65-9	Octane $H_3C\text{-}(CH_2)_6\text{-}CH_3$	568b, 1140, 1419, 1634, 3797, 4249, 5770, 5811b	568b, 619, 3797, 4249, 5811b	

(*continued*)

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
84.		Octane, dimethyl- $C_6H_{12}{=}(CH_3)_2$	222–224		
85.	61193-19-9	Octane, methyl- C_7H_{15}-CH_3	1822, 1884, 4249		
86.	2216-33-3	Octane, 3-methyl-	5811, 5811a, 5811b		
87.	2216-34-4	Octane, 4-methyl-		2917a	
88.	7194-85-6	Octatriacontane H_3C-$(CH_2)_{36}$-CH_3	625	208, 1893b, 3609	
89.	629-99-2	Pentacosane H_3C-$(CH_2)_{23}$-CH_3	172, 568b, 613, 619, 625, 727, 883, 1360, 1375, 1375a, 1375b, 1378, 1444, 1586, 2071, 2176, 2387, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 2777, 2875, 2939, 3308, 3557, 3608, 3768, 3797, 4249, 5811b	182, 404, 568b, 613, 619, 727, 832, 1893b, 1978, 2260, 2339a, 2595, 2939, 3547, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 4249, 4337, 4347, 5811b	1360, 1378, 2387
90.	629-87-8	Pentacosane, 2-methyl- H_3C-$(CH_2)_{22}$-$CH{=}(CH_3)_2$	3768, 4249, 4332	5811b	
91.	6902-54-1	Pentacosane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{21}$-CH_3	4249	4249	
92.	629-62-9	Pentadecane H_3C-$(CH_2)_{13}$-CH_3	568b, 619, 727, 1378, 1427, 1444, 1488, 2387, 2506, 2507, 2543, 2570, 2731, 2735, 2767, 2773, 2870, 3255, 3308, 3557, 3768, 3797, 4249, 5811b	182, 568b, 619, 1488, 1978, 2339a, 2753, 3547, 3797, 4249, 5657, 5811b	1378, 2387, 2506(0), 2507(0)
93.	1560-93-6	Pentadecane, 2-methyl- H_3C-$(CH_2)_{12}$-$CH{=}(CH_3)_2$	3302, 4249	925, 5657	
94.	2882-96-4	Pentadecane, 3-methyl- H_3C-$(CH_2)_{11}$-$CH(CH_3)$-CH_2-CH_3	3302, 4249	925	
95.	1921-70-6	Pentadecane, 2,6,10,14-tetramethyl- {pristane}	1282, 3226, 4249, 5811b		
96.	3892-00-0	Pentadecane, 2,6,10-trimethyl- {norpristane}	1282, 4249, 5811b		
97.	109-66-0	Pentane H_3C-$(CH_2)_3$-CH_3	85, 112, 142, 151, 199, 238, 239, 604, 605, 1140, 1153, 1154, 1284, 1374, 1375, 1375b, 1419, 1420, 1822, 2634, 2782, 2804, 2944, 2946, 3254, 3308, 3557, 3769, 3797, 3901, 4249, 5811b	1597, 3841, 4249, 5811b	
98.	1067-20-5	Pentane, 3,3-diethyl- $C(C_2H_5)_4$	1822, 4249		
99.	108-08-7	Pentane, 2,4-dimethyl- H_3C-$CH(CH_3)$-CH_2-$CH(CH_3)_2$	1140, 1419, 4068, 4249, 5811b		
100.	43133-95-5	Pentane, methyl- C_5H_{11}-CH_3	605, 1140, 4249		
101.	107-83-5	Pentane, 2-methyl- H_3C-$(CH_2)_2$-$CH{=}(CH_3)_2$	85, 604, 605, 1140, 1153, 1154, 1419, 1586, 1822, 2060, 2310, 2767, 2782, 2804, 2944, 2946, 3302, 3308, 3769, 3797, 4249	2339a	
102.	96-14-0	Pentane, 3-methyl- $(H_3C$-$CH_2)_2{=}CH$-CH_3	222–224, 605, 1140, 1586, 1822, 2060, 2310, 2767, 2782, 2804, 2944, 2946, 3302, 3308, 3769, 3797, 4249, 5811b	404, 2339a	
103.	630-07-9	Pentatriacontane H_3C-$(CH_2)_{33}$-CH_3	625, 727, 1375, 1375b, 1586, 2176, 2767, 2939, 3265, 3557, 3797, 4249, 4320, 4333, 5811b	727, 1893b, 1978, 2939, 3607, 3609, 3613a, 3616, 3679, 3755, 3797, 4249, 4320, 5811b	

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
104.	66576-73-6	Pentatriacontane, 2-methyl- H_3C-$CH(CH_3)$-$(CH_2)_{32}$-CH_3		2689c	
105.	78692-70-3	Pentatriacontane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{31}$-CH_3		3609, 4249	
106.	74-98-6	Propane H_3C-CH_2-CH_3	85, 168, 173a, 199, 238, 239, 544–546, 604, 605, 621, 722, 1067, 1140, 1153, 1154, 1284, 1306, 1365, 1375a, 1377, 1420, 1634, 1966, 2060, 2079, 2142, 2171, 2270, 2309, 2310, 2634, 2782, 2804, 2857, 2866, 2909, 2939, 2942, 2944, 2946, 3059, 3255, 3308, 3583, 3584, 3692, 3769, 3797, 3876, 3882, 3901, 3939, 3940, 4005–4007, 4052, 4056, 4135, 4162, 4249, 4319, 4394, 5770, 5811b		1375a, 1377, 3901, 4052, 4056
107.	75-28-5	Propane, 2-methyl-{isobutane} $(H_3C)_2$═CH-CH_3	199, 241, 544, 604, 605, 1140, 1153, 1154, 1284, 1375a, 1377, 2060, 2270, 2309, 2310, 2782, 2804, 2857, 2909, 2944, 2946, 3059, 3308, 3901, 3939, 3940, 4052, 4056, 4162, 4249, 4319, 5770, 5811b		1375a, 1377, 3901, 4052, 4056
108.	4181-95-7	Tetracontane H_3C-$(CH_2)_{38}$-CH_3	625, 1659		
109.	646-31-1	Tetracosane H_3C-$(CH_2)_{22}$-CH_3	568b, 613, 619, 625, 727, 1378, 1444, 1586, 2176, 2570, 2767, 2875, 3308, 3557, 3768, 3797, 4248, 4249, 5811b	248, 404, 568b, 619, 1378, 1978, 2339a, 2917a, 3604, 3609, 3703, 3797, 4249, 5811b	
110.	28503-88-0	Tetracosane, methyl-	4249	3226, 4249	
111.	1560-78-7	Tetracosane, 2-methyl- H_3C-$CH(CH_3)$-$(CH_2)_{21}$-CH_3	1900, 3557	2595, 4249, 5811, 5811b	
112.		Tetracosane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{20}$-CH_3	3327b	2595, 3327b, 4249	
113.	629-59-4	Tetradecane H_3C-$(CH_2)_{12}$-CH_3	336, 568b, 727, 1371, 1425, 1427, 1488, 1586, 1646, 2387, 2506, 2507, 2543, 2570, 2767, 2773, 2875, 3308, 3555, 3557, 3768, 3797, 4249, 4570a, 5811b	336, 404, 568b, 619, 1488, 2339a, 2753, 3547, 3555, 3797, 4249, 5657, 5811b	2387, 2506, 2507
114.	1560-95-8	Tetradecane, 2-methyl-H_3C-$(CH_2)_{11}$-CH═$(CH_3)_2$		925, 5657	
115.	18435-22-8	Tetradecane, 3-methyl- H_3C-$(CH_2)_{10}$-$CH(CH_3)$-CH_2-CH_3		925, 5657	
116.	14905-56-7	Tetradecane, 2,6,10-trimethyl-		2917a	
117.	14167-59-0	Tetratriacontane H_3C-$(CH_2)_{32}$-CH_3	613, 625, 727, 1375, 1375b, 1586, 1651, 2176, 2767, 2939, 3308, 3557, 3608, 3768, 3797, 4249, 5811b	619, 727, 832, 840, 1651, 1893b, 1978, 2939, 3607–3609, 3613a, 3616, 3679, 3755, 3797, 4249, 4337, 5811b	
118.	14167-65-8	Tetratriacontane, 2-methyl- H_3C-$CH(CH_3)$-$(CH_2)_{31}$-CH_3	2176, 4249	727, 3607, 3609, 3613a, 3616, 3679, 4249, 5811b	
119.	66309-88-4	Tetratriacontane, 3-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{30}$-CH_3	2767, 2769, 4249	3607, 3616, 3679, 5811b	

(*continued*)

TABLE 1.10 (continued)
Alkanes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
120.	638-68-6	Triacontane $H_3C\text{-}(CH_2)_{28}\text{-}CH_3$	568b, 613, 619, 625, 727, 883, 1375, 1375b, 1378, 1444, 1445, 1586, 1651, 2176, 2387, 2570, 2761, 2762, 2765–2767, 2777, 2939, 3308, 3608, 3768, 3797, 4249, 5811b	182, 404, 568b, 619, 727, 832, 840, 883, 1591, 1651, 1893b, 2595, 2939, 3604, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4249, 4337, 5079, 5388, 5811b	1378, 2387
121.	1560-72-1	Triacontane, 2-methyl- $H_3C\text{-}CH(CH_3)\text{-}(CH_2)_{27}\text{-}CH_3$	613, 727, 1360, 1375, 1375a, 1375b, 1586, 2387, 2570, 2761, 2762, 2765, 2766, 2777, 3557, 3797, 4249, 5811b	619, 727, 832, 840, 1591, 2595, 3607, 3609, 3613a, 3616, 3679, 4249, 4337, 5081, 5811b	1360, 1375a, 2387
122.	72227-01-1	Triacontane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{26}\text{-}CH_3$	2387, 2570, 4249, 4652, 5811b	832, 840, 1591, 3607, 3609, 3613a, 3616, 3679, 5682	2387
123.	638-67-5	Tricosane $H_3C\text{-}(CH_2)_{21}\text{-}CH_3$	568b, 619, 625, 727, 1378, 1586, 2176, 2387, 2570, 2601a, 2761, 2762, 2765–2767, 2777, 2875, 3308, 3557, 3768, 3797, 4249, 5811b	182, 404, 568b, 619, 727, 1978, 2339a, 2595, 2917a, 3547, 3604, 3703, 3797, 4249, 4337, 5811b	1378, 2387
124.	1928-30-9	Tricosane, 2-methyl- $H_3C\text{-}CH(CH_3)\text{-}(CH_2)_{20}\text{-}CH_3$	3302, 4249	2595, 4337, 5811b	
125.	13410-45-2	Tricosane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{19}\text{-}CH_3$		2595, 3609, 4249, 4337, 4573	
126.	629-50-5	Tridecane $H_3C\text{-}(CH_2)_{11}\text{-}CH_3$	568b, 727, 1075, 1371, 1425, 1427, 1488, 1586, 1646, 2387, 2506, 2507, 2570, 2731, 2735, 2767, 2875, 3186, 3308, 3410, 3557, 3768, 3797, 4249, 4570a, 5811b	182, 404, 568b, 619, 1488, 2339a, 2753, 3186, 3547, 3797, 5657, 5811b	2387, 2506, 2507
127.	1560-96-9	Tridecane, 2-methyl- $H_3C\text{-}(CH_2)_{10}\text{-}CH{=}(CH_3)_2$		925, 5657	
128.	6418-41-3	Tridecane, 3-methyl- $H_3C\text{-}(CH_2)_9\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$		925, 5657	
129.	630-05-7	Tritriacontane $H_3C\text{-}(CH_2)_{31}\text{-}CH_3$	613, 619, 625, 727, 776, 1360, 1375, 1375a, 1375b, 1444, 1445, 1586, 1651, 2176, 2177, 2570, 2601a, 2761, 2762, 2765, 2766, 2939, 3247, 3251, 3308, 3557, 3608, 3768, 3797, 4030, 4249, 5811b	613, 619, 727, 832, 840, 1308, 1591, 1651, 1893b, 1978, 2595, 2939, 3607–3609, 3613a, 3616, 3679, 3755, 3797, 4337, 5811b	1360, 1375a
130.	66214-27-5	Tritriacontane, 2-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{30}\text{-}CH_3$	727, 2767, 3557, 3797, 5811b	619, 727, 832, 840, 3607, 3609, 3613a, 3616, 3679, 3797	
131.	14167-69-2	Tritriacontane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{29}\text{-}CH_3$	1375, 1375b, 1586, 2570, 2761, 2762, 2765–2767, 3557, 4249, 5811b	832, 840, 2595, 3607, 3609, 3613a, 3616, 3679, 3797, 4249, 4337, 5811b	
132.	1120-21-4	Undecane $H_3C\text{-}(CH_2)_9\text{-}CH_3$	222–224, 568b, 1425, 1427, 1445, 1488, 1646, 2387, 2543, 2570, 2767, 2773, 3557, 4249, 4570a, 5770, 5811b	182, 568b, 619, 1488, 2339a, 3547, 3797, 4249, 5657, 5811b	2387
133.		Undecane, dimethyl-	222–224		
134.	17301-23-4	Undecane, 2,6-dimethyl-		404	
135.	7045-71-8	Undecane, 2-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_8\text{-}CH_3$	2769, 3557, 4249	925, 5657, 5811b	
136.	1002-43-3	Undecane, 3-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_7\text{-}CH_3$	2769, 3557	925, 5657, 5811b	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

of a particular alkane. Comparison of this updated list with that reported in the earlier edition indicates that very few new alkanes are included in our up-to-date Table 1.10.

1.2 ALKENES AND ALKYNES

In his summary of the identified components of tobacco smoke, Kosak (2170) listed only one unequivocally identified alkene or alkyne. It was ethyne (acetylene). Johnstone and Plimmer (1971) listed the following alkenes and alkynes identified in tobacco smoke: *cis*- and *trans*-butene, 1,3-butadiene, methyl-1,3-butadiene (isoprene), ethene, ethyne, methylethyne, propene, methylpropene, squalene and isosqualene, and several phytadienes. Less than a decade later, Stedman (3797) described and/or discussed nearly 235 acyclic alkenes and alkynes identified in tobacco smoke. This number includes the *cis* and *trans* isomers in the homologous monoalkene series discussed later.

In Table 1.11 are listed 392 acyclic alkenes and alkynes in tobacco smoke whose identifications have been reported to date. Comparison of this updated list with that reported in the earlier edition indicates that nearly 60 additional acyclic alkenes and alkynes are now included in our up-to-date Table 1.11.

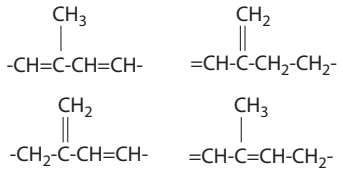
The lower molecular weight acyclic unsaturated hydrocarbons (alkenes, alkadienes, alkynes, etc.) occur primarily, if not totally, in the vapor phase of mainstream smoke (MSS). Even though some of the vapor-phase components of cigarette MSS have been shown to be significant in in vitro ciliastats, the low molecular weight hydrocarbons (alkanes, alkenes, alkynes) were not considered by Caroff et al. (604, 605) to be involved because of their low concentrations in the smoke. The smoke components (aldehyde, ketones, hydrogen cyanide, formic and acetic acids, phenol) reported to be significant in vitro ciliastats are relatively highly water soluble, whereas the low molecular weight hydrocarbons, generally considered nonciliastatic in in vitro systems, show extremely low solubility in water. Rodgman et al. (3306) and Dalhamn et al. (892, 893) described the differences in oral absorption of the tobacco smoke components isoprene (20%) *vs*. acetaldehyde (60%) or acetone (56%). It has also been noted by Wynder and Hoffmann (4332) that these compounds do not appear to play a significant role in tobacco smoke carcinogenesis: "Their [the alkenes] level in the smoke is rather low (0.01%) and they would, therefore, not be active even if they were tumor promoters."

In the National Cancer Institute study on the "less hazardous" cigarette, which involved chemical and biological (mouse skin-painting bioassay) studies on four series* (1329, 1330, 1332, 1333) of experimental cigarettes and appropriate controls, an interesting correlation was reported with the first series of cigarettes (1329): While no correlations were observed between the benzo[*a*]pyrene (B[*a*]P) content or the benz[*a*]anthracene (B[*a*]A) content of the cigarette smoke condensate (CSC) and the % tumor-bearing animals, a correlation—classified as significant—was observed between the isoprene content of the MSS and the % tumor-bearing animals. This observed isoprene—% tumor-bearing animal correlation—was heatedly discussed and debated for the following year. In the second, third, and fourth series of cigarette, the isoprene—% tumor-bearing animal correlation—was not observed, i.e., it had disappeared! It should be noted that the manipulations involved in the collection and preparation of the CSCs for the bioassay virtually preclude the presence of isoprene in the material applied to the host animals.

In its review of smoke composition and the relationship between smoke components and health, the IARC (1870) devoted very little space to the volatile acyclic hydrocarbons and just two paragraphs to the nonvolatile members of this compound group.

Among the alkenes listed as tobacco smoke components are several series of isomeric isoprenoid compounds, including the phytadienes (3247), the solanesenes (3297), and the squalenes (2175, 3297, 4033) plus several homologous series of monoalkenes (1144).

A series of phytadiene isomers with a pair of conjugated double bonds in different internal and terminal positions were identified in the MSS from cigarettes containing the American blend (3247). Similar series of phytadienes were identified in the MSSs from cigarettes containing individual tobaccos (flue cured, burley, Oriental). The evidence indicated the presence of at least the following four basic combinations of the conjugated linkages within an isoprenoid unit or between contiguous units:



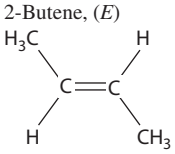
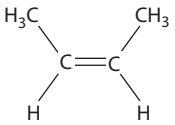
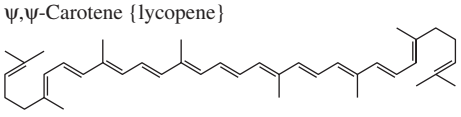
The mixture of smoke phytadienes was separated into groups of phytadienes by alumina column chromatography. Because Rowland (3345) had used the Diels–Alder reaction of neophytadiene with 1,4-naphthoquinone to great advantage in its characterization, this same reaction sequence was used in the phytadiene study. Treatment of each phytadiene fraction with 1,4-naphthoquinone gave Diels–Alder adducts which were converted to anthraquinonecarboxylic acids by sequential oxidations, first to alkylanthraquinones and then to carboxylic acids. The number and positions of the carboxyl groups permitted assignment of the conjugated double bonds in the phytadiene. The phytadiene series contained 3-methylene-7,11,15-trimethyl-1-hexadecene (neophytadiene); 3,7,11,15-tetramethyl-1,3-hexadecadiene; 2,6,10,14-tetramethyl-1,3-hexadecadiene; 1,2,4-trialkyl-1,3-butadiene; and possibly as many as nine other conjugated phytadienes (excluding *cis* and *trans* isomers). No evidence was obtained to indicate that six of the possible isomeric conjugated phytadienes were present in MSS. They may have either been unreactive in the Diels–Alder reaction with 1,4-naphthoquinone or, if reactive, gave an adduct which was not oxidizable to an alkylanthraquinone.

* The four series of cigarettes involved a total of 98 test cigarettes and about 30 reference (Kentucky Reference 1R1) and standard cigarettes, divided almost equally among the four series.

TABLE 1.11
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	25339-57-5	Butadiene	143, 1140, 1286, 1419, 1971, 2079, 2270, 3059, 3308, 3882, 3939, 4104, 4249, 4319, 5835		
2.	590-19-2	1,2-Butadiene $H_2C{=}C{=}CH\text{-}CH_3$	348, 1140, 1472, 2060, 2310, 2782, 2804, 2946, 3302, 3308, 3797, 4052, 4056, 4249		4052, 4056
3.	106-99-0	1,3-Butadiene $H_2C{=}CH\text{-}CH{=}CH_2$	73, 126a, 143, 154, 174b, 174c, 199, 216, 329, 402, 493–495, 603–605, 621, 688, 710, 722, 966, 1037a, 1037b, 1099, 1100, 1140, 1153, 1154, 1243, 1262a, 1386, 1472, 1557, 1571a, 1632, 1740, 1741, 1743, 1744, 1842, 1971, 2060, 2270, 2293, 2310, 2313a, 2634, 2644, 2645, 2782, 2804, 2857, 2866, 2942, 2946, 3007, 3260, 3265, 3300, 3302, 3308, 3370, 3441a, 3583, 3584, 3713, 3797, 3876, 3882, 3897, 3901, 4052, 4056, 4078, 4135, 4150, 4153, 4150, 4153, 4162, 4166, 4249, 4319, 4360, 5034, 5049, 5070, 5508, 5512, 5531, 5547, 5554, 5679, 5692, 5692a, 5770, 5811b, 5836, 5869a		4052, 4056
4.	513-81-5	1,3-Butadiene, 2,3-dimethyl-	568b, 4249		
5.	78-79-5	1,3-Butadiene, 2-methyl- {isoprene} $H_2C{=}C(CH_3)\text{-}CH{=}CH_2$	73, 112, 142, 143, 172, 173a, 174b, 174c, 199, 216, 239, 298, 299, 314, 323, 329, 402, 494, 495, 544–546, 568b, 603–605, 628, 639, 643, 645, 688, 722, 892, 893, 966, 1050, 1099, 1100, 1063–1066, 1068–1074, 1140, 1153, 1154, 1217, 1243, 1262a, 1284, 1286, 1329, 1330, 1332–1334, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1418–1420, 1437, 1445, 1449, 1492, 1497, 1586, 1589, 1634, 1637–1639, 1642, 1643, 1693, 1699, 1709, 1740, 1741, 1743, 1744, 1760, 1842, 1875, 1956, 1974, 2002, 2003, 2060, 2062, 2063, 2073, 2079, 2091, 2131, 2171, 2270, 2293, 2301, 2310, 2313a, 2520, 2543, 2570, 2582, 2589, 2634, 2644, 2645, 2683, 2761, 2762, 2767, 2775, 2777, 2782, 2799a, 2800, 2804, 2822, 2857, 2864b, 2866, 2874, 2939, 2942, 2946, 3007, 3059, 3105, 3106, 3132, 3254, 3255, 3257, 3260, 3265, 3300, 3302, 3306, 3308, 3370, 3373, 3418, 3482, 3493, 3551, 3557, 3583, 3584, 3692, 3714, 3797, 3862, 3876, 3882, 3897, 3901, 3939, 3973, 3976, 3999, 4005–4007, 4052, 4056, 4057, 4078, 4104, 4135, 4150, 4166, 4249, 4254–4256, 4258, 4290, 4319, 4360, 4636, 4731, 4830, 4998, 5034, 5049, 5512, 5547, 5554, 5679, 5692, 5811b, 5692a, 5770, 5836, 4A02	568b, 4249, 4731, 5811b	1330, 1332, 1354, 1375a, 1377, 1378, 4052, 4056
6.		1,3-Butadiene, 2-methyl-radical (isoprene radical}	27A33		
7.		1,3-Butadiene, 1,2,4-trialkyl- $R\text{-}CH{=}C(R_1)\text{-}CH{=}CH\text{-}R_2$	3247, 3251, 4249		
		1,3-Butadiene, 2-(4′,8′,12′-trimethyltridecyl)-	See1-hexadecene,3-methylene-7,11,15-trimethyl-		
8.	460-12-8	1,3-Butadiyne $HC{\equiv}C\text{-}C{\equiv}CH$	1243		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
9.	9003-28-5	Butene	546, 4249, 5811b		
10.		Butene, dimethyl-	5034		
11.		Butene, methyl-	1637, 4249, 5034		
12.	26760-64-5	Butene, 2-methyl-	5811a, 5811b		
13.	106-98-9 9003-28-5	1-Butene $H_2C{=}CH\text{-}CH_2\text{-}CH_3$	85, 112, 151, 199, 544–546, 604, 605, 722, 1140, 1153, 1154, 1243, 1375a, 1377, 2060, 2079, 2270, 2293, 2310, 2634, 2767, 2782, 2804, 2857, 2939, 2946, 3302, 3308, 3583, 3584, 3692, 3882, 3901, 4104, 4135, 4249, 5770		1375a, 1377, 3901
14.	563-78-0	1-Butene, 2,3-dimethyl- $H_2C{=}C(CH_3)\text{-}CH{=}(CH_3)_2$	568b, 1140, 1153, 1154, 2944, 3219, 3308, 3797, 4249, 5811b	568b, 2339a, 4249	
15.	558-37-2	1-Butene, 3,3-dimethyl- $H_2C{=}CH\text{-}C{\equiv}(CH_3)_3$	568b, 1140, 1153, 1154, 1419, 2944, 2946, 3302, 3308, 3797, 4249, 5811b		
16.	563-46-2	1-Butene, 2-methyl- $H_2C{=}C(CH_3)\text{-}CH_2\text{-}CH_3$	604, 605, 722, 1140, 2060, 2310, 2327, 2782, 2804, 2946, 3302, 3308, 3769, 3797, 3901, 4249, 5811b		
17.	563-45-1	1-Butene, 3-methyl- $H_2C{=}CH\text{-}CH{=}(CH_3)_2$	604, 605, 1140, 2060, 2310, 2782, 2804, 2946, 3302, 3308, 3769, 3797, 3901, 4249. 5770, 5811b		
18.	107-01-7	2-Butene $H_3C\text{-}CH{=}CH\text{-}CH_3$	85, 199, 298, 544–546, 621, 722, 1243, 2079, 2270, 2293, 2767, 3302, 3692, 3797, 3901, 4005–4007, 4135, 4249, 4449, 5811b		3901
19.	624-64-6	2-Butene, (*E*) 	199, 544–546, 604, 605, 1140, 1153, 1154, 2060, 2310, 2767, 2782, 2804, 2857, 2939, 3302, 3308, 3789, 3797, 3882, 4052, 4056, 4162, 4249, 4319, 5770, 5811b		4052, 4056
20.	590-18-1	2-Butene, (*Z*)- 	199, 544–546, 604, 605, 1140, 1153, 1154, 2060, 2310, 2767, 2782, 2804, 2857, 2939, 2946, 3302, 3308, 3769, 3797, 3882, 4052, 4056, 4162, 4249, 4319, 5770, 5811b		4052, 4056
21.	563-79-1	2-Butene, 2,3-dimethyl- $(H_3C)_2{=}C{=}C{=}(CH_3)_2$	568b, 1140, 1154, 2944, 3308, 3478, 4249		
22.	513-35-9	2-Butene, 2-methyl- $(H_3C)_2{=}C{=}CH\text{-}CH_3$	199, 604, 1140, 1153, 1154, 1374, 1375, 1375b, 2060, 2310, 2767, 2782, 2804, 2946, 3254, 3302, 3308, 3557, 3769, 3797, 4249, 5770, 5811b	5811b	
23.	689-97-4	1-Buten-3-yne $H_2C{=}CH\text{-}C{\equiv}CH$	1140, 1243, 2946, 3302, 3769, 3797, 4249, 5811b		
24.		Butyne $H\text{-}(CH_2)_n\text{-}C{\equiv}C\text{-}(CH_2)_{(2-n)}\text{-}H$	642, 2946, 3479, 4249		
25.	107-00-6	1-Butyne $H_3C\text{-}CH_2\text{-}C{\equiv}CH$	1140, 2946, 3302, 3769, 3797, 3882, 4249, 5034		
26.	503-17-3	2-Butyne $H_3C\text{-}C{\equiv}C\text{-}CH_3$	3882	3797, 4249	
27.	502-65-8	ψ,ψ-Carotene {lycopene} 	1572	367, 1572, 3218	

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

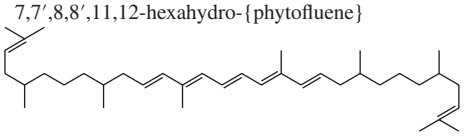
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
28.	540-04-5	ψ,ψ-Carotene, 7,7′,8,8′,11,11′,12,12′-octahydro-{phytoene}		367, 1156, 1157, 2939, 3194, 3797, 3973, 3974a, 4090, 4249	
29.	540-05-6 27664-65-9	ψ,ψ-Carotene, 7,7′,8,8′,11,12-hexahydro-{phytofluene} 		1156, 1157, 2939, 3194, 3797, 3973, 3974a, 4090, 4249, 5811	
30.	872-05-9	1-Decene $H_2C{=}CH\text{-}(CH_2)_7\text{-}CH_3$	568b, 1140, 1144, 1419, 2543, 2570, 3797, 4249, 5811b	404, 568b, 4249	
31.		1-Decene, 5-methyl- $H_2C{=}CH\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}(CH_2)_4\text{-}CH_3$	1882, 4249		
32.	6816-17-7	2-Decene $H_3C\text{-}CH{=}CH\text{-}(CH_2)_6\text{-}CH_3$	3797	4249	
33.	29730-67-4	Docosene	5811, 5811a, 5811b		
34.	1599-67-3	1-Docosene $H_3C\text{-}(CH_2)_{19}\text{-}CH{=}CH_2$	1144, 2387, 2570, 2601a, 2769, 3797, 4249, 5811b		2387
35.		1-Docosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{19}\text{-}CH_3$	1144		
36.		2-Docosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{18}\text{-}CH_3$	1144, 3797		
37.		2-Docosene, (*E*)-	1144, 3797		
38.		2-Docosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{18}\text{-}CH_3$	1144		
39.		2-Docosene, 20-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{16}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
40.		2-Docosene, 20-methyl-, (*E*)-	1144		
41.		2-Docosene, 21-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{17}\text{-}CH(CH_3)_2$	1144		
42.		2-Docosene, 21-methyl-, (*E*)-	1144		
43.	502-61-4	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (*E,E*)- {α-farnesene} $H_2C{=}CH\text{-}C(CH_3){=}CH\text{-}[CH_2\text{-}CH_2\text{-}C(CH_3){=}CH]_2\text{-}H$	343, 2731, 2735, 3302, 4249, 4570a, 5811b	131, 4249	
44.	18794-84-8	1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (*E*)- {β-farnesene} $H\text{-}[CH_2\text{-}C(CH_3){=}CH\text{-}CH_2\text{-}]_2\text{-}CH_2\text{—}(=CH_2\text{-})\text{-}CH{=}CH_2$	343, 2731, 2735, 3219, 3297, 3308, 3797, 4249	5811b	
45.	3899-18-1	2,6,10-Dodecatriene, 2,6,10-trimethyl-, (*E,E*)-	1375		
46.		2,6,10-Dodecatriene, 3,7,11-trimethyl- = 2,6,10-Dodecatriene, 2,6,10-trimethyl- $H\text{-}[CH_2\text{-}CH(CH_3){=}CH\text{-}CH_2]_3\text{-}H$	900, 901, 1375, 4249		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
47.	25378-22-7	Dodecene	2387, 2543, 2570, 2735, 4249	937, 4249	
48.	112-41-4	1-Dodecene $H_2C{=}CH\text{-}(CH_2)_9\text{-}CH_3$	1144, 2387, 2767, 3469, 3557, 3797, 4249		2387
49.	16435-49-7	1-Dodecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_9\text{-}CH_3$	1144		
50.		2-Dodecene $H_3C\text{-}CH{=}CH\text{-}(CH_2)_8\text{-}CH_3$	3797		
51.		2-Dodecene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_8\text{-}CH_3$	1144		
52.		2-Dodecene, 10-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_6\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
53.		2-Dodecene, 10-methyl-, (*E*)-	1144		
54.		2-Dodecene, 11-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}CH(CH_3)_2$	1144		
55.		2-Dodecene, 11-methyl-, (*E*)-	1144		
56.	110053-56-0	2,6,10,14,18,22,26,30-Dotriacontaoctaene, 3,7,11,15,19,23,27-heptamethyl-	5811		
57.	66309-89-5	2,6,10,14,18,22,26,30-Dotriacontaoctaene, 2,6,10,14,18,22,26,30-octamethyl-, (all-*E*)-	1586, 2769, 4249		
58.	85792-05-8	Dotriacontene	5811b, 1E01		
59.	18435-55-7	1-Dotriacontene $H_2C{=}CH\text{-}(CH_2)_{29}\text{-}CH_3$	3469, 4249		
60.		2-Dotriacontene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{28}\text{-}CH_3$	1144		
61.		2-Dotriacontene, (*E*)-	1144		
62.	7431-92-7	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl-, (all-*E*)- $H\text{-}[CH_2\text{-}C(CH_3){=}CH\text{-}CH_2]_5\text{-}H$	900, 1375, 1375b, 1586, 2601a, 3308		
63.	75581-03-2	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl-	2601a		
64.		2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl- {isomer}	2601a		
65.	27400-78-8	Eicosene	5811, 5811a, 5811b, 1E01		
66.	3452-07-1	1-Eicosene $H_2C{=}CH\text{-}(CH_2)_{17}\text{-}CH_3$	1144, 2387, 2570, 2769, 3797, 4249, 5811b, 1E01	404	2387
67.		1-Eicosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{17}\text{-}CH_3$	1144		
68.		2-Eicosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{16}\text{-}CH_3$	1144		
69.	42448-85-2	2-Eicosene, (*E*)-	1144, 3797		
70.		2-Eicosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{16}\text{-}CH_3$	1144		
71.		2-Eicosene, 18-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{14}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
72.		2-Eicosene, 18-methyl-, (*E*)-	1144		
73.		2-Eicosene, 19-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{15}\text{-}CH(CH_3)_2$	1144		

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
74.		2-Eicosene, 19-methyl-, (*E*)-	1144		
75.	74-85-1	Ethene {ethylene} $H_2C{=}CH_2$	85, 141, 143, 147, 151, 173a, 216, 239, 298, 544–546, 604, 605, 710, 722, 966, 1099, 1140, 1243, 1365, 1375a, 1377, 1437, 1445, 1472, 1664, 1821, 1842, 2060, 2079, 2252, 2270, 2293, 2310, 2583, 2634, 2782, 2799a, 2804, 2857, 2866, 2909, 2939, 2942, 2946, 3059, 3105, 3255, 3302, 3308, 3493, 3729, 3797, 3880, 3882, 3883, 3888, 3901, 3939, 4052, 4056, 4057, 4135, 4162, 4249, 4319, 4393, 5835, 5811b	2913a, 3633, 3973, 5811b	1228, 1375a, 1377, 3901, 4052, 4056
76.	74-86-2	Ethyne {acetylene} $HC{\equiv}CH$	85, 112, 143, 151, 172, 216, 239, 394, 604, 621, 722, 966, 1067, 1119, 1140, 1202, 1375a, 1377, 1437, 1472, 1664, 1744, 1842, 1966, 2060, 2079, 2142, 2170, 2270, 2583, 2781, 2782, 2799a, 2804, 2857, 2868, 2909, 2939, 2942, 2946, 3059, 3255, 3302, 3308, 3493, 3692, 3729, 3797, 3876, 3901, 4005–4007, 4052, 4056, 4104, 4162, 4249, 4319, 4354, 4393, 5079, 5154, 5512		1228, 1375a, 1377, 4052, 4056
77.	27400-79-9	Heneicosene	5811, 5811a		
78.	1599-68-4	1-Heneicosene $H_3C\text{-}(CH_2)_{18}\text{-}CH{=}CH_2$	1144, 2387, 2570, 2769, 3797, 4249		2387
79.		1-Heneicosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{18}\text{-}CH_3$	1144		
80.		2-Heneicosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{17}\text{-}CH_3$	3797		
81.		2-Heneicosene, (*E*)-	1144		
82.		2-Heneicosene, 2-methyl- $H_3C\text{-}C(CH_3)H{=}CH\text{-}(CH_2)_{17}\text{-}CH_3$	1144		
83.		2-Heneicosene, 19-methyl-,(*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{15}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	4249		
84.		2-Heneicosene, 19-methyl-, (*E*)-	1144		
85.		2-Heneicosene, 20-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{16}\text{-}CH(CH_3)_2$	4249		
86.		2-Heneicosene, 20-methyl-, (*E*)-	4249		
87.	77046-64-1	Hentriacontene	5811b, 1E01		
88.	18435-54-6	1-Hentriacontene $H_3C\text{-}(CH_2)_{28}\text{-}CH{=}CH_2$	3469, 4249		
89.		1-Hentriacontene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{28}\text{-}CH_3$	1144		
90.		2-Hentriacontene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{27}\text{-}CH_3$	1144		
91.		2-Hentriacontene, (*E*)-	1144		
92.		2-Hentriacontene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{27}\text{-}CH_3$	1144		
93.		2-Hentriacontene, 29-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{25}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
94.		2-Hentriacontene, 29-methyl-, (*E*)-	1144		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
95.		2-Hentriacontene, 30-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{26}$-CH$(CH_3)_2$	1144		
96.		2-Hentriacontene, 30-methyl-, (*E*)-	1144		
97.	67537-80-8	Heptacosene	2601a, 5811b, 1E01		
98.	15306-27-1	1-Heptacosene H_3C-$(CH_2)_{24}$-CH═CH_2	3469, 4249		
99.		2-Heptacosene, (*Z*)- H_3C-CH═CH-$(CH_2)_{23}$-CH_3	1144		
100.		2-Heptacosene, (*E*)-	1144		
101.		2-Heptacosene, 2-methyl- H_3C-C(CH_3)═CH-$(CH_2)_{23}$-CH_3	1144		
102.		2-Heptacosene, 25-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{21}$-CH(CH_3)-CH_2-CH_3	1144		
103.		2-Heptacosene, 25-methyl-, (*E*)-	1144		
104.		2-Heptacosene, 26-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{22}$-CH$(CH_3)_2$	1144		
105.		2-Heptacosene, 26-methyl-, (*E*)-	1144		
106.	26266-05-7	Heptadecene H-$(CH_2)_{15-n}$-CH═CH-$(CH_2)_n$-H	2543, 2570, 2731, 2735, 3226, 3557, 4249	2339a	
107.	6765-39-5	1-Heptadecene H_3C-$(CH_2)_{14}$-CH═CH_2	1144, 2735, 2387, 2845, 3557, 4249		2387
108.		1-Heptadecene, 2-methyl- H_2C═C(CH_3)-$(CH_2)_{14}$-CH_3	1144		
109.		2-Heptadecene, (*Z*)- H_3C-CH═CH-$(CH_2)_{13}$-CH_3	1144		
110.		2-Heptadecene, (*E*)-	1144, 3797		
111.	13287-12-2	2-Heptadecene, 2-methyl- H_3C-C(CH_3)═CH-$(CH_2)_{13}$-CH_3	1144		
112.		2-Heptadecene, 15-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{11}$-CH(CH_3)-CH_2-CH_3	1144		
113.		2-Heptadecene, 15-methyl-, (*E*)-	1144		
114.		2-Heptadecene, 16-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{12}$-CH$(CH_3)_2$	1144		
115.		2-Heptadecene, 16-methyl-, (*E*)-	1144		
116.	36232-39-0	2-Heptadecene, 4-methylene-8,12,16-trimethyl- H_3C-CH═CH-C(═CH_2)-CH_2-{$(CH_2)_2$-CH(CH_3)-CH_2}$_3$-H	2731, 2735, 3557, 4249, 5811b		
117.	74630-29-8	1,5-Heptadiene, 3,3,5-trimethyl- H_3C-CH═C(CH_3)-CH_2-C$(CH_3)_2$-CH═CH_2		404	
118.	74421-05-9	2,4-Heptadiene, 2,4-dimethyl-	5770		
119.	4634-87-1	2,4-Heptadiene, 2,6-dimethyl-	4570a		
120.	3511-27-1	1,5-Heptadien-3-yne H_3C-CH═CH-C≡C-CH═CH_2	568b, 1153, 1154, 4249, 5811b		
121.	1632-16-2	Heptane, 3-methylene- H_3C-$(CH_2)_3$-C(═CH_2)-CH_2-CH_3		4249, 5811b	
122.	24587-25-5	1,3,5-Heptatriene	4570a		
123.		1,3,5-Heptatriene, 1.6-dimethyl-	5770		

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
124.		1,3,5-Heptatriene, 1.6-dimethyl- {isomer}	5770		
125.		1,3,6-Heptatriene, 2.5.6-trimethyl-	5770		
126.		Heptene	5777		
127.	592-76-7	1-Heptene $H_2C{=}CH\text{-}(CH_2)_4\text{-}CH_3$	348, 1472, 3449, 4249, 5770, 5811b		
128.		1-Heptene, 2-methyl-	5770		
129.	592-77-8	2-Heptene $H_3C\text{-}CH{=}CH\text{-}(CH_2)_3\text{-}CH_3$	112, 348, 1472, 4249, 5811b		
130.	14686-13-6	2-Heptene, (*E*)-	5811, 5811a, 5811b		
131.	628-71-7	1-Heptyne $H_3C\text{-}(CH_2)_4\text{-}C{\equiv}CH$	3882		
132.	2586-89-2	3-Heptyne $H_3C\text{-}(CH_2)_2\text{-}C{\equiv}C\text{-}CH_2\text{-}CH_3$	156, 157, 2628, 2629, 2636, 2799a, 4249		
133.	84808-91-9	Hexacosene	5811, 5811a, 5811b, 1E01		
134.	18835-33-1	1-Hexacosene $H_2C{=}CH\text{-}(CH_2)_{23}\text{-}CH_3$	1144, 3469, 4249		
135.		1-Hexacosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{23}\text{-}CH_3$	1144		
136.		2-Hexacosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{22}\text{-}CH_3$	1144		
137.		2-Hexacosene, (*E*)-	1144, 3797		
138.		2-Hexacosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{22}\text{-}CH_3$	1144		
139.		2-Hexacosene, 24-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{20}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
140.		2-Hexacosene, 24-methyl-, (*E*)-	1144		
141.		2-Hexacosene, 25-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{21}\text{-}CH(CH_3)_2$	1144		
142.		2-Hexacosene, 25-methyl-, (*E*)-	1144		
143.	30917-33-0 100210-90-0	1,3-Hexadecadiene, 2,6,10,14-tetramethyl- $H[CH_2CH_2CH(CH_3)CH_2]_3\text{-}CH{=}CH\text{-}C(CH_3){=}CH_2$	2939, 3247, 3251, 3302, 4249, 5811b		
144.	21980-71-2	1,3-Hexadecadiene, 3,7,11,15-tetramethyl-{phytadiene} $H[CH_2CH(CH_3)CH_2CH_2]_3\text{-}CH{=}CH\text{-}C(CH_3){=}CH_2$	900, 2731, 2735, 2767, 2939, 3247, 3251, 3295, 3302, 3396, 3557, 3797, 3857, 4249		
145.		1,3-Hexadecadiene, 2,6,105-trimethyl-	2767, 4249		
146.		2.4-Hexadecadiene, 3,7,11,15-tetramethyl-		3345, 4249, 4680	
147.	36232-38-9	Hexadecane, 2,6,10-trimethyl-14-methylene- $H\text{-}\{CH_2\text{-}CH(CH_3)\text{-}(CH_2)_2\}_3\text{-}CH_2\text{-}C(=CH_2)\text{-}CH_2\text{-}CH_3$	2731, 2735, 4249, 5811b		
148.	34083-18-6	2,6,10,14-Hexadecatetraene, 2,6,10,14-tetramethyl- $H\text{-}[CH_2\text{-}C(CH_3){=}CH\text{-}CH_2]_4\text{-}H$	900, 1375, 1375b, 1586, 3219, 3308, 3797, 4249, 4562		
149.	7481-01-8	2,6,10,14-Hexadecatetraene, 2,6,10,14-tetramethyl-, (*E,E*)-		5811b	
150.	70901-63-2	1,6,10,14-Hexadecatetraene, 7,11,15-trimethyl-3-methylene-, (*E,E*)-		1156, 1248, 2917a, 3547, 4090, 4249, 4927	
151.	26952-14-7	Hexadecene	2543, 2570, 2773, 4249		
152.	629-73-2	1-Hexadecene {1-cetene} $H_2C{=}CH\text{-}(CH_2)_{13}\text{-}CH_3$	1144, 2387, 2769, 3797, 4249	404, 2339a, 3797	2387

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
153.	61868-19-7	1-Hexadecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{13}\text{-}CH_3$	1144		
154.	71278-20-1	1-Hexadecene, 2,6,10-trimethyl- $H_2C{=}CH\text{-}CH(CH_3)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)CH_2\}_2\text{-}(CH_2)_3\text{-}CH_3$	1282, 1283, 2767, 4249		
155.	504-96-1	1-Hexadecene, 3-methylene-7,11,15-trimethyl- {neophytadiene} $H_2C{=}CH\text{-}C(=CH_2)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)CH_2\}_3\text{-}H$	84, 172, 173a, 239, 337, 568b, 636, 723, 1138, 1063–1066, 1068–1074, 1089a, 1099, 1100, 1307, 1332, 1333, 1338, 1339, 1348, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1423, 1427, 1437, 1444, 1445, 1586, 1598, 1615, 1637, 1651, 1842, 1882, 1887a, 1973, 2387, 2493, 2506, 2507, 2524a, 2543, 2545, 2570, 2601a, 2630, 2683, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 2857, 2874, 2939, 3059, 3251, 3255, 3295, 3302, 3397, 3454, 3457, 3557, 3559, 3608, 3779, 3795, 3797, 3826, 4103, 4249, 4271, 4317, 4336, 4418, 5512, 5706, 5811b	120, 84, 330, 404, 524, 537, 543a, 568b, 840, 908, 911, 984, 1307, 1550, 1590a, 1598, 1615, 1651, 1751, 1893b, 1973, 1978, 2260, 2336, 2338, 2339a, 2386, 2389, 2394a, 2529, 2544, 2611, 2914, 2917a, 2939, 3059, 3188, 3194, 3198, 3215, 3219, 3295, 3329, 3345, 3350, 3430, 3435, 3461, 3470, 3472, 3482, 3493, 3511, 3543, 3545, 3547, 3549, 3560, 3561, 3604, 3605, 3608, 3609, 3611, 3613b, 3616, 3755, 3797, 3811, 3905, 3924, 3973, 3974a, 3976, 4098a, 4103, 4236, 4249, 4276, 4336, 5056, 5682, 5867	1332 (0), 1333, 1360, 1375a, 2387, 2506 (0), 2507 (0)

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
156.	30221-44-4	1-Hexadecene, 3,7,11,15-tetramethyl- {phytene-1}		3430, 5811	
157.		2-Hexadecene, (*Z*)- H_3C-CH═CH-$(CH_2)_{12}$-CH_3	1144		
158.	26741-29-7	2-Hexadecene, (*E*)-	3797		
159.	73120-40-8	2-Hexadecene, 2-methyl- H_3C-C(CH_3)═CH-$(CH_2)_{12}$-CH_3	1144		
160.		2-Hexadecene, 14-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{10}$-CH(CH_3)-CH_2-CH_3	1144		
161.		2-Hexadecene, 14-methyl-, (*E*)-	1144		
162.		2-Hexadecene, 15-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{11}$-CH(CH_3)$_2$	1144		
163.		2-Hexadecene, 15-methyl-, (*E*)-	4249		
164.	51806-25-8	4-Hexadecene, 3-methylene-7,11,15-trimethyl- H_3C-CH_2-C(═CH_2)-CH═CH-CH_2-CH(CH_3)-CH_2-{$(CH_2)_2$-CH(CH_3)-CH_2}$_2$-H		4249, 4434	
165.	54612-24-7	Hexadiene, dimethyl-	157, 4249		
166.		Hexadiene, methyl-	2506, 2507, 4249		2506, 2507
167.	592-48-3	1,3-Hexadiene	568b, 4249		
168.	62338-07-2	1,3-Hexadiene, 2,5-dimethyl-3-ethyl-	4570a		
169.	592-45-0	1,4-Hexadiene	568b, 4249		
170.	927-97-9	1,4-Hexadiene, 2,5-dimethyl- H_2C═C(CH_3)-CH_2-CH═C(CH_3)-CH_3	1153, 1154		
171.	592-42-7	1,5-Hexadiene	568b, 4249, 5811b		
172.	592-46-1	2,4-Hexadiene	568b, 4249, 5770, 5811b		
173.		2,4-Hexadiene {isomer}	568b, 4249		
174.	764-13-6	2,4-Hexadiene, 2,5-dimethyl- H_3C-C(CH_3)═CH-CH═C(CH_3)-CH_3	568b, 1153, 1154, 4249, 5811b		
175.	21293-01-6	2,4-Hexadiene, 3,4-dimethyl-	4570a		
176.	10420-90-3	1,3-Hexadien-5-yne H_2C═CH-CH═CH-C≡CH	348, 1153, 1154, 4249, 5811b		
177.	821-08-9	1,5-Hexadien-3-yne {divinylacetylene} H_2C═CH-CH═CH-C≡CH	1348–1350, 1354, 1375a, 1586, 1589, 2543, 2765, 2767, 2777, 4249		1354, 1375a
178.		Hexadiyne	5777		
179.	70322-25-7 71278-21-2	1,3,6,10,14,18,22,26,30,34-Hexatriacontadecaene, 3,7,11,15,19,23,27,31,35-nonamethyl-{solanesene}	3059, 3251, 3295, 3297, 3302, 3797, 4249, 4562	3059, 3616, 3971, 4275 5811, 5811b	
180.	71278-22-3	1,6,10,14,18,22,26,30,34-Hexatriacontanonaene, 7,11,15,19,23,27,31,35-octamethyl-3-methylene-	3059, 3251, 3295, 3297, 3302, 3797, 4249		
181.	66327-99-9	2,6,10,14,18,22,26,30,34-Hexatriacontanonaene, 2,6,10,14,18,22,26,30,34-nonamethyl-, (all-*E*)-	1586, 2769, 4249		
182.	2235-12-3	1,3,5-Hexatriene H_2C═CH-CH═CH-CH═CH_2	200, 329, 1153, 1154, 4249, 5811b		
183.	41233-72-1	1,3,5-Hexatriene, 2-methyl-	4570a		
184.	24587-26-6	1,3,5-Hexatriene, 3-methyl-	4570a		
185.	25264-93-1	Hexene H-$(CH_2)_n$-CH═CH-$(CH_2)_{(4-n)}$-H	1140, 1637, 2767, 4249, 5034		
186.	592-41-6	1-Hexene H_3C-$(CH_2)_3$-CH═CH_2	329, 568b, 1140, 1153, 1154, 1313, 1472, 2767, 2944, 3219, 3308, 3797, 4249, 5811b		
187.	6094-02-6	1-Hexene, 2-methyl-	5811		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
188.	3404-61-3	1-Hexene, 3-methyl-	5811		
189.	3769-23-1	1-Hexene, 4-methyl-	5811		
190.	3524-73-0	1-Hexene, 5-methyl- $(H_3C)_2$═CH-$(CH_2)_2$-CH═CH_2	4249, 5811b		
191.	592-43-8	2-Hexene	5811		
192.	4050-45-7	2-Hexene, (*E*)- H_3C-$(CH_2)_2$-CH═CH-CH_3	112, 568b, 1140, 2697, 2944, 3308, 4249, 5811b		
193.	7688-21-3	2-Hexene, (*Z*)-	1140, 2387, 2944, 3308		
194.	3404-78-2	2-Hexene, 2,5-dimethyl- H_3C-CH(CH_3)-CH_2-CH═C(CH_3)-CH_3	1153, 1154, 4249, 5811b		
195.	2738-19-4	2-Hexene, 2-methyl- H_3C-$(CH_2)_2$-CH═C(CH_3)-CH_3	1153, 1154, 4249, 5811b		
196.	3404-62-4	2-Hexene, 5-methyl- H_3C-CH(CH_3)-CH_2-CH═CH-CH_3	1472		
197.	592-47-2	3-Hexene H_3C-CH_2-CH═CH-CH_2-CH_3	1153, 1154, 2944, 4249, 5811b		
198.	13269-52-8	3-Hexene, (*E*)-	568b, 1154, 2944, 3219, 3308, 4249	984	
199.	7642-09-3	3-Hexene, (*Z*)-	2944, 3308		
200.	26856-30-4	Hexyne H-$(CH_2)_n$-C≡C-$(CH_2)_{(4-n)}$-H	1154, 1884, 4249		
201.	693-02-7	1-Hexyne HC≡C-$(CH_2)_3$-CH_3	1153, 1154, 5811b		
202.	2203-80-7	1-Hexyne, 5-methyl- HC≡C-$(CH_2)_2$-CH$(CH_3)_2$	2769, 4249		
203.	764-35-2	2-Hexyne H_3C-C≡C-$(CH_2)_2$-CH_3	1153, 1154, 4249, 5811b		
204.	53566-37-3	2-Hexyne, 5-methyl- H_3C-C≡C-CH_2-CH$(CH_3)_2$	2767, 4249		
205.	928-49-4	3-Hexyne H_3C-CH_2-C≡C-CH_2-CH_3	157, 1153, 1154, 4249, 5811b		
206.	18835-35-3	1-Nonacosene H_2C═CH-$(CH_2)_{26}$-CH_3	3469, 4249		
207.		1-Nonacosene, 2-methyl- H_2C═C(CH_3)-$(CH_2)_{26}$-CH_3	1144		
208.		2-Nonacosene, (*Z*)- H_3C-CH═CH-$(CH_2)_{25}$-CH_3	1144		
209.		2-Nonacosene, (*E*)-	1144		
210.		2-Nonacosene, 2-methyl- H_3C-C(CH_3)═CH-$(CH_2)_{25}$-CH_3	1144		
211.		2-Nonacosene, 27-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{23}$-CH(CH_3)-CH_2-CH_3	1144		
212.		2-Nonacosene, 27-methyl-, (*E*)-	1144		
213.		2-Nonacosene, 28-methyl-, (*Z*)- H_3C-CH═CH-$(CH_2)_{24}$-CH$(CH_3)_2$	1144		
214.		2-Nonacosene, 28-methyl-, (*E*)-	1144		
215.	27400-77-7	Nonadecene H-$(CH_2)_n$-CH═CH-$(CH_2)_{(17-n)}$-H	1427, 2387, 2506, 2507, 2570, 3226, 3557, 4249, 5811b		2387, 2506, 2507
216.	18435-45-5	1-Nonadecene H_2C═CH-$(CH_2)_{16}$-CH_3	1144, 1427, 3797, 4249	404	

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
217.	52254-50-9	1-Nonadecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{16}\text{-}CH_3$	1144		
218.		2-Nonadecene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{15}\text{-}CH_3$	1144		
219.	94434-40-9	2-Nonadecene, (*E*)-	1144, 3797		
220.	110746-39-9	2-Nonadecene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{15}\text{-}CH_3$	1144		
221.		2-Nonadecene, 17-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{13}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
222.		2-Nonadecene, 17-methyl-, (*E*)-	1144		
223.		2-Nonadecene, 18-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{14}\text{-}CH(CH_3)_2$	1144		
224.		2-Nonadecene, 18-methyl-, (*E*)-	1144		
225.	71030-52-9	Nonadiene		84, 4249	
226.	51655-64-2	Nonane, 3-methylene-	4570a		
227.	124-11-8	1-Nonene $H_3C\text{-}(CH_2)_6\text{-}CH{=}CH_2$	568b, 1313, 1472, 3797, 4249, 5770, 5811b		
228.	2216-39-8	2-Nonene $H_3C\text{-}(CH_2)_5\text{-}CH{=}CH\text{-}CH_3$	3797		
229.	17003-99-5	2-Nonene, 3-methyl-	4570a		
230.	53966-53-3	3-Nonene, 2-methyl- $H_3C\text{-}(CH_2)_4\text{-}CH{=}CH\text{-}CH{=}(CH_3)_2$	4249		
231.	2198-23-4	4-Nonene	5770		
232.	3452-09-3	1-Nonyne $H_3C\text{-}(CH_2)_6\text{-}C{\equiv}CH$	1822, 4249		
233.	66328-00-5	2,6,10,14,18,22,26-Octacosaheptaene, 2,6,10,14,18,22,26-heptamethyl-, (all-*E*)-	1586, 2769, 4249		
234.	18835-34-2	1-Octacosene $H_3C\text{-}(CH_2)_{25}\text{-}CH{=}CH_2$	1144, 3469, 3797		
235.		1-Octacosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{25}\text{-}CH_3$	1144		
236.		2-Octacosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{24}\text{-}CH_3$	1144		
237.		2-Octacosene, (*E*)-	1144, 3797, 4249		
238.		2-Octacosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{24}\text{-}CH_3$	1144		
239.		2-Octacosene, 26-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{23}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
240.		2-Octacosene, 26-methyl-, (*E*)-	1144		
241.		2-Octacosene, 27-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{23}\text{-}CH(CH_3)_2$	1144		
242.		2-Octacosene, 27-methyl-, (*E*)-	1144		
243.	27070-58-2	Octadecene $H\text{-}(CH_2)_n\text{-}CH{=}CH\text{-}(CH_2)_{(16-n)}\text{-}H$	2570, 2767, 4249		
244.	112-88-9	1-Octadecene $H_2C{=}CH\text{-}(CH_2)_{15}\text{-}CH_3$	1144, 1472, 2339a, 2387, 3469, 3797, 4249, 5811b		2387
245.	61868-20-0	1-Octadecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{15}\text{-}CH_3$	1144		
246.		2-Octadecene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{14}\text{-}CH_3$	1144		
247.	7206-18-0	2-Octadecene, (*E*)-	1144, 3797		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
248.		2-Octadecene, 2-methyl- $H_3C\text{-}C(CH_3)=CH\text{-}(CH_2)_{14}\text{-}CH_3$	1144		
249.		2-Octadecene, 16-methyl-, (*Z*)- $H_3C\text{-}CH=CH\text{-}(CH_2)_{12}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
250.		2-Octadecene, 16-methyl-, (*E*)-	1144		
251.		2-Octadecene, 17-methyl-, (*Z*)- $H_3C\text{-}CH=CH\text{-}(CH_2)_{13}\text{-}CH(CH_3)_2$	1144		
252.		2-Octadecene, 17-methyl-, (*E*)	1144		
253.	71899-42-8	5-Octadecyne $H_3C\text{-}(CH_2)_3\text{-}C\equiv C\text{-}(CH_2)_{11}\text{-}CH_3$		404	
254.	71607-91-5	1,6-Octadiene, 4,7-dimethyl- {2,5-dimethyl-2,7-octadiene} $H_2C=CH\text{-}C(CH_3)=CH\text{-}CH_2\text{-}CH=C(CH_3)_2$	1153, 4249		
255.	123-35-3	1,6-Octadiene, 7-methyl-3-methylene- {myrcene} $H_2C=CH\text{-}C(=CH_2)\text{-}(CH_2)_2\text{-}CH=C(CH_3)_2$	568b, 1140, 1419, 4249, 5811b	568b, 909, 1156, 2336, 2339a, 2389, 2544, 3971, 4090, 4249, 5811b	
256.	2216-70-8	2,4-Octadiene, 7-methyl- $H_3C\text{-}CH=CH\text{-}CH=CH\text{-}CH_2\text{-}CH(CH_3)_2$	1153, 1154, 4249, 5811b		
257.	40195-09-3	1,6-Octadiene, 2,7-dimethyl- = {2,7-dimethyl-2,7-octadiene} $H_2C=C(CH_3)\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH=C(CH_3)_2$	4570a, 5770		
258.	128241-35-0	1,6-Octadiene, 3,7-dimethyl- = {2,6-dimethyl-2,7-octadiene} $H_2C=CH\text{-}CH(CH_3)\text{-}CH_2\text{-}\ CH_2\text{-}CH=C(CH_3)_2$	5770		
259.	71607-92-6	2,5-Octadiene, 7-methyl- $H_3C\text{-}CH=CH\text{-}CH_2\text{-}CH=CH\text{-}CH(CH_3)_2$	1153, 1154, 4249		
260.	2792-39-4	2,6-Octadiene, 2,6-dimethyl-	4570a, 5770		
261.	18476-57-8	2,6-Octadiene, 4,5-dimethyl-	5770		
262.	929-20-4	1,3,6-Octatriene $H_2C=CH\text{-}CH=CH\text{-}CH_2\text{-}CH=CH\text{-}CH_3$	4249		
263.	13877-91-3	1,3,6-Octatriene, 3,7-dimethyl- {ocimene} $H_2C=CH\text{-}C(CH_3)=CH\text{-}CH_2\text{-}CH=C(CH_3)_2$	1365, 1371, 3266, 4249, 4579	1053, 3266, 4249	
264.	3779-61-1	1,3,6-Octatriene, 3,7-dimethyl-, (*E*)-	4249	4249, 5811b	
265.	673-84-7	2,4,6-Octatriene, 2,6-dimethyl- {alloöcimene} $(H_3C)_2=C=CH\text{-}CH=CH\text{-}C(CH_3)=CH\text{-}CH_3$	2597, 3302, 4249, 4316		
266.	71607-54-0	Octene, methyl-	199, 4249		
267.	111-66-0	1-Octene {caprylene} $H_2C=CH\text{-}(CH_2)_5\text{-}CH_3$	348, 568b, 1472, 3797, 4249, 5770, 5811b		
268.	4588-18-5	1-Octene, 2-methyl- $H_2C=C(CH_3)\text{-}(CH_2)_5\text{-}CH_3$	200, 1153, 4249, 5811b		
269.	111-67-1	2-Octene $H_3C\text{-}CH=CH\text{-}(CH_2)_4\text{-}CH_3$	1153, 4249		
270.	592-99-4	4-Octene $H_3C\text{-}(CH_2)_2\text{-}CH=CH\text{-}(CH_2)_2\text{-}CH_3$	4249		
271.		Octyne	5777		
272.	30551-31-6	Pentacosene	2570, 2769, 3226, 3557, 4249		
273.	16980-85-1	1-Pentacosene $H_3C\text{-}(CH_2)_{22}\text{-}CH=CH_2$	1144, 2570, 2769, 3557, 3797, 4249		

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
274.		1-Pentacosene, 2-methyl- $H_2C{=}CH\text{-}(CH_2)_{22}\text{-}CH_3$	1144		
275.		2-Pentacosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{21}\text{-}CH_3$	1144		
276.		2-Pentacosene, (*E*)-	1144, 3797, 4249		
277.		2-Pentacosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{21}\text{-}CH_3$	1144		
278.		2-Pentacosene, 23-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{19}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
279.		2-Pentacosene, 23-methyl-, (*E*)-	1144		
280.		2-Pentacosene, 24-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{20}\text{-}CH(CH_3)_2$	1144		
281.		2-Pentacosene, 24-methyl-, (*E*)-	1144		
282.		Pentadecadiene, 2,6,10,14-tetramethyl-	1282, 4249		
283.	27251-68-9	Pentadecene $H\text{-}(CH_2)_n\text{-}CH{=}CH\text{-}(CH_2)_{(13-n)}\text{-}H$	1427, 2543, 2570, 2773, 4248, 4249		
284.	13360-61-7	1-Pentadecene $H_3C\text{-}(CH_2)_{12}\text{-}CH{=}CH_2$	1144, 2387, 2731, 2735, 3797, 4249		2387
285.	29833-69-0	1-Pentadecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{11}\text{-}CH_3$	1144		
286.		2-Pentadecene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{11}\text{-}CH_3$	1144		
287.	74392-36-2	2-Pentadecene, (*E*)-	3797		
288.		2-Pentadecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{12}\text{-}CH_3$	1144		
289.		2-Pentadecene, 13-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_9\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
290.		2-Pentadecene, 13-methyl-, (*E*)-	4249		
291.		2-Pentadecene, 14-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{10}\text{-}CH(CH_3)_2$	1144		
292.		2-Pentadecene, 14-methyl-, (*E*)-	4249		
293.	2140-82-1 60976-73-0 100404-00-0	1-Pentadecene, 2,6,10,14-tetramethyl-{norphytene} $H_2C{=}C(CH_3)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\}_3\text{-}H$	1360, 1371, 1663, 2524a, 2630, 2761, 2762, 2765, 2766, 2777, 3302, 3797, 4249	3971, 5811b	1360
294.	36232-37-8	6-Pentadecene, 2,6,10,14-tetramethyl- $(H_3C)_2CH\text{-}(CH_2)_3\text{-}C(CH_3){=}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\}_2\text{-}H$	2731, 2735, 4249, 5811b		
295.	41050-31-1	Pentadiene	1140, 1348–1350, 1354, 1375a, 1412–1414, 1416, 1418, 1586, 1589, 2543, 2570, 2765, 2767, 2777, 3308, 3692, 4005–4007, 4104, 4249, 5811b		1354, 1375a
296.	51064-12-1	Pentadiene, methyl-	1637, 5811a		
297.	591-95-7	1,2-Pentadiene {ethylallene} $H_3C\text{-}CH_2\text{-}CH{=}C{=}CH_2$	605, 1140, 1153, 1154, 3308, 3797, 4249, 5811b		
298.	504-60-9	1,3-Pentadiene {piperylene} $H_3C\text{-}CH{=}CH\text{-}CH{=}CH_2$	299, 314, 568b, 722, 1243, 1063–1066, 1068–1074, 1348–1350, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1419, 1586, 1589, 2003, 2543, 2545, 2570, 2634, 2767, 2822, 2946, 3254, 3302, 3557, 3797, 4249, 5034, 5770, 5811b	5811b	1375a, 1377, 1378
299.	2004-70-8	1,3-Pentadiene, (*E*)-	329, 605, 1140, 1153, 1154, 2777, 2782, 2946, 3308, 4249		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
300.	1574-41-0	1,3-Pentadiene, (*Z*)-	329, 605, 1140, 2782, 2804, 3308, 4249		
301.	1118-58-7	1,3-Pentadiene, 2-methyl- H_3C-CH═CH-C(CH_3)═CH_2	568b, 1153, 1154, 4249, 5811b		
302.	4549-74-0	1,3-Pentadiene, 3-methyl-	568b, 4249		
303.	2787-45-3	1,3-Pentadiene, 3-methyl-, (*Z*)-	568b, 4249		
304.	2787-43-1	1,3-Pentadiene, 3-methyl-, (*E*)-	568b, 4249		
305.	926-56-7	1,3-Pentadiene, 4-methyl- H_3C-C(CH_3)═CH-CH═CH_2		984, 4249	
306.	591-93-5	1,4-Pentadiene H_2C═CH-CH_2-CH═CH_2	1140, 1374, 1419, 2060, 2782, 2804, 2946, 3302, 3308, 3557, 3797, 4249		
307.	763-30-4	1,4-Pentadiene, 2-methyl-	568b, 4249		
308.	1115-08-8	1,4-Pentadiene, 3-methyl-	568b, 4249		
309.	760-21-4	Pentane, 3-methylene- {2-ethyl-1-butene} (H_3C-CH_2)$_2$═C═CH_2	2310, 2944, 3302, 3308, 4249		
310.	34044-64-9 34786-54-4	1,5,9,13,17,21,25,29,33-Pentatriacontanonaene, 2,6,10,14,18,22, 26,30,34-nonamethyl- {norsolanesene} H-{CH_2-C(CH_3)═CH-CH_2}$_8$-CH_2-C(CH_3)═CH_2		1149, 1149a, 1155, 4249, 5811, 5811b	
311.	25377-72-4	Pentene	1140, 4249, 5034, 5811, 5811a, 5811b		
312.	37275-41-5	Pentene, methyl-	1637, 5811a		
313.	109-67-1	1-Pentene H_3C-(CH_2)$_2$-CH═CH_2	112, 199, 568b, 604, 605, 1140, 1154, 1375, 1375b, 1414, 1419, 1472, 2060, 2310, 2767, 2782, 2804, 2946, 3254, 3302, 3308, 3797, 3901, 4249, 5770, 5811b		
314.	3404-73-7	1-Pentene, 3,3-dimethyl- H_3C-CH_2-C(CH_3)$_2$-CH═CH_2	348, 4249		
315.	763-29-1	1-Pentene, 2-methyl- H_3C-(CH_2)$_2$-C(CH_3)═CH_2	1140, 1348–1350, 1354, 1375a, 1586, 1589, 2543, 2570, 2765, 2767, 2777, 2944, 3219, 3308, 3797, 4249, 5811b		1354, 1375a
316.	760-20-3	1-Pentene, 3-methyl- H_3C-CH_2-CH(CH_3)-CH═CH_2	1140, 1586, 2944, 3219, 3308, 3797, 4249, 5811b		
317.	691-37-2	1-Pentene, 4-methyl- (H_3C)$_2$═CH-CH_2-CH═CH_2	568b, 1140, 2060, 2545, 2777, 2782, 2804, 2944, 3302, 3308, 3797, 4249, 5811b		
318.	109-68-2	2-Pentene H_3C-CH_2-CH═CH-CH_3	604, 605, 2310, 3302, 3308, 3797, 3901, 4249, 5770, 5811b	3186, 3188, 4249	
319.	646-04-8	2-Pentene, (*E*)-	604, 1140, 2060, 2782, 2804, 2946, 3308, 4249, 5811b		
320.	627-20-3	2-Pentene, (*Z*)-	604, 1140, 1153, 1154, 2060, 2782, 2804, 2946, 3308, 4249, 5811b		
321.	625-27-4	2-Pentene, 2-methyl- H_3C-CH_2-CH═C═(CH_3)$_2$	568b, 605, 1140, 1153, 1154, 2944, 3219, 3308, 3797, 4249, 5811b		
322.	922-61-2	2-Pentene, 3-methyl- (*Z*), H_3C-CH_2-C(CH_3)═CH-CH_3	568b, 1140, 2767, 4249, 5811b		
323.	616-12-6	2-Pentene, 3-methyl-, (*E*)-	1140, 4249		
324.	4461-48-7	2-Pentene, 4-methyl- H_3C-CH(CH_3)-CH═CH-CH_3	1586, 2060, 2545, 2767, 3302, 3308, 3797, 4249, 5811b		
325.	674-76-0	2-Pentene, 4-methyl-, (*E*)-	1140, 1153, 1154, 2060, 2944, 2782, 2804, 3308, 4249		
326.	691-38-3	2-Pentene, 4-methyl-, (*Z*)-	1140, 2060, 2782, 2804, 4249		
327.	627-21-4	2-Pentyne H_3C-C≡C-CH_2-CH_3	1153, 1154, 4249		

(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

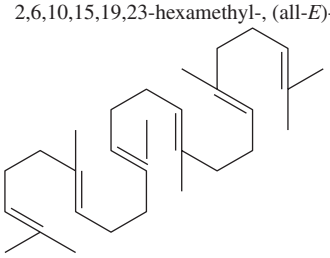
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
328.	71010-49-6	Phytadiene C	2628, 2939	2939, 5794, 5797	
329.	2437-92-5	Phytodienes		900, 3247, 3251, 3297	
330.	463-49-0	1,2-Propadiene {allene} $H_2C{=}C{=}CH_2$	160, 1140, 2060, 2767, 2781, 2782, 2804, 2946, 3302, 3308, 3882, 3897, 4052, 4056, 4162, 4249, 4360, 5811b		4052, 4056
331.	115-07-1	1-Propene $H_3C\text{-}CH{=}CH_2$	85, 126a, 142, 143, 151, 173a, 199, 544–546, 604, 605, 722, 966, 1099, 1140, 1153, 1154, 1243, 1365, 1445, 1472, 1634, 2060, 2079, 2142, 2171, 2270, 2293, 2310, 2634, 2782, 2804, 2866, 2909, 2939, 2946, 3059, 3105, 3255, 3302, 3308, 3692, 3797, 3876, 3882, 3897, 3901, 3939, 3940, 3973, 4005–4007, 4052, 4056, 4104, 4162, 4249, 4319, 4360, 4394, 5034, 5811b, 5835		3901, 3192, 4052, 4056
332.	115-11-7	1-Propene, 2-methyl- {isobutylene} $H_3C\text{-}C(CH_3){=}CH_2$	604, 605, 722, 966, 1140, 1634, 2060, 2270, 2293, 2310, 2782, 2804, 2939, 2942, 2946, 3059, 3302, 3308, 3797, 3876, 3901, 4249, 4319, 5034, 5811b		
333.	74-99-7	1-Propyne $H_3C\text{-}C{\equiv}CH$	394, 397, 605, 1140, 1966, 2060, 2310, 2782, 2857, 2939, 2946, 3302, 3308, 3797, 3882, 4052, 4056, 4104, 4249, 4319, 5034, 5811b		4052, 4056
334.	11030-10-7	1,6,10,14,18,23-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- {isosqualene} $H_2C{=}C(CH_3)CH_2CH_2\,[CH_2C(CH_3){=}CHCH_2]_2\text{-}[CH_2CH{=}C(CH_3)CH_2]_3\text{-}H$	1139, 2174–2176, 2939, 3059, 3251, 3295, 3297, 3302, 3797, 5811, 5811a		
335.	7683-64-9	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-	1375, 1375b, 1586, 3308	404, 1229	
336.	111-02-4	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-*E*)- {squalene} 	722, 900, 1139, 1286, 2174–2176, 2601a, 2767, 2939, 3059, 3219, 3251, 3295, 3297, 3302, 3308, 3797, 3810, 3971, 3999, 4033, 5811b	404, 433, 722, 1102, 1229, 1651, 3611, 3612, 3616, 3797, 3971, 3973, 5581	
337.		2,6,14,18,22-Tetracosapentaene, 2,6,10,15,19,23-pentamethyl-		2339a	
338.	10192-32-2	1-Tetracosene $H_2C{=}CH\text{-}(CH_2)_{21}\text{-}CH_3$	2387, 2570, 2769, 3557, 4249		2387
339.		1-Tetracosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{21}\text{-}CH_3$	1144		
340.		2-Tetracosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{20}\text{-}CH_3$	1144		
341.		2-Tetracosene, (*E*)-	1144		
342.		2-Tetracosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{20}\text{-}CH_3$	1144		
343.		2-Tetracosene, 22-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{18}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
344.		2-Tetracosene, 22-methyl-, (*E*)-	1144		
345.		2-Tetracosene, 23-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{19}\text{-}CH(CH_3)_2$	1144		

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
346.		2-Tetracosene, 23-methyl-, (*E*)-	1144		
347.	1120-36-1	1-Tetradecene $H_2C{=}CH\text{-}(CH_2)_{11}\text{-}CH_3$	1144, 1427, 2387, 2543, 2570, 2731, 2735, 2773, 3797, 4249	404, 2339a	2387
348.	52254-38-3	1-Tetradecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{11}\text{-}CH_3$	1144, 2735, 4249		
349.	1652-97-7	2-Tetradecene	5811, 5811b		
350.	35953-54-9	2-Tetradecene, (*E*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{10}\text{-}CH_3$	1144, 2731, 2735, 3797		
351.	35953-53-8	2-Tetradecene, (*Z*)-	1144		
352.	52254-38-3	2-Tetradecene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{10}\text{-}CH_3$	1144		
353.		2-Tetradecene, 12-methyl-,(*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_8\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
354.		2-Tetradecene, 12-methyl-, (*E*)-	1144		
355.		2-Tetradecene, 13-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_9\text{-}CH(CH_3)_2$	1144		
356.		2-Tetradecene, 13-methyl-, (*E*)-	1144		
357.	18435-53-5	1-Triacontene $H_2C{=}CH\text{-}(CH_2)_{27}\text{-}CH_3$	1144, 3469, 4249		
358.		1-Triacontene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{27}\text{-}CH_3$	1144		
359.		2-Triacontene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{26}\text{-}CH_3$	4249		
360.		2-Triacontene, (*E*)-	1144		
361.		2-Triacontene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{26}\text{-}CH_3$	1144		
362.		2-Triacontene, 28-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{24}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
363.		2-Triacontene, 28-methyl-, (*E*)-	1144		
364.		2-Triacontene, 29-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{25}\text{-}CH(CH_3)_2$	1144		
365.		2-Triacontene, 29-methyl-, (*E*)-	1144		
366.	18835-32-0	1-Tricosene $H_3C\text{-}(CH_2)_{20}\text{-}CH{=}CH_2$	1144, 2387, 2570, 2769, 3557, 3797, 4249	404	2387
367.		1-Tricosene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{20}\text{-}CH_3$	1144		
368.		2-Tricosene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{19}\text{-}CH_3$	1144, 3797		
369.		2-Tricosene, (*E*)-	1144		
370.		2-Tricosene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{19}\text{-}CH_3$	1144		
371.		2-Tricosene, 21-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{17}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
372.		2-Tricosene, 21-methyl-, (*E*)-	1144		
373.		2-Tricosene, 22-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_{18}\text{-}CH(CH_3)_2$	1144		
374.		2-Tricosene, 22-methyl-, (*E*)-	1144		
375.	27519-02-4	9-Tricosene		404	
376.	19780-80-4	Tridecane, 7-methylene- $[H_3C\text{-}(CH_2)_5]_2{=}C{=}CH_2$	1365	404	

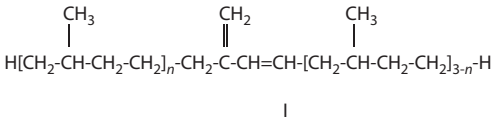
(*continued*)

TABLE 1.11 (continued)
Alkenes and Alkynes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

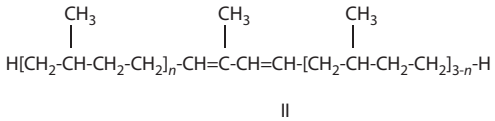
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
377.		Tridecene $H\text{-}(CH_2)_n\text{-}CH{=}CH\text{-}(CH_2)_{(11-n)}\text{-}H$	112, 1644, 1645, 2506, 2507, 2543, 2570, 4249		2506 (0), 2507 (0)
378.	2437-56-1	1-Tridecene $H_3C\text{-}(CH_2)_{10}\text{-}CH{=}CH_2$	37, 38, 1144, 1427, 2387, 2731, 2735, 3797, 4249, 5811b	5811b	2387
379.	18094-01-4	1-Tridecene, 2-methyl- $H_2C{=}C(CH_3)\text{-}(CH_2)_{10}\text{-}CH_3$	1144		
380.	19150-20-0	2-Tridecene, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_9\text{-}CH_3$	1144, 2731, 2735, 3797, 4249, 5811b		
381.	25377-82-6	2-Tridecene, (*E*)-	1144, 5811b		
382.	62060-10-0	2-Tridecene, 2-methyl- $H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_9\text{-}CH$	1144		
383.		2-Tridecene, 11-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1144		
384.		2-Tridecene, 11-methyl-, (*E*)-	1144		
385.		2-Tridecene, 12-methyl-, (*Z*)- $H_3C\text{-}CH{=}CH\text{-}(CH_2)_8\text{-}CH(CH_3)_2$	1144		
386.		2-Tridecene, 12-methyl-, (*E*)-	1144		
387.	55976-13-1	1,4-Undecadiene, (*E*)- $H_3C\text{-}(CH_2)_5\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}CH_2$	4249	4249	
388.	16356-11-9	1,3,5-Undecatriene	5770		
389.	28761-27-5	Undecene	5811		
390.	821-95-4	1-Undecene $H_3C\text{-}(CH_2)_8\text{-}CH{=}CH_2$	568b, 1144, 1472, 1644, 1645, 2387, 2543, 2570, 2769, 2773, 3797, 4249, 5770		2387
391.	2244-02-2	2-Undecene	3797		
392.	31613-73-7	5-Undecene, 5-methyl- $H_3C\text{-}(CH_2)_4\text{-}CH{=}C(CH_3)\text{-}(CH_2)_3\text{-}CH_3$		404	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

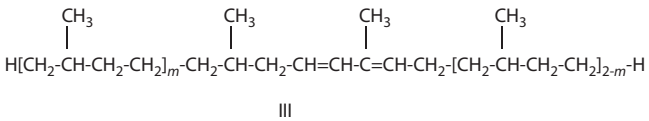
The several groups of possible conjugated phytadienes are more completely defined in structures I through VI:



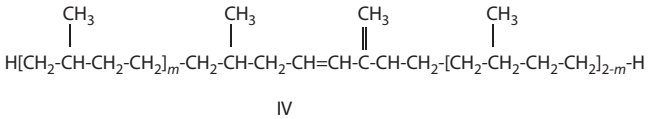
I



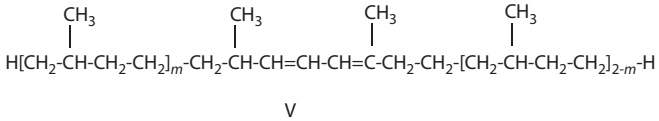
II



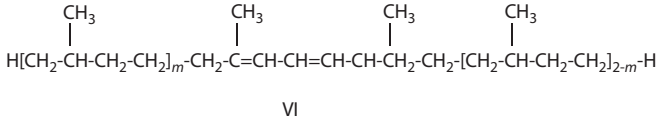
III



IV



V



VI

Phytadienes I–IV with the potential to generate anthraquinonecarboxylic acids in the reaction sequence described are shown in Figure 1.1. Phytadienes I, II ($n = 3$), and IV can exist as *cis* and *trans* isomers. The remaining phytadienes in Figure 1.1 can exist as *cis cis*, *cis trans*, *trans cis*, and *trans trans* isomers. In Figure 1.2 are shown the phytadienes (V, VI) that do not appear to form Diels–Alder adducts.

As noted previously, even if they did form the Diels–Alder adducts, they would not yield alkylanthraquinones because of the absence of hydrogen atoms at the 1 and/or

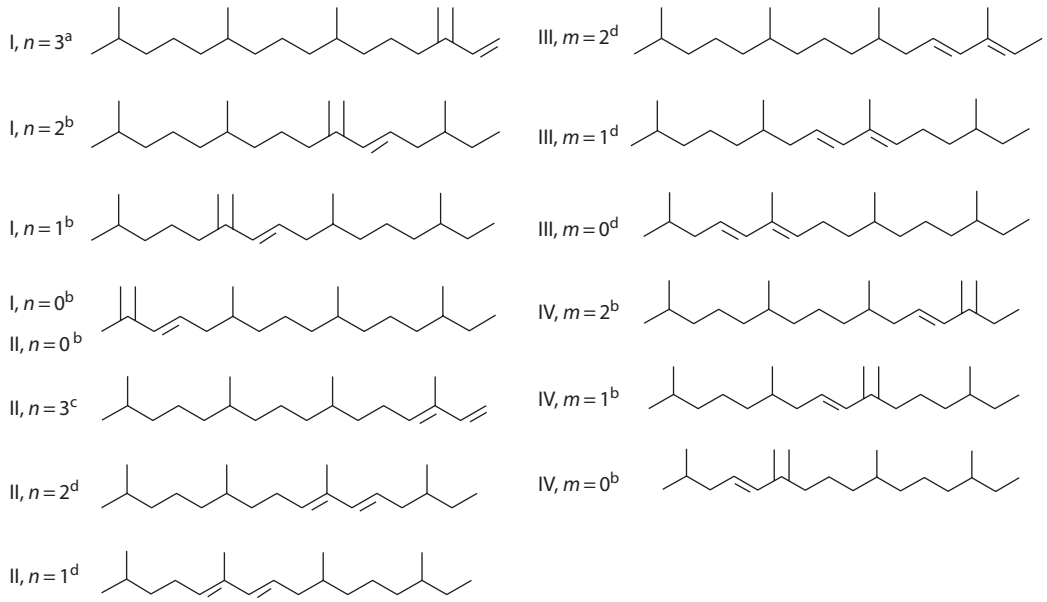


FIGURE 1.1 Phytadienes with potential to yield Diels–Alder adducts and subsequently alkylanthraquinones and anthraquinonecarboxylic acids. [a]Yields anthraquinone-2-carboxylic acid; [b]Yields anthraquinone-1,3-dicarboxylic acid; [c]Yields anthraquinone-1,2-dicarboxylic acid; [d]Yields anthraquinone-1,2,4-tricarboxylic acid.

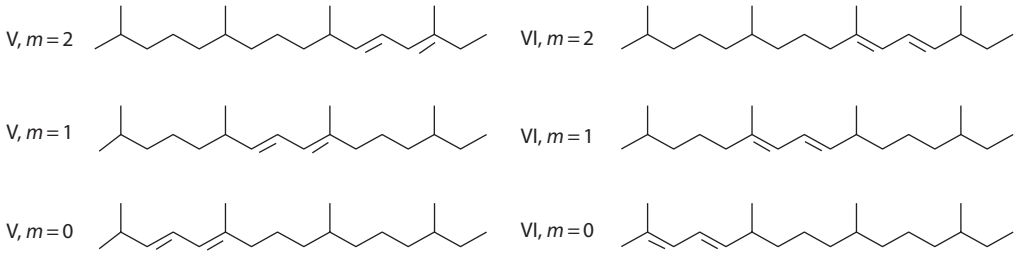


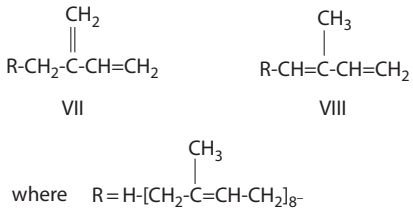
FIGURE 1.2 Phytadienes with little or no potential to form Diels–Alder adducts.

4 positions. Figure 1.1 also summarizes the various anthraquinonecarboxylic acids which could arise from the phytadienes depicted.

In their study of the smoke from British cigarettes, Johnstone and Quan (1973) reported that at least 99% of the acyclic phytadienes comprised neophytadiene. They made no comment on the presence of phytadiene isomers in the remaining 1%. Since no quantitative data were provided by Rodgman (3247) in his study of the phytadiene isomers in tobacco smoke, comparisons of the two investigations are not possible. The Johnstone–Quan study involved the study of tobacco smoke from flue-cured tobacco cigarettes, whereas the Rodgman study involved smoke from cigarettes containing a cased American blend (flue-cured, burley, Oriental, and Maryland tobaccos).

Because of the similarities among the infrared absorption spectra of the gross phytadiene fraction in cigarette MSS (3247), the mixture of phytadiene isomers described by Rowland (3345), and the mixture of phytadienes generated by heating neophytadiene (180°C, 2.5 h), Rodgman suggested that the isomeric conjugated phytadienes in tobacco smoke resulted from thermal isomerization of neophytadiene during the smoking process. However, as Lam et al. (2260) suggested, it is highly possible that the various phytadienes may be generated during the smoking process from phytol or phytyl esters in the tobacco. Vandemeent et al. (4015) reported that chlorophyll-bound phytol yielded several phytadienes when various geological materials containing chlorophylls were pyrolyzed at 610°C. Lam et al. (2260) reported the presence of at least five different phytadienes in a pyrolysate from phytol heated at 550°C. Neither Vandemeent et al. nor Lam et al. described the structures of the phytadienes they had identified.

Another series of isoprenoid hydrocarbons isolated from cigarette MSS by Rodgman et al. (3297) comprised the solanesol-related solanesenes. Dehydration of solanesol or pyrolysis of solanesyl acetate yields a mixture of solanesenes similar to that isolated from cigarette MSS. VII and VIII are the major components of the solanesene mixture in tobacco smoke.



Sodium–alcohol reduction of the mixture gave dihydrosolanesene whose infrared spectrum *vs.* that of the solanesenes was consistent with the migration of the terminal double bond to an internal position. The Diels–Alder reaction sequence used by Rowland (3345) in the characterization of neophytadiene from tobacco and the various phytadienes in cigarette MSS by Rodgman (3247) was applied to the solanesene mixture. It provided confirmatory evidence for the presence of the solanesene VII: Reaction of the isolated solanesene mixture with 1,4-naphthoquinone, followed by air oxidation of the adduct, apparently yielded a single 2-alkylanthraquinone rather than the anticipated mixture of 2-alkyl- and 1,2-dialkylanthraquinones. Only anthraquinone-2-carboxylic acid was isolated and identified as a product of the alkylanthraquinone-to-anthraquinonecarboxylic acid oxidation. The failure to demonstrate the presence of anthraquinone-1,2-dicarboxylic acid was attributed to the inertness of solanesene VIII in the Diels–Alder reaction.

Wynder and Hoffmann (4319) reported that the phytadienes did not produce hyperplasia or destroy sebaceous glands when applied to mouse skin. They also reported (4316) that removal of terpenoid hydrocarbons such as the phytadienes from a polycyclic aromatic hydrocarbon (PAH)-enriched fraction did not significantly alter its sebaceous gland suppression. From this result, they concluded that "the terpenes may not contribute significantly to the tumorigenic activity of tobacco smoke."

Entwhistle and Johnstone (1144) described six homologous series of monoalkenes isolated from tobacco smoke, including all of the possible *cis* and *trans* isomers. They reported the total delivery of these series in cigarette MSS to be about 3 µg/cigarette. These series did not appear to be present in tobacco leaf. Their precursors in tobacco have not been defined. However, Carruthers and Johnstone (614) earlier had reported that long-chained alkenes in tobacco smoke did not result from the dehydration of the corresponding alcohol during the smoking process.

Monoalkene Series	*n* =
$H_2C{=}CH\text{-}(CH_2)_n\text{-}CH_3$	7 through 25
$H_2C{=}C(CH_3)\text{-}(CH_2)_n\text{-}CH_3$	9 through 28
$CH_3\text{-}CH{=}CH\text{-}(CH_2)_n\text{-}CH_3$[a]	9 through 28
$CH_3\text{-}C(CH_3){=}CH\text{-}(CH_2)_n\text{-}CH_3$	8 through 27
$CH_3\text{-}CH{=}CH\text{-}(CH_2)_n\text{-}CH{=}(CH_3)_2$[a]	7 through 26
$CH_3\text{-}CH{=}CH\text{-}(CH_2)_n\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$[a]	6 through 25

[a] *cis* and *trans* isomers.

Rodgman et al. (3294) described the composition of an aliphatic ester fraction isolated from MSS generated by cigarettes fabricated from an American tobacco blend, burley tobacco, or Oriental tobacco. Aliphatic ester fractions almost identical with those from the smokes were also isolated from flue-cured tobacco, burley, and Oriental tobaccos. With the analytical technology available in the early 1960s, the aliphatic ester fraction was shown to consist of a series of esters whose alcohol moiety varied from 1-dodecanol (C_{12}) to 1-heptacosanol (C_{27}), inclusive. The acid moiety ranged from tetradecanoic acid (C_{14}) to octacosanoic acid (C_{28}), inclusive, plus the C_{18} unsaturated acids, oleic, and linolenic.

More than two decades later, Arrendale et al. (103) extended the identification of the components of the aliphatic ester fraction from tobacco. The alcohol moiety ranged from 1-hexadecanol (C_{16}) to 1-tetratriacontanol (C_{34}). Esters with 1-hentriacontanol and 1-tritriacontanol as the alcohol moieties were not detected. The acid moiety ranged from dodecanoic acid (C_{12}) to dotriacontanoic acid (C_{32}). An ester with hentriacontanoic acid as the acid moiety was not detected. For a given number of carbons, the acid moiety not only included the *normal* acid but also in several cases included the *iso* and/or *anteiso* acid, e.g., esters were identified with *n*-, *iso*-, and *anteiso*-pentadecanoic acid as the acid moieties.

Even though Arrendale et al. (103) limited their study to an ester fraction isolated from tobacco, it seems logical to assume, based on the findings of Rodgman et al. (3294) on the equivalence of the aliphatic ester fractions isolated from various smokes and tobaccos, that each ester identified by Arrendale et al. would appear in tobacco smoke.

Controlled thermal degradation of higher molecular weight aliphatic esters generates an alkene and an acid (950c, 3294). Thermal degradation during the smoking process of the aliphatic esters identified in tobacco could conceivably yield some of the alkenes in the series described by Entwhistle and Johnstone (1144).

$$R\text{-}CH_2\text{-}CH_2\text{-}OOC\text{-}R_1 \rightarrow R\text{-}CH{=}CH_2 + R_1\text{-}COOH$$

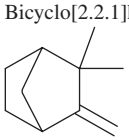
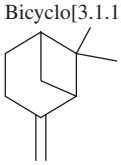
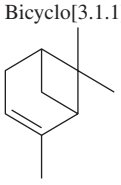
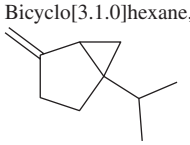
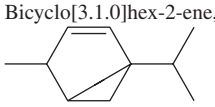
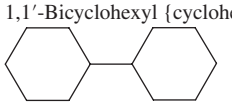
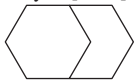
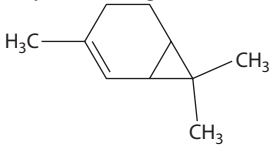
2,6-Dimethyl-2,4,6-octatriene (alloöcimene) was reported by Wynder and Hoffmann (4316) as a significant tobacco smoke component (0.5% of CSC) with cocarcinogenic activity. However, Mold et al. (2597) presented contradictory data which indicated that if 2,6-dimethyl-2,4,6-octatriene were present in smoke, its level was less than 0.006%.

1.3 ALICYCLIC HYDROCARBONS

The cyclic aliphatic hydrocarbons in tobacco and tobacco smoke include compounds whose ring sizes range from cyclopropane through cyclooctane, cyclononane, cycloundecane, and cyclotetradecane. Theoretically, cyclooctatetraene could be included in the listing of monocyclic aromatic hydrocarbons. Numerous hydrocarbons with cyclopentane and cyclohexane rings were reported as tobacco and tobacco smoke components in the late 1950s through the mid-1960s (see Table 1.12). Tobacco smoke hydrocarbons with a cyclobutane ring were reported by Stedman in 1963 (3795). Three dimethylcyclopropanes were reported in 1970 by Bartle and Novotny (200). 1,3,5-Cycloheptatriene and cyclooctatetraene were reported by Enzell et al. (1154) and Mauldin (2506), respectively. A hydrocarbon with the cycloheptatriene ring had been reported previously as a tobacco smoke component in 1947 by Ikeda (1857): The bicyclic aromatic hydrocarbon azulene, an isomer of naphthalene.

Several fused-ring alicyclic hydrocarbons obviously derived from tobacco sterols were reported in 1989 in tobacco smoke by Benner et al. (273).

TABLE 1.12
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	121-46-0	Bicyclo[2.2.1]hepta-2,5-diene {norbornadiene}		3973	
2.	79-92-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-{camphene} 	3266, 3302, 4249	2282	
3.	498-66-8	Bicyclo[2.2.1]hept-2-ene {norbornene} 	568b, 1067, 1505, 4249		
4.		Bicyclo[2.2.1]hept-2-ene, 5-ethyl-	5770		
5.	127-91-3 18172-67-3	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- {β-pinene} 	314, 1140, 1168, 1365, 1375, 1375b, 1416, 1422, 3224, 3254, 3266, 3302, 3795, 3797, 4249	131, 172a, 909, 1053, 2282, 2339a, 3266, 4249	
6.	80-56-8 7785-26-4	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- {α-pinene} 	1168, 1375, 1375b, 1822, 2870, 2939, 3254, 3266, 3451, 4249, 4259	131, 172a, 909, 1053, 1157, 2282, 2339a, 3266, 3547, 3971, 4249	
7.	4889-83-2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-		4249	
8.	3387-41-5	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-		2339a, 2917a, 4249	
9.	2867-05-2	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-		2917a, 4249	
10.	3387-41-5	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- {sabinene} 		2339a, 2917a	
11.	2867-05-2	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)- {3-thujene} 		2917a	
12.	3917-48-4	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-, (1R)-		2407a, 5811b	
13.	92-51-3	1,1′-Bicyclohexyl {cyclohexylcyclohexane} 	1375, 1375b, 1822, 2769	2753	
14.	280-65-9	Bicyclo[3.3.1]nonane 	1375, 1375b, 1822, 2769, 3890, 4249	2753, 4249	2506, 2507
15.	4497-92-1	Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-, (1R, 6R)- {(+)-2-carene} 		5811	

(*continued*)

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

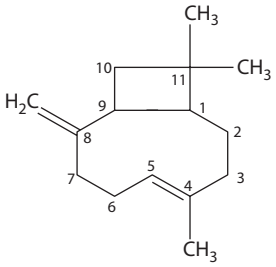
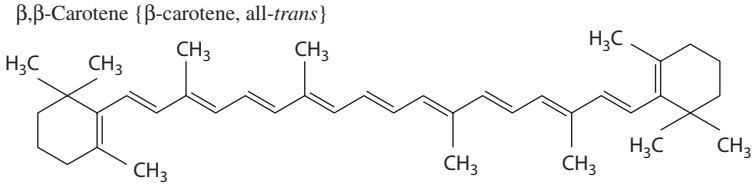
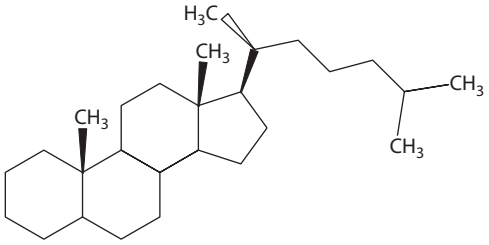
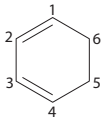
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
16.	498-15-7 13466-78-9	Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- {(+)-3-carene; δ-3-carene}		131, 568b, 2339a, 4249, 5811	
17.	87-44-5	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)] {β-caryophyllene} 		172a, 174b, 937, 1053, 1156, 1254, 1256, 2611, 3266, 3370, 4073b, 4090, 4249, 5811b	
18.		Carotene		5867	
19.	7235-40-7	β,β-Carotene {β-carotene, all-*trans*} 	3257	120, 367, 433, 543a, 585, 830a, 832, 835, 838, 922a, 943, 971, 972, 1053, 1063–1066, 1068–1074, 1110, 1156, 1254, 1256, 1927a, 1941, 1956, 2079, 2270, 2283, 2338, 2339b, 2543, 2545, 2611, 2761, 2762, 2765, 2766, 2939, 3059, 3194, 3218, 3266, 3616, 3645, 3797, 3971, 3973, 3974a, 4090, 4159, 4222, 4249, 4286, 5079, 5189, 5300, 5811b	
20.	6811-73-0	β,β-Carotene, 13-*cis*-		1053, 3266, 4249	
21.	68295-84-1	β,β-Carotene, *neo*		2939, 3797, 3974a, 4249	

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
22.	7488-99-5	β,ε-Carotene, (6′R)- {α-carotene}		120, 971, 972, 1156, 3194, 3218, 3797, 3973, 3974a, 4090, 4249	
23.	119973-28-3	Chol-3-ene, 23-methyl-, (5α)-	273, 429c		
24.	747-90-0	Cholesta-3,5-diene	273, 2601a, 3263		
25.		Cholesta-3,5-diene, 24-ethyl-	1099, 1100, 3255		
26.	481-21-0	Cholestane, (5α)- {coprostane} 		429c, 3867, 4249	
27.		Cholesta-3,5,22-triene, 24-methyl-	1099, 1100, 3255		
28.	544-25-2	1,3,5-Cycloheptatriene {tropilidene} 	1153, 1154, 4249, 5811b	1153, 4249	
29.	29797-09-9	Cyclohexadiene	314, 1054, 1154, 1637, 2310, 2545, 3302, 3897, 4249		3401
30.	592-57-4	1,3-Cyclohexadiene 	299, 568b, 1063–1066, 1068–1074, 1153, 1154, 1365, 2310, 3302, 4249, 4360, 5811b		
31.	99-86-5	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- {α-terpinene}	3410	404, 1156, 2336, 2339a, 2389, 2544, 4090, 4249, 5811b	
32.	99-83-2 1329-99-3	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- {α-phellandrene}	1154, 3266, 4249	172a, 1053, 3266	
33.	4221-98-1	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)-, (R)- {α-phellandrene}	568b, 3266, 4249	172a, 174b, 568b, 1053, 3266	
34.	514-96-5	1,3-Cyclohexadiene, 1,2,6,6-tetramethyl-		1053, 3266	

(*continued*)

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

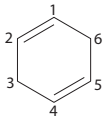
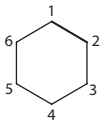
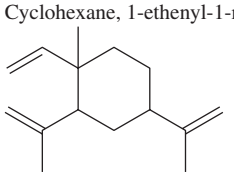
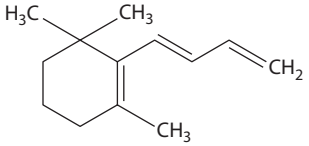
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
35.	628-41-1	1,4-Cyclohexadiene 	568b, 2309, 4249		
36.	4313-57-9	1,4-Cyclohexadiene, 1-methyl-	568b, 4249		
37.	99-85-4	1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-		2339a	
38.	110-82-7	Cyclohexane 	142, 151, 222–224, 239, 1140, 1413–1416, 1422, 1437, 1637, 2799a, 2944, 2946, 3302, 3308, 3557, 3769, 3797, 4249, 4319, 5811b	5811b	
39.	27195-67-1	Cyclohexane, dimethyl-	222–224	4249, 4807, 5811b	
40.	1678-91-7	Cyclohexane, ethyl-	1822, 5811b		
41.	30677-34-0	Cyclohexane, ethyl-methyl-	5811, 5811a, 5811b		
42.	108-87-2	Cyclohexane, methyl-	222–224, 568b, 1822, 4249		
43.	1678-92-8	Cyclohexane, propyl-	1822, 5811b		
44.	27013-35-0	Cyclohexane, methyl-(1-methylethenyl)-	1822		
45.	590-66-9	Cyclohexane, 1,1-dimethyl-	1822, 4249, 5811b		
46.	2207-01-4	Cyclohexane, 1,2-dimethyl-, (*Z*)	568b, 4249		
47.	6876-23-9	Cyclohexane, 1,2-dimethyl-, (*E*)	568b, 4249		
48.	591-21-9	Cyclohexane, 1,3-dimethyl-	1822, 4249, 5811b		
49.	624-29-3	Cyclohexane, 1,4-dimethyl-, (*Z*)	568b, 4249		
50.	2207-04-7	Cyclohexane, 1,4-dimethyl-, (*E*)	568b, 4249		
51.	33880-83-0	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, (1α,2β,4β)- 		1156, 1256, 4090, 4249, 5811b	
52.	515-13-9	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-		1156, 1256, 4090, 4249	
53.	62238-31-7	Cyclohexane, 1-ethyl-1,3-dimethyl-, (*Z*)-	1974, 3302, 4249		
54.	62238-29-3	Cyclohexane, 1-ethyl-1,3-dimethyl-, (*E*)-	1974, 3302, 4249		
55.	62238-30-6	Cyclohexane, 1-ethyl-1,4-dimethyl-, (*Z*)-	1974, 3302		
56.	62238-32-8	Cyclohexane, 1-ethyl-1,4-dimethyl-, (*E*)-	1974, 3302		

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
57.	62238-33-9	Cyclohexane, 1-ethyl-2-propyl-	4570a		
58.	13828-34-7	Cyclohexane, 1-methyl-3-(1-methylethylidene)-	1153, 1154, 4249		
59.	99-62-1	Cyclohexane, 1-methyl-4-(1-methylethyl)- {*p*-menthane}	1936		
60.	61142-00-5	Cyclohexane, 1,2,4,5-tetramethyl-	4570a		
61.	3073-66-3	Cyclohexane, 1,1,3-trimethyl-	1822, 4249		
62.	110-83-8	Cyclohexene	568b, 1140, 1419, 1822, 2944, 3308, 3797, 4249, 5034, 5811b		
63.		Cyclohexene, dimethyl-	5777		
64.		Cyclohexene, methyl-	5777		
65.	74423-06-6	Cyclohexene, 2-(1,3-butadienyl)-1,3,3-trimethyl-, (*E*)- {megastigmatriene} 		3760a, 3780b, 4249	
66.	2808-76-6	Cyclohexene, 1,3-dimethyl-	568b, 4249		
67.	70688-47-0	Cyclohexene, 1,4-dimethyl-	568b, 4249		
68.	1743-61-9	Cyclohexene, 1,4-dimethyl-4-ethenyl-	5770		
69.	495-62-5	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl- {bisabolene}		174b, 3266	
70.	70941-91-2	Cyclohexene, 6-(3,7-dimethyl-1,3,5,7-octatetraenyl)-1,5,5-trimethyl-, (*E,E,E*)-		4249, 4286	
71.	25168-07-4	Cyclohexene, ethenyl-	3308, 3508, 4249		
72.		Cyclohexene, 3-ethenyl-1,3-di(4′,8′,12′-trimethyltridecyl)-	1973		
73.	100-40-3	Cyclohexene, 4-ethenyl-	1286, 3302, 4249		
74.	20307-84-0	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-{δ-elemene)		404	
75.		Cyclohexene, 4-ethenyl-1,4-di(4′,8′,12′-trimethyltridecyl)-	1973		
76.	1611-21-8	Cyclohexene, 5-ethenyl-1,5-dimethyl-	798, 900, 1974, 2870, 3302, 3308, 3797, 4249		
77.	591-49-1	Cyclohexene, 1-methyl-	568b, 1153, 1154, 4249, 5811b		
78.		Cyclohexene, 3-(1-methylethyl)-	5770		
79.	38738-60-2	Cyclohexene, 1-methyl-3-(1-methylethenyl)- {sylvestrene}	299, 314, 1063–1066, 1068–1074, 1140, 1153, 1154, 1365, 1371, 1419, 2545, 4068, 4249		

(*continued*)

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

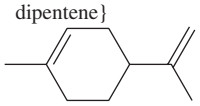
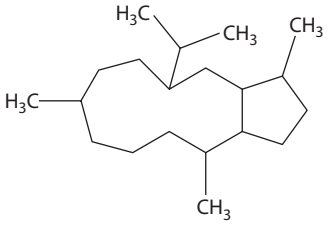
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
80.	138-86-3	Cyclohexene, 1-methyl-4-(1-methylethenyl)- {limonene; *p*-mentha-1,8-diene; dipentene} 	111, 112, 156, 157, 172, 199, 239, 299, 314, 315, 462, 568b, 765, 900, 1063–1066, 1068–1074, 1099, 1140, 1153, 1154, 1262a, 1286, 1313, 1338, 1348–1350, 1354, 1364, 1365, 1371, 1373–1375, 1375a, 1375b, 1377, 1416–1419, 1427, 1431, 1432, 1437, 1445, 1586, 1589, 1634, 1637, 1638, 1663, 1842, 1882, 1947, 1971, 1974, 1975, 2002, 2003, 2173, 2174, 2387, 2493, 2506, 2507, 2508, 2543, 2545, 2570, 2597, 2628, 2629, 2636, 2722, 2765, 2767, 2777, 2799a, 2857, 2870, 2874, 2939, 3255, 3257, 3265, 3302, 3308, 3397, 3410, 3451, 3508, 3530, 3557, 3797; 3826, 4068, 4121, 4249, 4259, 4570a, 5034, 5770, 5811b	404, 568b, 909, 984, 2282, 2339a, 2611, 2917a, 3186, 3188, 3905, 4249, 5811b	1354, 1375a, 1377, 2387, 2506, 2507

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
81.	5989-27-5	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- {*d*-limonene}	2543, 2601a, 3300, 4249, 4570a		
82.	5989-54-8	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)- {*l*-limonene}	5811, 5811a, 5811b		
83.	5502-88-5	Cyclohexene, 1-methyl-4-(1-methylethyl)-	299, 314, 1063–1066, 1068–1074, 1140, 1365, 1419, 1422, 2387, 2506, 2507, 2545, 3797, 4068, 4249, 5770		2387, 2506, 2507
84.	13828-33-6	Cyclohexene, 5-methyl-1-(1-methylethyl)-{*m*-menthene}	5811b	5811, 5811a, 5811b	
85.	586-62-9	Cyclohexene, 1-methyl-4-(1-methylethylidene)- {terpinolene}		172a, 174b, 1053, 2339a, 3266	
86.	1461-27-4	Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)-	4249, 5811b		
87.	591-48-0	Cyclohexene, 3-methyl-	568b, 1354, 1375a, 1586, 1589, 2543, 2570, 2765, 2777		1354, 1375a
88.	591-47-9	Cyclohexene, 4-methyl-	568b, 4249		
89.	586-67-4	Cyclohexene, 4-methyl-1-(1-methylethenyl)- {3,8-menthadiene}	314, 2174, 3557, 4249		
90.	5256-65-5	Cyclohexene, 3-methyl-6-(1-methylethyl)-	2508, 4249		
91.	23733-91-7	Cyclohexene, 3-methylene-4-(1-methylethenyl)-, (R)-		4249	
92.		Cyclohexene, 3-(1″-methylene-5″,9″,13″-trimethyltetradecyl)-1-(4′,8′,12′-trimethyltridecyl)-	1973		
93.		Cyclohexene, 4-(1″-methylene-5″,9″,13″-trimethyltetradecyl)-1-(4′,8′,12′-trimethyltridecyl)-	1973		
94.		Cyclohexene, 3-(1-methylethyl)-	5770		
95.	14072-82-3	Cyclohexene, 4-(1-methylethyl)-	5811, 5811a, 5811b		
96.	13828-33-6	Cyclohexene, 5-methyl-1-(1-methylethyl)-{*m*-menthene}		5811, 5811a, 5811b	
97.	503-45-7	Cyclohexene, 3,3,5-trimethyl-	5770		
98.	629-20-9	1,3,5,7-Cyclooctatetraene 	2506, 2507, 3397, 5811b		2506 (0), 2507 (0)
99.	149331-19-1	Cyclononane, 1,1,4,4,7,7-hexamethyl-		2917a	
100.	142750-43-4	Cyclopentacycloundecene, tetradecahydro-1,4,8-trimethyl-11-(1-methylethyl)- 		4249	

(*continued*)

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

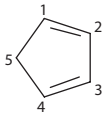
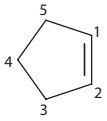
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
101.	542-92-7	1,3-Cyclopentadiene {pyropentylene} 	199, 299, 314, 1063–1066, 1068–1074, 1140, 1153, 1154, 1348–1350, 1354, 1365, 1375a, 1586, 1589, 1637, 1822, 2079, 2310, 2543, 2545, 2570, 2765, 2767, 2777, 2857, 2946, 3302, 3797, 4249, 4360, 4570a, 4996, 5034, 5770, 5811b	5811b	1354, 1375a, 3401
102.	77208-25-4	1,3-Cyclopentadiene, dimethyl-	3530, 4249		
103.	26519-92-6	1,3-Cyclopentadiene, ethyl-	1422, 4249		
104.	26519-91-5	1,3-Cyclopentadiene, methyl-	1067, 1153, 1348–1350, 1354, 1375a, 1586, 1589, 1637, 2543, 2570, 2765, 2767, 2777, 3897, 4249, 4360		1354, 1375a
105.	4784-86-5	1,3-Cyclopentadiene, 1,2-dimethyl-	4570a		
106.	4045-53-8	1,3-Cyclopentadiene, 1,3-dimethyl-	3530, 4249		
107.	96-39-9	1,3-Cyclopentadiene, 1-methyl-	1422, 4249, 4570a, 5770		
108.	96-38-8	1,3-Cyclopentadiene, 5-methyl-	1422, 4249, 4570a		
109.	497-20-1	1,3-Cyclopentadiene, 5-methylene- {fulvene}	4249		
110.	287-92-3	Cyclopentane {pentamethylene}	142, 143, 604, 605, 1140, 1154, 1822, 2060, 2648, 2781, 2782, 2804, 2944, 2946, 3302, 3308, 3797, 4249, 5811b		
111.	2452-99-5	Cyclopentane, 1,2-dimethyl-, (*Z*)-	1822, 5811b		
112.	822-50-4	Cyclopentane, 1,2-dimethyl-, (*E*)-	1153, 1154, 1822, 4249		

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References		
			Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
113.	96-37-7	Cyclopentane, methyl-	568b, 1140, 1153, 1154, 2060, 2781, 2782, 2804, 2944, 2946, 3302, 3308, 4249, 5811b	5811b	
114.	53366-54-4	Cyclopentane, (2-methylbutylidene)-	4570a		
115.	53366-58-8	Cyclopentane, (2-methylpropylidene)-	4570a		
116.	79637-61-9	Cyclopentane, propenyl-	4249		
117.	2040-96-2	Cyclopentane, propyl-	1822		
118.	30498-64-7	Cyclopentane, trimethyl-	1822		
119.	142-29-0	Cyclopentene 	568b, 1140, 1153, 1154, 1637, 2060, 2782, 2804, 2944, 2946, 3302, 3308, 3797, 4249, 5034, 5811b		
120.		Cyclopentene, ethenyl-	156, 157		
121.	28638-58-6	Cyclopentene, 1-ethenyl-	156, 157, 4249		
122.	30233-85-3	Cyclopentene, ethyl-	156, 157, 2628, 2629, 2636, 2799a		
123.	2146-38-5	Cyclopentene, 1-ethyl-	156, 642, 4249		
124.		Cyclopentene, methyl-	5034		
125.	693-89-0	Cyclopentene, 1-methyl-	568b, 1140, 2782, 2944–2946, 3308, 3797, 4249, 4570a, 5811b		
126.	1120-62-3	Cyclopentene, 3-methyl-	1140, 1348–1350, 1354, 1375a, 1586, 1589, 2543, 2570, 2767, 2777, 2944, 2946, 3797, 4249, 5811b		1354, 1375a
127.	1759-81-5	Cyclopentene, 4-methyl-	2782, 2944, 2946, 3308, 3797, 4249, 5811b		
128.		Cyclopentene, 3-(1-methylethyl)-	5770		
129.	3074-61-1	Cyclopentene, 1-propyl-	2506, 4249		

(*continued*)

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

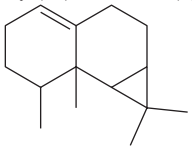
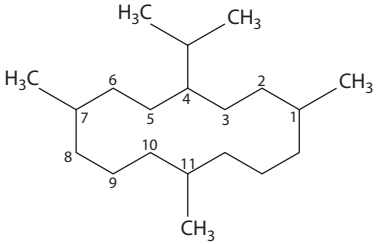
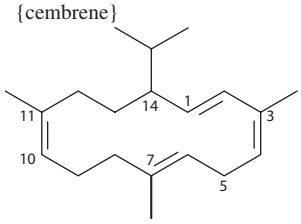
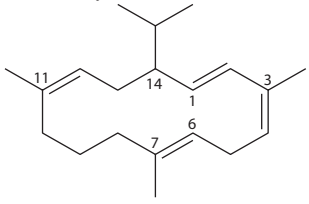
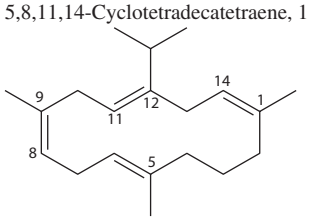
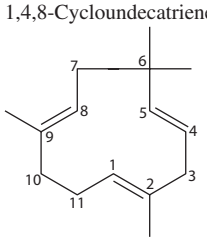
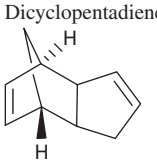
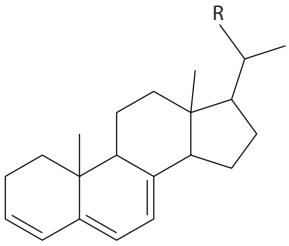
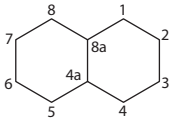
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
130.	17334-55-3	1aH-Cyclopropa[a]naphthalene, 1,1,7,7a-tetramethyl-2,3,5,6,7,7b-hexahydro {1(10)-aristolene, (+)} 		5811, 5811b	
131.	1630-94-0	Cyclopropane, 1,1-dimethyl-	199, 200, 1153, 1154, 4249, 5811b		
132.	2511-95-7	Cyclopropane, 1,2-dimethyl-	199, 200, 1153, 1154, 4249, 5811b		
133.	930-18-7	Cyclopropane, 1,2-dimethyl-, (*Z*)-	199, 200, 1154, 4249, 5811b		
134.	2402-06-4	Cyclopropane, 1,2-dimethyl-, (*E*)-	199, 200, 1154, 4249, 5811b		
135.	1786-12-5	Cyclotetradecane, 1,7,11-trimethyl-4-(1-methylethyl)- 		1495a, 4086a, 5811b	
136.	150405-76-8	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-		671, 4249	
137.	101159-08-4	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)- {cembrene} 	2726, 4249	9, 671, 943, 1149, 1149a, 1157, 1248, 3853, 4073b, 4089, 4249, 5811b	
138.	1898-13-1	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(*E,Z,E,E*)]-		2917a, 4073b, 4098a, 5811b	
139.		1,3,6,11-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)- 		671	

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
140.		5,8,11,14-Cyclotetradecatetraene, 1,5,9-trimethyl-12-(1-methylethyl)- 		671	
141.	101159-07-3	1,4,7,10-Cyclotetradecatetraene, 1,7,11-trimethyl-4-(1-methylethenyl)-		671, 4249, 5811b	
142.	62376-15-2	Cycloundecane, 1,1,2-trimethyl-	2601a		
143.	6753-98-6	1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (*E,E,E*)- 		1156, 1256, 4090, 4249, 5811b	
144.	77-73-6	Dicyclopentadiene 	5777		
145.	119973-29-4	26,27-Dinorergosta-3,5-diene	273	429c	
146.	119973-31-8	26,27-Dinorergosta-3,5,22-triene, (22*E*)-	273	429c	
147.	119973-30-7	26,27-Dinorergost-3-ene, (5α)-	273	429c	
148.	77327-07-2	Ergosta-3,5-triene, (24ξ)-  R═$-(CH_2)_2-CH(CH_3)-CH(CH_3)_2$	273, 278, 1099, 1100		
149.	475-20-7	1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-,[1S-(1α,3aβ,4α,8aβ)]-		131, 568b, 4249	
150.	469-61-4 11028-42-5	1*H*-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,7β,8aα)]-		1256, 4249, 5811, 5811b	
151.	91-17-8	Naphthalene, decahydro- 	222–224, 568b, 4249		

(*continued*)

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

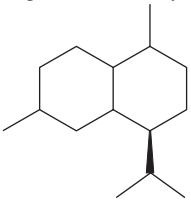
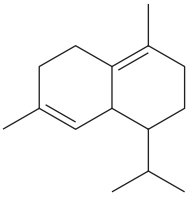
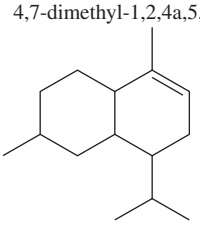
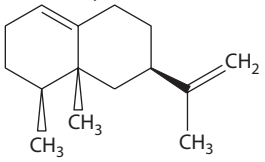
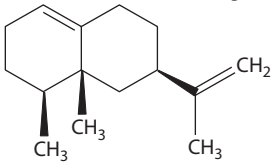
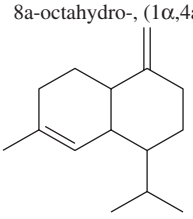
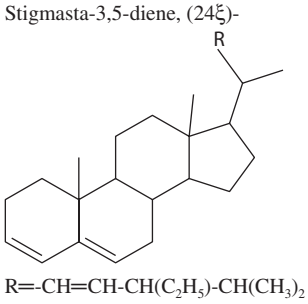
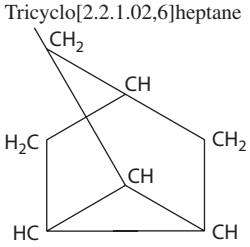
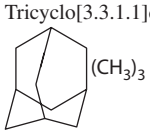
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
152.	29350-73-0	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)- {cadinene} 		1053, 2339a, 2917a, 3266, 4249	
153.	3242-05-5	Naphthalene, decahydro-1,8a-dimethyl-7-(1-methylethyl)-, [1S-(1α,4aα,7α,8aα)]-		4249	
154.	483-76-1	Naphthalene, 4,7-dimethyl-1,2,3,5,6,8a-hexahydro-1-(1-methylethyl)-, (1S-*cis*)-{δ-cadinene} 		1156, 1256, 4090, 4249	
155.	31983-22-9	Naphthalene, 4,7-dimethyl-1,2,4a,5,6,8a-hexahydro-1-(1-methylethyl)- {α-muurolene} 		404, 2339a	
156.	4630-07-3	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7β,8a α] {valencene} 		172a, 404, 568b, 1053, 2917a, 3266	
157.	10219-75-7	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7 α,8a α] {eremophilene} 		404	
158.	39029-41-9	Naphthalene, 7-methyl-4-methylene-1-(1-methylethyl)- 1,2,3,4,4a,5,6, 8a-octahydro-, (1α,4aβ,8aα)- {γ-cadinene} 		1156, 2339a, 4090, 4249, 4812	
159.	102491-96-3	Stigmasta-3,5,22-triene, (22*E*)-	1098, 5811b	429c	
160.	81531-12-6	Stigmasta-3,5,22-triene, (22*E*,24ξ)-	273, 2601a	429c	

TABLE 1.12 (continued)
Alicyclic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
161.	86709-50-4	Stigmasta-3,5,24(28)-triene	273	429c	
162.	79897-80-6	Stigmasta-3,5-diene, (24ξ)-  R═-CH═CH-CH(C_2H_5)-CH(CH_3)$_2$	273, 1099, 1100, 3263		
163.	279-19-6	Tricyclo[2.2.1.02,6]heptane 		4249	
164.	707-35-7	Tricyclo[3.3.1.1]decane, 1,3,5-trimethyl- 		2917a	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

In addition to a low level of cholesterol {1a}, tobacco usually contains substantial levels of several phytosterols [campesterol {Ib}, β-sitosterol {Ic}, stigmasterol {Id}, ergosterol {1e}] structurally similar to cholesterol. These phytosterols differ slightly from cholesterol in the structure of the long side chain (Figure 1.3). They are present in tobacco in both the free and bound form (as glycosides, esters, etc.), and they are transferred as such to mainstream smoke (MSS). The sterols constitute about 0.2% of the tobacco weight. As shown in Figure 1.3, pyrolysis of cholesterol {Ia} yields chrysene {III}, Diels hydrocarbon {IV}—a methylcyclopentaphenanthrene—and numerous other polycyclic aromatic hydrocarbons (PAHs). Both PAHs noted have also been identified in pyrolysates of the major tobacco phytosterols [Wynder et al. (4356); Van Duuren (4022)]. While none of the sterols {Ia–Ie} has been shown to generate the potent tumorigen 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) on pyrolysis, Falk et al. (1171) reported that cholesterol and cholesterol esters do generate the mouse-skin tumorigens 4-cholesten-3-one {Va} and 3,5-cholestadiene {VIa}. Veldstra (4042a) reported that the pyrolysis of cholesteryl oleate also yielded 3,5-cholestadiene {VIa}. Cholesteryl oleate was probably a component of the mixture of steryl esters described in flue-cured tobacco by Rowland and Latimer (3358) and in tobacco smoke by Rodgman et al. (3296). The steryl esters included sterols esterified with a series of saturated (palmitic, stearic, etc.) and unsaturated (oleic, linoleic, etc.) acids.

In the late 1950s/early 1960s, Rodgman proposed that the tobacco phytosterols—campesterol, β-sitosterol, stigmasterol, ergosterol—might generate compounds analogous to those generated from cholesterol, i.e., 4-campesten-3-one {Vb}, 3,5-campestadiene {VIb}, β-4-sitosten-3-one {Vc}, 3,5-sitostadiene {VIc}, 4-stigmasten-3-one {Vd}, 3,5-stigmastadiene {VId}, ergosten-3-one {Ve}, 3,5-ergostatriene {VIe}, on thermal degradation of these tobacco phytosterols or their esters during the smoking process. These campesterol-, β-sitosterol-, stigmasterol-, and ergosterol-related compounds might also be mouse-skin tumorigens as are their cholesterol counterparts. For nearly a decade, Rodgman and Cook (3286) were unsuccessful in their periodic efforts to isolate any of these steryl ketones or dienes from cigarette smoke condensate (CSC) and identify them. However, Benner et al. (273) did subsequently identify two

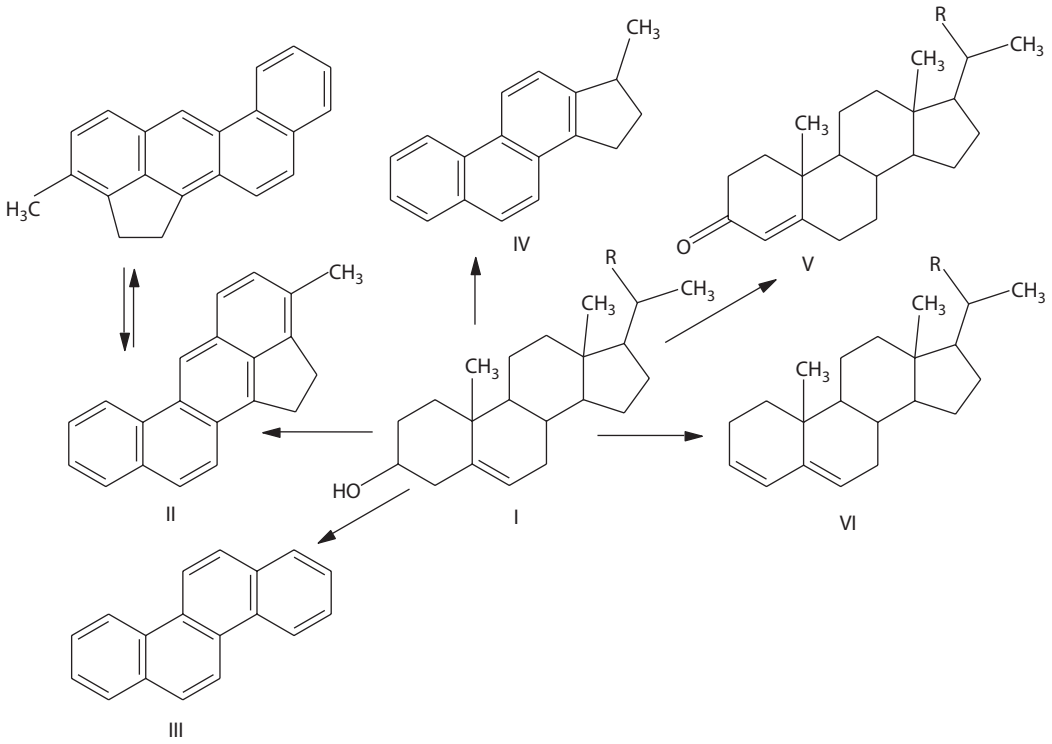


FIGURE 1.3 Possible sterol degradation products. *Sterol*, R═; Ia, cholesterol -$(CH_2)_3$-$CH(CH_3)_2$; Ib, campesterol -$(CH_2)_2$-$CH(CH_3)$-$CH(CH_3)_2$; Ic, β-sitosterol -$(CH_2)_2$-$CH(C_2H_5)$-$CH(CH_3)_2$; Id, stigmasterol -CH═CH-$CH(C_2H_5)$-$CH(CH_3)_2$; Ie, ergosterol[a] -CH═CH-$CH(CH_3)$-$CH(CH_3)_2$; II, 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene); III, chrysene; IV, Diels hydrocarbon; Va, 4-cholesten-3-one; Vb, 4-campesten-3-one; Vc, β-4-sitosten-3-one; Vd, stigmasten-3-one; Ve, ergostadien-3-one; VIa, 3,5-cholestadiene; VIb, 3,5-campestadiene; VIc, β-3,5-sitostadiene; VId, 3,5-stigmastadiene; VIe, 3,5,7-ergostatriene. [a]Ergosterol has a double bond at the 7 position.

of these 3,5-dienes, 3,5-campestadiene {VIb} and 3,5-stigmastadiene {VId}, in tobacco smoke, see also Eatough et al. (1099,1100).

Johnstone and Quan (1973) reported that flue-cured tobacco smoke contains several hydrocarbons related to neophytadiene: an aliphatic acyclic hydrocarbon norphytene (2,6,10,14-tetramethyl-1-pentadecene) and the four alicyclic hydrocarbons {VII–X, Figure 1.4} that are dimers of neophytadiene. These dimers are identical with the major products generated when neophytadiene is heated at 190°C–200°C. The dialkylethenylcyclohexenes {IX and X} were a small proportion of the mixture. The more plentiful pair {VII and VIII} each absorbed two equivalents of hydrogen to form saturated hydrocarbons and were readily dehydrogenated to *p*- and *m*-alkylbenzene derivatives readily separable by column chromatography on alumina. Nitric acid oxidation of these benzenoid hydrocarbons generated *p*-benzenedicarboxylic (terephthalic) and *m*-benzenedicarboxylic (isophthalic) acids, respectively. Johnstone and Quan (1973) considered and rejected the possibility that the dimer mixture may have been artifactually produced during the laboratory generation, collection, and fractionation of the CSC. They noted that "At no time was the condensate subjected to temperatures above 80°C, and that only for short periods, so it is likely that the dimers were formed during the smoking process."

The isolation and identification in the late 1950s and early 1960s of several polyhydronaphthalene derivatives in tobacco

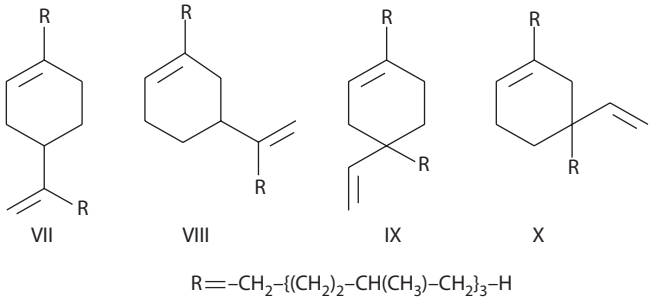


FIGURE 1.4 Phytadiene dimers.

and smoke, e.g., α- and β-levantenolide* (799, 801, 1299), α_2-levantanolide† (1290, 1300), 12α-hydroxy-13-epimanoyl oxide‡ (800, 1298, 3281), sclareolide§ (3272, 3533), and sclaral¶ (3534), subsequently led to the identification of many

* α- and β-Levantenolide are listed by Chemical Abstracts as decahydro-3,3′a,6′,6′,9′a-pentamethyl- and 3′a,4′,5′,5′a,6′,7′,8′,9′,9′a,9′b-decahydro-3,3′a,6′,6′,9′a-pentamethylspiro[furan-2(3*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5(4*H*)-one, respectively.

† α_2-Levantanolide is listed by Chemical Abstracts as dodecahydro-3,3′a,6′,6′,9′a-pentamethylspiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one.

‡ 12α-Hydroxy-13-epimanoyl oxide is listed by Chemical Abstracts as 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl1*H*-Naphtho[2,1-*b*]pyran-2-ol.

§ Sclareolide is listed by Chemical Abstracts as decahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2(1*H*)-one.

¶ Sclaral is listed by Chemical Abstracts as dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2-ol.

more such derivatives [see Enzell and Wahlberg reviews (1156, 1157, 4089, 4090)] among which were several polyhydronaphthalenes, e.g., decahydronaphthalene (222–224), 4,7-dimethyl-1,2,3,5,6,8a-hexahydro-1-(1-methylethyl)-naphthalene, (1156, 1256, 4090), and its isomer 4,7-dimethyl-1,2,4a,5,6,8a-hexahydro-1-(1-methylethyl)-naphthalene (α-muurolene) (404), and two isomers of 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydronaphthalene (valencene and eremophilene) (404).

A similar situation occurred with the cyclotetradecanes. Subsequent to the isolation and identification of several hydroxy derivatives and epoxy derivatives of unsaturated cyclotetradecane from tobacco (3195, 3220, 3221, 3361) and smoke (3361), several trimethyl-(1-methylethyl)-substituted cyclotetradecatrienes and tetraenes were identified in tobacco (1149, 1149a, 3853) and/or smoke (2726).

Table 1.12 lists the alicyclic aliphatic hydrocarbons identified in tobacco and tobacco smoke. Comparison of this updated list with that reported in the earlier edition indicates that over 20 additional alicyclic hydrocarbons are now included in our up-to-date Table 1.12.

1.4 MONOCYCLIC AROMATIC HYDROCARBONS

In this section, monocyclic aromatic hydrocarbons are defined as those compounds with one or more *nonfused* aromatic rings, e.g., benzene, biphenyl, terphenyl, stilbene. Some authors might classify the aromatic hydrocarbons with two or more nonfused rings as polycyclic aromatic hydrocarbons (PAHs). Table 1.13 lists the monocyclic aromatic hydrocarbons identified in tobacco and/or tobacco smoke. None of these compounds was included in Kosak's 1954 catalog of tobacco smoke components (2170). Johnstone and Plimmer (1971) listed only five such compounds [benzene, ethenylbenzene (styrene), methylbenzene (toluene), 1,2,4-trimethylbenzene (pseudocumene), 1,3,5-trimethylbenzene (mesitylene)]. By 1964, Elmenhorst and Reckzeh (1139) listed 11 such hydrocarbons (see Table 1.13). In 1968, Stedman (3797) listed 20 monocyclic aromatic hydrocarbons. The list presented in 1980 by Ishiguro and Sugawara (1884) indicated this number had doubled. To date, over 110 monocyclic aromatic hydrocarbons have been identified in tobacco and/or its smoke. Comparison of our current Table 1.13 with that in our previous edition indicates that over a dozen monocyclic aromatic hydrocarbons have been newly reported over the past 4 years.

In its 1986 review of tobacco smoke components and their relationship to health, the IARC (1870) discussed only three monocyclic aromatic hydrocarbons, namely, benzene, methylbenzene (toluene), and ethenylbenzene (styrene):

> Tobacco smoke contains traces of other volatile compounds found to be carcinogenic in humans or in experimental animals.
>
> Benzene, a human carcinogen [IARC (1868)], has been reported in the MS of cigarettes (12-48 µg/cigarette) and in the SS of a 100-mm US filter cigarette (453 µg/cigarette) [Wynder and Hoffmann (4332); Elmenhorst and Schultz (1140); Jermini et al. (1947)]. It can be assumed that benzene is formed during the burning of tobacco either from precursors with an aromatic or cyclohexane ring or by pyrosynthesis from primary radicals such as C_6H_5… The most abundant volatile hydrocarbon in tobacco smoke is toluene [methylbenzene], which has been reported to occur at levels of up to 164 µg/cigarette in MS and 904 µg in the SS of a 100-mm US nonfilter cigarette (1140, 1947, 4332).

With regard to the carcinogenic activity (actually its leukemogenic activity) of benzene, it was noted:

> Sufficient evidence in animals with new data from US National Toxicology Program (sufficient evidence in humans).

The carcinogenicity of ethenylbenzene was described as follows:

> Limited evidence [in] animals (inadequate evidence in humans).

In 1989, Hoffmann and Hecht (1727) included benzene in their list of 43 tumorigens in tobacco and tobacco smoke. They discussed the role of exposure to benzene in tobacco smoke as follows:

> Significant amounts of benzene are found in cigarette MS (up to 50 µg/cigarette). Sufficient evidence exists that this aromatic hydrocarbon causes leukemia in humans [IARC (1868)]. On the basis of analytical data for exhaled breath, it has been calculated that a smoker inhales about 2 mg of benzene per day while a nonsmoker inhales only 0.2 mg per day [Wallace et al. (4111)]. Former epidemiological studies have not demonstrated a strong association of smoking and leukemia [IARC (1868)]. However, a recent prospective study among 248,000 U.S. veterans indicates that cigarette smokers have a significant increase in mortality from leukemia [Kinlen and Rogot (2096)].

Examination of the compendia of compounds tested for carcinogenicity [Hartwell (1543, 1544); Shubik and Hartwell (3664, 3665); Thompson et al. (3908)] reveals that benzene has not only been tested for its carcinogenicity per se to skin (mouse, rat, guinea pig, rabbit, monkey) but also has been used as the solvent for application of hundreds of compounds (PAHs, their alkyl and other derivatives, plus their nitrogen, oxygen, and sulfur analogs; quinones; aromatic aza-arenes; aromatic amines; sterols and sterol-related compounds) to the skin of a variety of laboratory animals. In many of these latter experiments, groups of "solvent control" animals were painted with benzene at the same time as other test groups were painted with benzene solutions of the compound(s) under investigation. Despite the hundreds of animals skin-painted with benzene, only in very few cases were carcinomas or other tumors observed at the painting site in the "solvent control" benzene-treated animals or in the animals treated in the benzene carcinogenicity studies.

TABLE 1.13
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

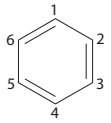
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	71-43-2	Benzene 	73, 111, 112, 126, 126a, 126b, 141–143, 147, 151, 156, 157, 167, 172, 173a, 174a, 174b, 174c, 174e, 199, 203, 222–224, 237, 239, 299, 314, 315, 402, 414, 462, 493–495, 544–546, 566, 568, 568b, 603, 605, 643, 645, 688, 705, 902, 966, 1026, 1050, 1063–1074, 1139, 1140, 1148, 1153, 1154, 1168, 1217, 1243, 1262a, 1313, 1348–1351, 1354, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1412–1414, 1416, 1418, 1423, 1443, 1445, 1472, 1485, 1571a, 1586, 1589, 1634, 1637, 1639, 1643, 1649, 1673, 1674, 1701, 1727, 1740, 1741, 1743, 1744, 1751, 1760, 1773, 1842, 1849–1852, 1868, 1870, 1871, 1873, 1947, 1966, 1975, 2002, 2063, 2079, 2088, 2090, 2096, 2114, 2133, 2142, 2256, 2270, 2293, 2310, 2313a, 2354, 2520, 2543, 2545, 2570, 2589, 2601b, 2634, 2644, 2645, 2765, 2767, 2777, 2782, 2799a, 2800, 2804, 2822, 2825, 2857, 2870, 2939, 2942, 3003, 3007, 3059, 3106, 3135–3137, 3190, 3251, 3254, 3255, 3257, 3260, 3265, 3300, 3302, 3308, 3370, 3368, 3441a, 3410, 3418, 3464–3470, 3482, 3493, 3498, 3500, 3530, 3557, 3692, 3711, 3729, 3794, 3797, 3876, 3897, 3901, 3992, 4005–4007, 4052, 4056, 4078, 4104, 4111, 4135, 4151, 4162, 4166, 4249, 4257, 4259, 4319, 4360, 5012, 5034, 5049, 5070, 5508, 5512, 5531, 5547, 5554, 5692a, 5770, 5811b, 5869a	568b, 984, 4249, 5811b	1228, 1354, 1375a, 1377, 1378, 2244, 3401, 4052, 4056
2.		Benzene, C_3-alkyl-	157, 1371, 1427, 1445, 2508, 2570, 2767, 2773, 2777, 3397		
3.		Benzene, C_4-alkyl-	157, 1371, 1427, 1445, 2570, 2773, 3397		
4.		Benzene, C_5-alkyl-	157, 1427, 1445, 2570, 2773		
5.	886-66-8	Benzene, 1,1′-(1,3-butadiyne-1,4-diyl)bis- C_6H_5-C≡C-C≡C-C_6H_5	4249, 4746		
6.	824-90-8	Benzene, 1-butenyl- C_6H_5-CH═CH-$(CH_2)_2$-CH_3	1959, 4249		
7.	104-51-8	Benzene, butyl- C_6H_5-C_4H_9	152, 3557, 4249		
8.	25340-17-4	Benzene, diethyl-	157, 4249	84	
9.	135-01-3	Benzene, 1,2-diethyl-	5811		
10.	141-93-5	Benzene, 1,3-diethyl-	5811		
11.	105-05-5	Benzene, 1,4-diethyl-	4249, 4832		
12.	25550-13-4	Benzene, diethylmethyl-	3557, 4249		
13.	1330-20-7	Benzene, dimethyl- {xylene}	37, 38, 104, 222–224, 1365, 1445, 1472, 1649, 2088, 2506, 2799a, 3308, 3530, 4249, 4570a, 5034	984, 5811b	
14.	95-47-6	Benzene, 1,2-dimethyl- {*o*-xylene}	84, 112, 156, 157, 199, 222–224, 299, 314, 568b, 797, 1139, 1140, 1153, 1154, 1168, 1313, 1338, 1348–1350, 1354, 1365, 1374, 1375a, 1377, 1416, 1418, 1419, 1443, 1586, 1589, 1634, 1637, 1947, 1975, 2002, 2003, 2142, 2310, 2543, 2545, 2570, 2628, 2731, 2735, 2765, 2767, 2777, 2799a, 2870, 3255, 3302, 3308, 3508, 3530, 3557, 3797, 4104, 4249, 5770, 5811b, 5869a	84, 568b, 2917a, 3186, 4249, 5811b	1354, 1375a, 1377, 2244, 3401

TABLE 1.13 (continued)
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
15.	1014-60-4	Benzene, 1,3-bis(1.1-dimethylethyl)-	5811	5811	
16.	108-38-3	Benzene, 1,3-dimethyl- {*m*-xylene}	84, 111, 112, 142, 143, 151, 156, 157, 172, 199, 222–224, 299, 314, 568b, 798, 1063–1066, 1068–1074, 1110, 1139, 1140, 1154, 1168, 1313, 1348–1350, 1354, 1365, 1374, 1375a, 1377, 1416, 1418, 1419, 1443, 1586, 1589, 1634, 1637, 1639, 1643, 1947, 1975, 2002, 2003, 2142, 2543, 2545, 2570, 2731, 2735, 2765, 2767, 2777, 2799a, 2857, 2870, 3255, 3302, 3308, 3508, 3530, 3557, 3797, 4249, 4354, 4570a, 5811b, 5869a	84, 404, 568b, 2339a, 2917a, 3186, 3188, 4249, 5811b	1354, 1375a, 1377, 2244, 3401
17.	2234-20-0	Benzene, 1,3-dimethyl-2-ethenyl- {2,4-dimethylstyrene}	568b, 4249		
18.	1012-72-2	Benzene, 1,4-bis(1.1-dimethylethyl)-	5811	5811	
19.	100-18-5	Benzene, 1,4-bis(1-methylethyl)-	5811	5811	
20.		Benzene, 3,5-bis(1,1-dimethylethyl)-1-methyl-	1063–1066, 1068–1074		
21.	106-42-3	Benzene, 1,4-dimethyl- {*p*-xylene}	84, 111, 112, 142, 143, 151, 156, 157, 199, 222–224, 299, 314, 315, 568b, 1063–1066, 1068–1074, 1140, 1154, 1168, 1313, 1348–1350, 1354, 1374, 1375a, 1377, 1416, 1418, 1419, 1443, 1586, 1589, 1634, 1637, 1639, 1643, 1947, 1975, 2002, 2003, 2142, 2543, 2545, 2570, 2731, 2735, 2765, 2767, 2777, 2799a, 2870, 3255, 3302, 3308, 3508, 3530, 3557, 3797, 4249, 4570a, 5770, 5811b, 5869a	84, 404, 568b, 2917a, 3186, 3188, 4249, 5811b	1354, 1375a, 1377, 2244, 3401
22.	2039-89-6	Benzene, 1,4-dimethyl-2-ethenyl- {2,5-dimethylstyrene}	568b, 1884, 3757, 4249, 5811b	5811b	
23.	29224-55-3	Benzene, dimethylethyl-	5811, 5811a, 5811b		
24.	934-80-5	Benzene, 1,2-dimethyl-4-ethyl-	2767, 3557, 4249		
25.	874-41-9	Benzene, 1,3-dimethyl-4-ethyl-	2769, 3557, 4249, 4570a		
26.	1758-88-9	Benzene, 1,4-dimethyl-2-ethyl-	2767, 2769, 3557, 4249		
27.	98-06-6	Benzene, (1,1-dimethylethyl)- C_6H_5-$C(CH_3)_3$	348, 1153, 1154, 4249, 5811b	2339a	
28.	14411-56-4	Benzene, 1-(1,1-dimethylethyl)-3-ethyl-	5811		
29.	1075-38-3	Benzene, 1-(1,1-dimethylethyl)-3-methyl-	5811		
30.	644-30-4	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-		1156, 1256, 4090, 4249, 5811b	
31.	4176-17-4	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-, (R)-		1247, 4249	
32.	2049-95-8	Benzene, (1,1-dimethylpropyl)-	5811		
33.	1007-26-7	Benzene, (2,2-dimethylpropyl)- C_6H_5-CH_2-$C(CH_3)_3$		404	
34.	103-29-7	Benzene, 1,1′-(1,2-ethanediyl) bis- {bibenzyl} C_6H_5-CH_2-CH_2-C_6H_5	104, 142, 143, 151, 4249, 5811b	1248, 4249	
35.	588-59-0	Benzene, 1,1′-(1,2-ethenediyl) bis- {stilbene} C_6H_5-CH═CH-C_6H_5	1427, 1981, 1983, 4249	1983	

(*continued*)

TABLE 1.13 (continued)
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

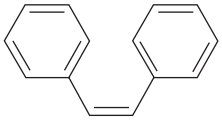
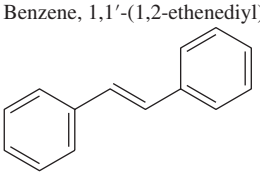
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
36.	645-49-8	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*Z*)- 	1427		
37.	103-30-0	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*E*)- 	1427, 4249		
38.	100-42-5	Benzene, ethenyl- {styrene} C_6H_5-CH═CH_2	73, 104, 111, 112, 141–143, 151, 156, 157, 174a, 174b, 174c, 174e, 299, 314, 315, 566, 568, 568b, 688, 798, 1063–1066, 1068–1074, 1139, 1140, 1153, 1154, 1168, 1217, 1262a, 1313, 1339, 1348–1350, 1354, 1365, 1374, 1375a, 1386, 1414, 1416, 1418, 1419, 1443, 1445, 1472, 1586, 1589, 1634, 1637, 1649, 1740, 1741, 1743, 1744, 1842, 1870, 1871, 1873, 1947, 1975, 1981, 2142, 2313a, 2543, 2570, 2765, 2767, 2777, 2799a, 2825, 2870, 3007, 3190, 3255, 3257, 3265, 3300, 3308, 3464, 3468, 3498, 3508, 3530, 3557, 3711, 3713, 3714, 3729, 3797, 3992, 4078, 4166, 4249, 4570a, 4998, 5012, 5034, 5049, 5512. 5554, 5770, 5811b, 5835, 5836, 5869a	568b, 984, 1983, 2260, 2339a, 2389, 2544, 2917a, 4249, 5811b	1354, 1375a, 3401
39.	27576-03-0	Benzene, ethenyl-, dimethyl-	104, 1472, 1649, 2570, 3757, 4249		
40.	28106-30-1	Benzene, ethenylethyl-	1472, 2494, 4249, 5811b		
41.	71607-81-3 77227-00-0	Benzene, ethenylethyldimethyl-	3757, 4249, 5811, 5811a, 5811b		
42.	27138-10-9 77220-33-8	Benzene, ethenylethylmethyl-	3757, 4249, 5811, 5811a, 5811b		
43.	637-69-4	Benzene, 1-ethenyl-4-methoxy-	4249, 4633		
44.		Benzene, ethenylmethyl-	1472, 5034		
45.	611-15-4	Benzene, 1-ethenyl-2-methyl-	126a, 1416, 3302, 3557, 3729, 3797, 4249, 5811b		
46.	100-80-1	Benzene, 1-ethenyl-3-methyl-	126a, 143, 568b, 1140, 1313, 1416, 3302, 3797, 4249, 5811b		
47.	622-97-9	Benzene, 1-ethenyl-4-methyl-	126a, 143, 568b, 1140, 1313, 1981, 4249, 5811, 5811a, 5811b		
48.	71607-82-4 77226-99-4	Benzene, ethenyltetramethyl-	3757, 4249, 5811, 5811a, 5811b		
49.	50976-21-1 77220-32-7	Benzene, ethenyltrimethyl-	3757, 4249, 5811, 5811a, 5811b		
50.	100-41-4	Benzene, ethyl-	37, 38, 141–143, 152, 199, 222–224, 299, 314, 315, 568b, 798, 1063–1066, 1068–1074, 1139, 1140, 1153, 1154, 1168, 1262a, 1313, 1348–1350, 1354, 1365, 1371, 1374, 1375a, 1416, 1418, 1419, 1586, 1589, 1637, 1975, 1981, 2002, 2003, 2543, 2545, 2570, 2765, 2767, 2775, 2777, 2804, 2870, 3255, 3302, 3308, 3410, 3465–3467, 3508, 3530, 3557, 3797, 4249, 4570a, 5034, 5770, 5811b, 5869a	84, 568b, 984, 2339a, 2389, 2544, 2917a, 3188, 4249, 5811b	1354, 1375a, 2244, 3401

TABLE 1.13 (continued)
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
51.	874-41-9	Benzene, 1-ethyl-2,4-dimethyl-	3557, 4249, 4570a		
52.	25550-14-5	Benzene, ethyl methyl-	1153, 1154, 4249, 4570a, 5034	1153, 4249	
53.	611-14-3	Benzene, 1-ethyl-2-methyl-	84, 568b, 1140, 1313, 1416, 1418, 1419, 2002, 2767, 3302, 3308, 3557, 3797, 4249, 5811b	84, 568b, 2339a, 4249, 5811b	
54.	620-14-4	Benzene, 1-ethyl-3-methyl-	84, 568b, 798, 1140, 1313, 1416, 1418, 1419, 2002, 2870, 3302, 3308, 3557, 3797, 4249, 5770, 5811b	84, 568b, 4249, 5811b	
55.	622-96-8	Benzene, 1-ethyl-4-methyl-	84, 568b, 798, 1140, 1313, 1416, 1418, 1419, 2870, 3302, 3308, 3557, 3797, 4249, 5811b	84, 568b, 4249, 5811b	
56.	18908-70-8	Benzene, 1-ethyl-2-(1-phenylethyl)-		2917a	
57.	18640-62-5	Benzene, 1-ethyl-4-(2-propenyl)-	2767, 4249		
58.	536-74-3	Benzene, ethynyl- {phenylacetylene}	394, 397, 568b, 1139, 2088, 2939, 3302, 3308, 3797, 4249, 5811b		3401
59.		Benzene, 1-(2-hepten-6-yl)-4-methyl-		1256, 4249	
60.	1077-16-3	Benzene, hexyl-	4249, 5811b		
61.	108-88-3	Benzene, methyl- {toluene} C_6H_5-CH_3	37, 38, 73, 104, 111, 112, 126a, 126b, 141–143, 151, 152, 156, 157, 167, 173a, 174a, 174b, 174c, 174e, 199, 222–224, 237, 239, 299, 314, 315, 402, 462, 480, 493–495, 544–546, 566, 568, 568b, 603, 605, 643, 645, 688, 892, 893, 966, 1050, 1063–1074, 1110, 1139, 1140, 1153, 1154, 1168, 1243, 1262a, 1313, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1412–1414, 1416, 1418, 1419, 1423, 1437, 1445, 1472, 1485, 1586, 1589, 1634, 1637, 1639, 1643, 1649, 1674, 1842, 1849–1852, 1947, 1966, 1975, 1981, 2002, 2003, 2060, 2063, 2079, 2088, 2091, 2133, 2134a, 2142, 2270, 2310, 2313a, 2520, 2543, 2545, 2570, 2589, 2634, 2644, 2645, 2731, 2735, 2765, 2767, 2777, 2782, 2799a, 2800, 2804, 2822, 2857, 2870, 2939, 2942, 3007, 3059, 3105, 3106, 3190, 3254, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3373, 3418, 3464–3470, 3482, 3493, 3498, 3500, 3508, 3530, 3557, 3692, 3794, 3797, 3876, 3897, 3939, 3992, 4005–4007, 4052, 4056, 4078, 4104, 4135, 4162, 4166, 4249, 4257, 4259, 4290, 4319, 4360, 4570a, 5012, 5025, 5034, 5049, 5547, 5554, 5692a, 5770, 5811b, 5836, 5869a, 4A02	568b, 984, 1590a, 2339a, 2917a, 3186, 3188, 4249, 5811b	1354, 1375a, 1377, 1378, 2244, 3401, 3402, 4052, 4056
62.		Benzene, ^{14}C-methyl- {toluene-^{14}C-methyl}		1850	
63.	101-81-5	Benzene, 1,1′-methylenebis- {diphenylmethane} C_6H_5-CH_2-C_6H_5	151, 1508, 3757, 4249, 5811b	1256, 4249, 5811b	
64.	98-83-9	Benzene, (1-methylethenyl)- {α-methylstyrene} C_6H_5-$C(CH_3)$=CH_2	142, 143, 151, 339, 1313, 3308, 3465–3467, 3557, 4249, 4570a		

(*continued*)

TABLE 1.13 (continued)
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

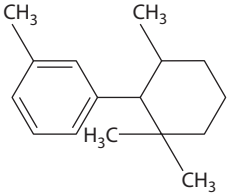
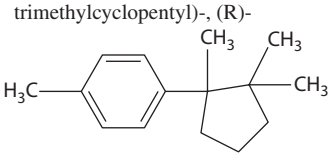
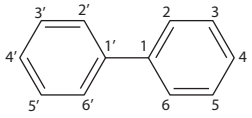
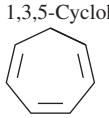
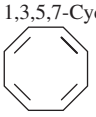
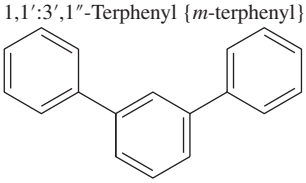
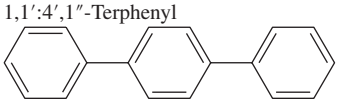
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
65.	98-82-8	Benzene, (1-methylethyl)- {cumene} C_6H_5-CH═$(CH_3)_2$	156, 157, 339, 568b, 1063–1066, 1068–1074, 1139, 1140, 1313, 1416, 1418, 2002, 2628, 2629, 2636, 2799a, 3255, 3308, 3797, 4249, 4570a, 5770, 5811b, 5869a	568b, 984, 4249	
66.	26444-18-8	Benzene, methyl (1-methylethenyl)-	5811, 5811a, 5811b		
67.	1124-20-5	Benzene, 1-methyl-3-(1-methylethenyl)-	143, 4249		
68.	1195-32-0	Benzene, 1-methyl-4-(1-methylethenyl)- {*p*,α-dimethylstyrene}	143, 1139, 1975, 2731, 2735, 3302, 3557, 3797, 4249		
69.	535-77-3	Benzene, 1-methyl-3-(1-methylethyl)- {*m*-cymene}	143, 2767	2339a	
70.	99-87-6	Benzene, 1-methyl-4-(1-methylethyl)- {*p*-cymene}	143, 299, 568b, 798, 1140, 1313, 1365, 1419, 2767, 3224, 3255, 3266, 3308, 3557, 3797, 4249, 5811b	568b, 1053, 1157, 3266, 3370, 4082, 4249, 5811b	
71.		Benzene, methyl-propenyl-	5034		
72.	28729-54-6	Benzene, methylpropyl-	5811b		
73.	17271-70-4	Benzene, 1-methyl-3-(1-propenyl)-	2767, 2769, 3555, 3557, 4249		
74.	1074-43-7	Benzene, 1-methyl-3-propyl-	2769, 3557, 4249		
75.	1074-55-1	Benzene, 1-methyl-4-propyl-	4249		
76.	538-93-2	Benzene, (2-methylpropyl)- C_6H_5-CH_2-CH$(CH_3)_2$	2328a, 4249, 5811, 5811a, 5811b		
77.	1139-49-7	Benzene, 1-methyl-3-(2,2,6-trimethylcyclohexyl)- {toluene, *m*-(2,2,6-trimethylcyclohexyl} 	1110, 3219, 3308, 3557, 4249		
78.	16982-00-6	Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)- 		1156, 1256, 4090, 4249	
79.	2189-60-8 71607-64-2	Benzene, octyl- {phenyloctane} C_6H_5-$(CH_2)_7$-CH_3	1822, 4249, 5811b		
80.	538-68-1	Benzene, pentyl- C_6H_5-$(CH_2)_4$-CH_3	37, 38	4249, 4425, 5811b	
81.	637-50-3	Benzene, 1-propenyl- C_6H_5-CH═CH-CH_3	1313, 2777, 3557, 4249, 4570a, 5811b	5811b	
82.	300-57-2	Benzene, 2-propenyl- {allyl benzene} C_6H_5-CH_2-CH═CH_2	568b, 348, 3557, 4249, 4570a, 5811b		
83.	103-65-1	Benzene, propyl- C_6H_5-$(CH_2)_2$-CH_3	152, 222–224, 299, 348, 568b, 1063–1066, 1068–1074, 1262a, 1313, 1472, 1649, 4249, 4570a, 5770, 5811b, 5869a	568b, 2339a, 4249	

TABLE 1.13 (continued)
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
84.	673-32-5	Benzene, 1-propynyl- C_6H_5-C≡C-CH_3	2570, 2769, 2777, 4249, 5811b		
85.	10147-11-2	Benzene, 2-propynyl-	5811, 5811a, 5811b		
86.	25619-60-7	Benzene, tetramethyl-	2731, 2735, 3226, 4249, 4570a	84, 2339a	
87.	488-23-3	Benzene, 1,2,3,4-tetramethyl-	1959, 4249		
88.	527-53-7	Benzene, 1,2,3,5-tetramethyl-	1959, 3557, 4249		
89.	95-93-2	Benzene, 1,2,4,5-tetramethyl-	1959, 4249, 5811b	5811b	
90.	25551-13-7	Benzene, trimethyl-	1649, 2767, 3226, 4248, 4570a, 5034, 5811b	1248, 2339a, 4101, 4249, 5811b	3401
91.	526-73-8	Benzene, 1,2,3-trimethyl-	37, 84, 568b, 1140, 1313, 1416, 2731, 2735, 3302, 3557, 3797, 4249, 5770, 5811b	84, 568b, 3186, 4249, 5811b	
92.	95-63-6	Benzene, 1,2,4-trimethyl- {pseudocumene}	84, 394, 568b, 1139, 1140, 1168, 1286, 1313, 1416, 1418, 1419, 1634, 1975, 2002, 2601a, 2767, 2870, 3302, 3308, 3557, 3797, 4249, 5811b	84, 568b, 3186, 3188, 4249, 5811b	
93.	108-67-8	Benzene, 1,3,5-trimethyl- {mesitylene}	394, 568b, 1139, 1140, 1262a, 1286, 1313, 1374, 1375a, 1377, 1416, 1418, 1419, 1975, 2088, 2113, 2870, 3302, 3308, 3557, 3797, 4249, 5770, 5811b	568b, 3186, 4249, 5811b	1375a, 1377
94.	92-52-4	1,1′-Biphenyl {diphenyl} 	142, 143, 151, 167, 568b, 1360, 1371, 1375, 1375a, 1375b, 1377, 1427, 1462, 1649, 1751, 2113, 2506, 2507, 2543, 2557, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 3191, 3308, 3410, 3465–3467, 3469, 3616, 3619, 3620, 3729, 3797, 4249, 5811b	84, 568b, 984, 2339a, 3547, 4249, 5811b	1360, 1375a, 1377, 2506, 2507
95.	61141-66-0	1,1′-Biphenyl, 3,4-diethyl-		2917a	
96.	7383-90-6	1,1′-Biphenyl, 3,4′-dimethyl-		984	
97.	613-33-2	1,1′-Biphenyl, 4,4′-dimethyl-	142, 143, 4249		
98.	28013-11-8	1,1′-Biphenyl, ar,ar′-dimethyl-	1360, 1375a, 2570, 2761, 2762, 2765–2767, 2777, 3410, 4249, 5811b	3547, 4249	1360, 1375a
99.	40529-66-6	1,1′-Biphenyl, ethyl-	2570, 3226, 4249		
100.	1812-51-7	1,1′-Biphenyl, 2-ethyl-	4248		
101.	71277-83-3	1,1′-Biphenyl, ethylmethyl-	2328, 4249, 5811b, 1D01, 1E01		
102.	28652-72-4	1,1′-Biphenyl, methyl-	1371, 1649, 2543, 2570, 2731, 2735, 2767, 2773	2339a, 3547, 4249	
103.	643-58-3	1,1′-Biphenyl, 2-methyl-	372, 2777, 4249		
104.	643-93-6	1,1′-Biphenyl, 3-methyl-	104, 1360, 1375a, 2570, 2761, 2762, 2765–2767, 2777, 3619, 3620, 3758, 3759, 4249, 5811b		1360, 1375a
105.	644-08-6	1,1′-Biphenyl, 4-methyl-	104, 1110, 1360, 1375a, 2761, 2762, 2765, 2766, 2777, 3492, 3619, 3620, 3758, 3759, 4249, 5811b		1360, 1375a
106.	71294-42-3	1,1′-Biphenyl, propyl-	2328, 4249		
107.	30581-97-6	1,1′-Biphenyl, trimethyl- {3 isomers detected}	2328, 2570, 4249		
108.	544-25-2	1,3,5-Cycloheptatriene (tropilidene) 	1153, 1154, 4249, 5811b	1153, 4249	

(*continued*)

TABLE 1.13 (continued)
Monocyclic Aromatic Hydrocarbons in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
109.	629-20-9	1,3,5,7-Cyclooctatetraene 	2506, 2507, 3397, 5811b		2506 (0), 2507 (0)
110.	530-45-0	Ethane, bis(4-methylphenyl)-		2917a	
111.	29036-02-0	Quaterphenyl	1884, 1900		
112.	92-06-8 26140-60-3	1,1′:3′,1″-Terphenyl {*m*-terphenyl} 	1462, 3308, 4249		
113.	92-94-4	1,1′:4′,1″-Terphenyl 	4248		

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

Examination of the references listed for benzene provides an indication of the amount of research and discussion pertinent to the presence of benzene in tobacco smoke.

Rodgman and Green (3300) in their discussion of toxicants in tobacco and tobacco smoke noted that subsequent lists and discussions generated after that of IARC (1870) included not only benzene but also ethenylbenzene (styrene) [see Table 1.15 in (3265) and Table 1 in (3300)] and methylbenzene (toluene) [see Table 1 in (3300)].

1.5 POLYCYCLIC AROMATIC HYDROCARBONS

Classified as toxicants in many of the substances to which humans are exposed are the polycyclic aromatic hydrocarbons (PAHs). Such exposures include air pollutants from a variety of sources, foodstuffs and beverages, and tobacco smoke. Since the early 1950s, the composition of the latter has been more completely defined than that of any other consumer product. Over 5200 components have been identified in tobacco smoke and among these are over 500 PAHs either completely or partially identified.

Because of the tumorigenicity of many PAHs, much research has been conducted in attempts to define the relationship between the PAH structures and their specific tumorigenicities in laboratory animals. None of the theories to date completely answers all the questions. In 2006, Rodgman and Perfetti (3306a) cataloged the PAHs completely or partially identified in cigarette smoke as a prelude to an attempt to develop a more reasonable PAH structure–tumorigenicity relationship. Additionally, they tabulated the PAHs considered in several previous studies on structure–tumorigenicity relationships, studies that dealt primarily with all-benzenoid PAHs. The majority of the information included in Section 1.5 comes from the 2006 article from Rodgman and Perfetti (3306a).

Tobacco and tobacco products in the forms of leaf, shredded or grounded tobacco, and various forms of cigars and cigarettes have been available to individuals for ages. For centuries, people have enjoyed tobacco but have been admonished of its potential health concerns. Health concerns for cigarette smokers have increased steadily since the early 1950s due to the rapid development and advancement in separation sciences, toxicology and medicine. In his 1954 publication, Kosak (2170) was the first person to catalog compounds reported in tobacco smoke. His list contained fewer than 100 compounds, and a significant number were incorrectly characterized. Today, over 5200 compounds have been identified as components in tobacco smoke [see Figure 1, p. 140 in (1373)]. Over the past 50 years, the tobacco industry has made significant progress in both the identification of tobacco and smoke components and the development of technologies to reduce cigarette smoke yields. Significant efforts continue in government, academia, and especially the tobacco industry to understand the health effects of smoking and to develop cigarette products with reduced health risks for smokers. One class of tobacco smoke components that has been studied extensively and intensively is the PAHs due to their potential health concerns.

Periodically, tobacco researchers have reported the progress on the identification of tobacco and smoke components. Review articles by Johnstone and Plimmer (1971) and Izawa (1900) detailed the tobacco and smoke research conducted over 100 years. Izawa listed 440 identified smoke components

by 1961. Quin (3059) published a review of components found in tobacco and smoke. Herrmann (1625) reviewed phenolic compounds in tobacco smoke. In 1963, Philip Morris (2939) published a monograph on tobacco and smoke composition, a copy of which was provided the Advisory Committee on smoking and health to the U.S. Surgeon General (3999). In 1964, Elmenhorst and Reckzeh (1139) tabulated the aromatic hydrocarbons identified in tobacco smoke. Kuhn (2226) published an article on alkaloids in tobacco and smoke. In their 1967 book, Wynder and Hoffmann (4332) discussed tobacco and smoke chemistry and the results of animal studies with tobacco smoke. Elmenhorst and Schultz (1140) listed 250 low-boiling components and vapor-phase components identified in tobacco smoke. In his 1968 review, Stedman (3797) listed nearly 1200 identified tobacco and smoke components. The next year, Neurath (2724) reported on the presence of 180 nitrogen-containing compounds in smoke. With the meaningful advancements in analytical methodology, the number of tobacco and smoke components increased dramatically (1371). At R. J. Reynolds Tobacco Company (RJRT), Schumacher et al. (3553), Heckman and Best (1587), and Newell et al. (2769) identified 1490 compounds in the water-soluble and ether-soluble fractions of tobacco smoke: 365 were confirmation of previously reported components and 1125 were newly identified components. In 1977, Schmeltz and Hoffmann (3491) cataloged nearly 500 *N*-containing compounds identified in tobacco smoke, but their catalog did not include the more than 230 *N*-containing compounds newly identified in tobacco smoke by Heckman and Best (1587). Between 1974 and 1978, Snook et al. (3732, 3756–3759) published the results of their massive study of the PAHs identified in tobacco smoke, a study that was followed by an equally definitive one published in 1981 on the aza-arenes in tobacco smoke (3750). In 1980, Ishiguro and Sugawara (1884) listed 1889 identified tobacco smoke components in their monograph. However, a tally of the reported tobacco smoke components at that time exceeded 2500. No additional catalogs of the total number of identified components of cigarette mainstream smoke (MSS) have been published since the 1980 Ishiguro and Sugawara (1884) publication. Smith et al. (3712) recently reported the chemical structures of the 253 identified phenols reported in cigarette MSS.

Numerous catalogs of PAHs identified in MSS have been compiled from 1955 through 2005. Table 1.14 is a chronology of catalogs of PAHs in MSS. It contains the year of each catalog, author (and reference), and the number of PAHs listed. The catalogs prior to 2006 contain much overlap in terms of the PAHs identified. In 2006, Rodgman and Perfetti (3306a) published a report that attempted to eliminate the overlap and clearly present the 539 PAHs identified in MSS. The intent of this chapter is to present a referenced catalog of the either completely or partially characterized* PAHs in tobacco, tobacco MSS, and MSS of tobacco substitutes. The catalog to follow (Table 1.19) contains the CAS registration number, chemical name, structure, and alphabetical listing of references on PAHs.

TABLE 1.14
Chronology of Catalogs of PAHs in MSS

Year	Author	No. of PAHs Listed	Reference
1954	Kosak	4[a]	2170
1955	Latimer	10	2270
1957	Latimer and Rodgman	33	2292a
1958	Rodgman	36	3245
1959	Johnstone and Plimmer	57	1971
1960	Rodgman and Menz	68	3301
1962	Rodgman et al.	77	3303
1963	Philip Morris	61	2939
1963	Rodgman et al.	77	3304
1964	Elmenhorst and Reckzeh	70	1139
1965	Rodgman et al.	85	3302
1967	Rodgman and Woosley	85	3308
1968	Stedman	79	3797
1975	Roberts et al.	206	3224
1976	Snook et al.	252[b]	3758
1977	Snook et al.	157[b]	3756
1978	Snook et al.	438[b]	3757
1980	Ishiguro and Sugawara	191	1884
1997	Williams et al.	427[c]	4249
2005	Rodgman and Perfetti	539[d]	3306a

[a] Three of the PAHs listed were identified in a destructive distillate of tobacco, not in tobacco smoke.

[b] In the three articles on the PAH study by Snook et al. (3756–3758), some identified PAHs were listed in more than one article.

[c] In several instances, more than one isomer was reported for some monoalkyl-, dialkyl-, trialkyl-, and tetraalkyl-PAHs, but the positions of the alkyl groups were not determined. In the case of such multiple alkyl isomers, only one was listed in this report.

[d] This list includes the number of isomers of monoalkyl-, dialkyl-, trialkyl-, and tetraalkyl-PAHs reported where the positions of the alkyl groups were not determined.

The significant increase in the number of studies on tobacco smoke composition was triggered by the following events: (1) the results in the early 1950s from several retrospective epidemiology studies (1026a, 1027, 3529, 4306b) in which it was reported that an association existed between cigarette smoking and the incidence of lung cancer in smokers, (2) a 1953 report of the production of skin carcinoma in susceptible laboratory animals skin painted repeatedly with a concentrated solution of cigarette MSS condensate supposedly produced under conditions simulating the human smoking of a cigarette (4306a), (3) the realization in 1954 that very little (2170) was known about the composition of tobacco smoke to which consumers had been exposed for nearly 400 years, and (4) the incorporation of chromatography into the overall methodology of the fractionation of complex mixtures such as tobacco smoke.

Naturally, these findings raised several questions. The first dealt with the identity of the cigarette MSS component(s)

* The term "partially characterized" or "partially identified" indicates that the position of one or more alkyl substituents was not determined.

responsible for the smoking–lung cancer association in smokers and the skin tumor induction in laboratory animals. Because of extensive data generated on the specific tumorigenicity of about 25% of the hundreds of PAHs synthesized between 1929 and the early 1950s (1543, 1544), PAHs were considered the most likely tumorigenic agents in cigarette MSS even though their presence was not certain. Eventually, numerous PAHs were identified in cigarette MSS. Because of its MSS level and its high specific tumorigenicity in several bioassays, one PAH was subjected to intense scrutiny: benzo[*a*]pyrene (B[*a*]P). As a carcinogen, B[*a*]P elicited carcinomas at the painting site in the mouse-skin bioassay. As a sarcogen, B[*a*]P elicited sarcomas in rodent bioassays involving subcutaneous injection.

One class of tobacco smoke components studied extensively is the PAHs. As reported by Rodgman (3262), between 1950 and 1970, an extensive amount of research was conducted on tobacco- and cigarette smoke-related topics. The information generated led to the development of several significant cigarette design technologies that resulted in the modification of the delivery and composition of cigarette MSS.

The following is a brief chronology of the events occurring in the tobacco smoke–PAH situation: In 1939, the PAHs anthracene, phenanthrene, and B[*a*]P were reported as components of a tobacco-related material by Roffo (3323–3325) and his son (3316, 3318). In discussions of tobacco smoke, the Roffo findings are generally disregarded because the three PAHs they reported were not detected in tobacco smoke but in a destructive distillate of tobacco. However, Roffo did report another finding that led to much research both within and outside the tobacco industry. Roffo reported that comparison of the destructive distillate of tobacco with that of an ethanol-extracted tobacco indicated (3327) that the PAH content and specific tumorigenicity of the extracted tobacco destructive distillate were reduced from those of the destructive distillate from the control tobacco. Roffo speculated that the precursors of the tumorigenic PAH components of his distillates were ethanol-soluble phytosterols. Eventually, his prediction, as far as it went, was found to be true for cigarette MSS (3269, 3616). Because he was unaware of the presence in tobacco of long-chained terpenoids such as solanesol, identified in flue-cured tobacco in 1957 by Rowland et al. (3359), Roffo obviously could not include them in his 1942 precursor prediction. It should be noted that the findings by Roffo on destructive distillates of tobacco were subsequently equivalent to the effects observed in smoked tobacco, i.e., organic solvent extraction of a tobacco or tobacco blend which was then incorporated into cigarettes gave MSS with reduced PAH levels and specific tumorigenicity to mouse skin compared to the MSS from control tobacco. However, usually the reduction in specific tumorigenicity was less than the reduction in PAHs, particularly B[*a*]P.

1.5.1 Controversies over the Roffo Investigations

Because the results of a 1930 biological study reported by Roffo (25A50) on a tobacco-related material, a destructive distillate from tobacco, coincided with the demonstration of the tumorigenicity to rodent skin of the PAH DB[*a*,*h*]A in 1930 (2078) and preceded the demonstration of similar tumorigenicity of B[*a*]P in 1932 (797), questions were frequently raised about the pertinence to tobacco smoke of the subsequent Roffo findings in which the destructive distillate tar was reported not only to be tumorigenic to laboratory animal skin but also to contain the tumorigenic B[*a*]P (see Table 1.15).

In their comments on the Roffos' reports of their investigations on the chemical composition and biological properties of a destructive distillate from tobacco and the presence of B[*a*]P in the distillate (claims based on spectroscopic data), Wynder et al. (4306a) noted that Roffo had claimed to have identified B[*a*]P in the tobacco destructive distillate, but his finding was not confirmed by Cooper et al. (813). However, Wynder et al. did note that Eby (25A21), in his examination of the cigarette tar used in the Wynder et al. 1953 biological study, did not detect B[*a*]P. They made little comment about Eby's failure to identify B[*a*]P or any other tumorigenic PAH in the Wynder et al. cigarette tar or the 1957 summary by Fieser (1181) on (1) the inadequacy of the spectroscopic data purported to indicate the presence of B[*a*]P in cigarette tar or (2) the failure of Fieser's colleagues to detect B[*a*]P in cigarette tar despite their success in identifying B[*a*]P in roast coffee.

Later, in their lengthy 1964 review [see p. 259 in (4319)] and 1967 book [see p. 94 in (4332)], Wynder and Hoffmann essentially dismissed the research by Roffo on a tobacco destructive distillate by tersely noting that the preparation by Roffo of a tobacco "tar" for a carcinogenicity test involved the mere destructive distillation of tobacco, thus excluding the Roffo investigations from any discussion of tobacco smoke.

Of course, most criticisms of Roffo's research findings were based on his production of a tobacco tar by destructive distillation of tobacco, a process not considered comparable to the normal combustion of tobacco in a cigarette in the presence of air and its oxygen. It is indeed true that, during the cigarette puff, the oxygen level immediately ahead of the fire cone is depleted from the ≈21% level of air, but as Newsome and Keith (2780) demonstrated, the oxygen level is not 0% as it might be during destructive distillation. During the smoking process, the cigarette system has access to air (and its oxygen content) surrounding the cigarette both during and between puffs. Cigarette paper porosity also dictates some air flow through the cigarette paper during the puff.

In 1961, Larson et al. [see pp. 422–424 in (5260)] provided a critique of Roffo's rabbit-skin-painting studies with destructive distillates from tobaccos. Roffo succeeded in producing tumors, many of which were described as carcinomas or epitheliomas, in the treated rabbits. Because of the small number of tumors generated in the Roffo biological studies, Larson et al. considered that one must be very hesitant in placing too great weight on Roffo's reiterated description of a solitary tumor.

Roffo also claimed that his tobacco tar generated by destructive distillation was more tumorigenic than equivalent doses of coal tar, a finding at odds with those of many investigators, even those who compared the tumorigenicity in mice of various tobacco-tar preparations with that of equivalent doses of coal-tar solutions (see Table 1.15).

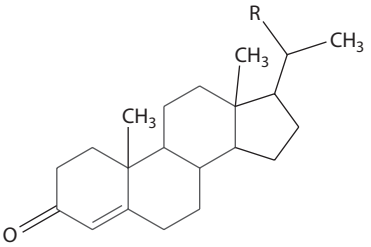
TABLE 1.15
Comparison of Roffo's Findings on the Destructive Distillate of Tobacco *vs.* Research Findings Reported by Others on Tobacco Smoke

Roffo and the Destructive Distillate of Tobacco and Other Related Research	Tobacco Smoke and Other Related Research
Roffo (5354) defined CO derived from tobacco as a hazard	Many investigators pre-1954 (see Table 1) and post-1953 proposed the CO in tobacco smoke as a hazard. Subsequently, because of its hazard, CO became categorized as a "Hoffmann analyte" [see Chapter 23 in (5078)]
A.E. Roffo (3316, 3318) identified several PAHs (anthracene, B[*a*]P, phenanthrene) in the destructive distillate of tobacco	In 1953, several PAHs (anthracene, pyrene) were identified in cigarette smoke by R.L. Cooper and Lindsey (818)
B[*a*]P was identified in the destructive distillate of tobacco (3323, 3325, 3326, 3327, 5360).	• E.A. Cooper et al. (813) stated that they could not confirm Roffo's finding of B[*a*]P in the destructive distillate of tobacco
Note: The Roffo's reported 1,2-benzpyrene in the tobacco destructive distillate. 1,2-Benzpyrene was the name originally assigned by Cook et al. (797) to their coal-tar isolate. Subsequently, the nomenclature 1,2-benzpyrene was changed to 3,4-benzpyrene and then to benzo[*a*]pyrene by the IUPAC	• However, it should also be noted that Eby (25A21) could not detect B[*a*]P in the "tar" used by Wynder et al. (4306a) in their noted 1953 biological study • In 1957, Fieser (1181) classified as inadequate the ultraviolet spectrographic data claimed by R.L. Cooper and Lindsey (820) and by Rand personnel (55, 593, 2335) as indicating B[*a*]P in cigarette "tar" • Fieser's colleague could not detect B[*a*]P in cigarette "tar" but identified it in roast coffee (1181) • B[*a*]P was eventually accepted universally as a cigarette smoke component after the published report in 1959 of its isolation in crystalline form from cigarette smoke by Wynder and Hoffmann (4307) • Fourteen PAHs, including benz[*a*]anthracene (B[*a*]A), B[*a*]P, and DB[*a,h*]A, had previously been isolated individually from cigarette smoke (3273), 12 in crystalline form, two as oils [see Table 1 in Rodgman(3262)]
In 1930 and 1939, Roffo reported the tumorigenicity to animal skin of the destructive distillate of tobacco (3320, 5361, 5362, 25A52)	In 1953, cigarette "tar" was reported to be tumorigenic to mouse skin in the renowned study by Wynder et al. (4306a, 5202) and subsequently reported to be tumorigenic to several other species [see Tables VII 1–3 in (4332)]
Roffo reported that the specific tumorigenicities of the destructive distillates from the different tobacco types were essentially the same (3324, 5359, 25A60)	As reported by Wynder and Hoffmann in 1963 (4317), subsequent findings with tobacco smoke did differ from those reported by Roffo (3324, 5359, 25A60). The specific tumorigenicities (mouse skin) of the cigarette "tars" from different tobacco types varied as follows: flue-cured = Oriental > Maryland > burley. The B[*a*]P levels in the CSC varied as follows: flue-cured > Oriental > Maryland > burley
Roffo (5357) claimed that the destructive distillate "tar" from tobacco showed greater specific tumorigenicity to laboratory animals than did coal tar	Later, Jaffe et al. (5233) and Hueper (5230) described findings that disagreed with those of Roffo, i.e., they reported that coal tar showed greater specific tumorigenicity to laboratory animals than did tobacco "tar"
The yields of B[*a*]P and other PAHs in the destructive distillate from organic solvent-extracted tobacco were less than those in the destructive distillate from the control (unextracted) tobacco (3327)	The per cigarette yields of B[*a*]P and other PAHs were less in the "tar" (CSC) from organic solvent-extracted tobacco than those in the CSC from control (unextracted) tobacco (116, 3241, 3246, 4353, 4354) [see Table 3 in Rodgman (3262)]
The destructive distillate from the organic solvent-extracted tobacco showed less tumorigenicity than the destructive distillate from the control (unextracted) tobacco (3327)	The CSC from organic solvent-extracted tobacco showed lower specific tumorigenicity than CSC from control tobacco but the % decrease in specific tumorigenicity was less than the % decrease in the B[*a*]P content (4353, 4354) of the CSC
Roffo proposed that the precursor in tobacco of the PAHs in the destructive distillate from tobacco (3327) was phytosterol. *Note*: In 1939 and 1941, cholesterol was not a known component of tobacco. Also, high molecular weight terpenoids such as solanesol, neophytadiene, and the cyclotetradecane derivatives had not yet been identified as tobacco components. Each cyclotetradecane derivative had a 14-carbon structure similar to that in anthracene or phenanthrene. Subsequently, the high molecular weight terpenoids and derivatives (solanesyl esters) were identified in tobacco (and tobacco smoke) as were cyclotetradecane derivatives plus numerous phytosterols and their long-chained aliphatic esters plus cholesterol, its glycoside, and many long-chained aliphatic cholesteryl esters	• Subsequently, identified in tobacco were several phytosterols [stigmasterol (1433), sitosterol (1080), campesterol (1082), ergosterol (1080)] and cholesterol (1434, 5152) and their long-chained aliphatic esters (3296). All were also identified in tobacco smoke components (612, 1434, 2178) • The saturated aliphatic hydrocarbons,[a] the phytosterols,[b] and terpenoids[c] (such as solanesol and its long-chained aliphatic esters) in tobacco, were demonstrated to be major precursors of PAHs in CSC in a 1979 study by Severson et al. (3616) of the USDA and in a 1958 study in which the levels of each category in the cigarette tobacco were doubled and tripled (3269) • In 1963 and 1964, Rowland et al. (3361) described the conversion of a cyclotetradecane derivative to a phenanthrene derivative

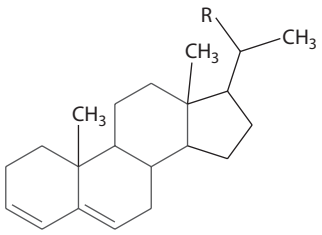
(*continued*)

TABLE 1.15 (continued)
Comparison of Roffo's Findings on the Destructive Distillate of Tobacco *vs.* Research Findings Reported by Others on Tobacco Smoke

Roffo and the Destructive Distillate of Tobacco and Other Related Research	Tobacco Smoke and Other Related Research
In 1939, Roffo demonstrated that the pyrolysate from cholesterol was tumorigenic (4A03, 25A58), a confirmation of the 1928 findings of Kennaway and Sampson (2080) and a prelude to the 1949 findings of Falk et al. (1171).	A cholesterol pyrolysate was demonstrated to be tumorigenic in 1928 by Kennaway and Sampson (2080), in 1945 by Beck et al. (5125), and again in 1949 by Falk et al. (1171)
Note: In 1939 and 1941, cholesterol was not a known component of tobacco	
Roffo reported that the tumorigenicity of his cholesterol pyrolysate was due to derivatives of phenanthrene (4A03)	• Pyrolysis of cholesterol and cholesteryl esters yielded two tumorigenic compounds, 4-cholesten-3-one and 3,5-cholestadiene (1171, 4042a), both of which may be considered as phenanthrene derivatives

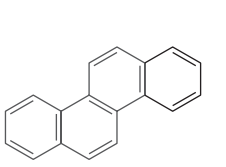


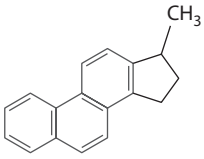
4-Cholesten-3-one



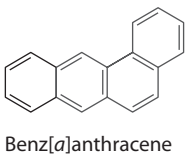
3,5-Cholestadiene

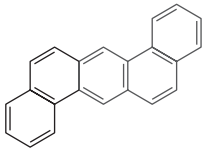
- In the 1935 report on his pyrolysis of cholesterol, Cohen et al. (5151) described the generation of phenanthrene derivatives, the so-called Diels hydrocarbon (17-methyl-17*H*-cyclopenta[*a*]phenanthrene) and chrysene. At one time, chrysene was classified as a carcinogen by the IARC (1868a), but subsequently, the IARC canceled its carcinogen classification
- By 1951, many phenanthrene derivatives had been reported as tumorigenic, e.g., 1,2,3,4-tetramethylphenanthrene (1544)
- Also, chrysene, the Diels hydrocarbon, and several tumorigenic PAHs such as benz[*a*]anthracene B[*a*]A, DB[*a,h*]A, and B[*a*]P are obviously related structurally to phenanthrene since each has one or more additional benzene rings fused to a phenanthrene structure

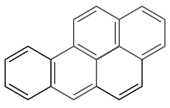

Chrysene

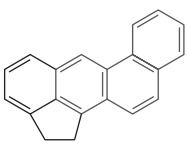


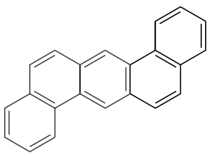
Diels hydrocarbons


Benz[*a*]anthracene






Cholanthrene


Dibenz[*a,h*]anthracene

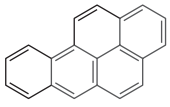

Benzo[*a*]pyrene

TABLE 1.15 (continued)
Comparison of Roffo's Findings on the Destructive Distillate of Tobacco *vs.* Research Findings Reported by Others on Tobacco Smoke

Roffo and the Destructive Distillate of Tobacco and Other Related Research	Tobacco Smoke and Other Related Research
In 1939, Roffo reported the tumorigenicity to laboratory animals of heated/oxidized "fat" (25A53, 25A55)	• Subsequent studies on heated fats essentially confirmed the findings of Roffo, e.g., Peacock and Beck (5327), Lane et al. (5257), but a study by Morris et al. (5292) did not • Fat components such as saturated hydrocarbons were shown to yield tumorigens on heating, e.g., (142, 2257) • Fat components such as high molecular weight aliphatic esters and triglycerides yield tumorigens on heating (1646, 2111a, 5212)
Duplicating his tobacco destructive distillate procedure, Roffo reported in 1940 that the destructive distillate from tea was tumorigenic (5356) as was the destructive distillate of Yerba mate (5358) *Note*: Yerba mate is a tea like substance containing xanthines and used for drink preparations, including toasted Yerba mate used in drink preparation	• In the late 1950s, tumorigenic PAHs were reported in tea and coffee by Kuratsune (2237) and Kuratsune and Hueper (2236) • In his 1988 review, Maga (2438) summarized the identification of numerous tumorigenic PAHs in foodstuffs and beverages, including tea and coffee
In 1939, Roffo reported that the destructive distillate from coffee was tumorigenic to laboratory animals (5355)	• In 1939, Widmark (5466) reported that an extract of roasted coffee was tumorigenic to laboratory animals • With improved analytical technology available in the mid-1950s, B[*a*]P was identified in roast coffee by Fieser's colleagues (1181, 2236, 2237), but no B[*a*]P was identified by them in cigarette "tar"

[a] Considered a major precursor of PAHs by Lam and by Wynder; demonstrated to be significant but less significant than phytosterols and terpenoids such as solanesol.
[b] Considered a major precursor of PAHs by Wynder and Wright (4353); demonstrated to be major by Rodgman and Cook (3260) and by Severson et al. (3616).
[c] Considered a major precursor of PAHs by Wright; demonstrated to be major by Rodgman and Cook (3269) and Severson et al. (3616).

Despite the numerous criticisms of the information provided by Roffo in his numerous publications issued in the 1930s and early 1940s on the destructive distillate from tobacco because of the purported lack of pertinence of such information to that derived from studies on tobacco-derived smoke, it is interesting to compare the results reported by Roffo on the chemical and biological properties of the tobacco destructive distillate with those obtained post-1953 with tobacco smoke, particularly cigarette smoke. Also interesting is the comparison of the findings of Roffo on the pyrolysis of several tobacco components with reports by other investigators. Such comparisons are also presented in Table 1.15.

Although many of the findings reported by Roffo on the tobacco destructive distillate differ in degree from findings reported for tobacco smoke, many of the tobacco destructive distillate and tobacco smoke findings do parallel each other generally. As indicated in Table 1.15, two Roffo findings do differ substantially from those reported by other investigators: (1) the relationship between the tumorigenicity of tobacco destructive distillate *vs.* coal-tar tumorigenicity and (2) the similarity of the tumorigenicities of the destructive distillates from different tobacco types reported by Roffo (3324, 5359, 25A60) *vs.* the difference in tumorigenicities of the MSS "tars" from various tobacco types reported by Wynder and Hoffmann (4317). Recently, Proctor (5341) summarized the contributions of Roffo to our tobacco-pertinent knowledge and noted several of the investigators who were either supportive of or critical of his findings.

The generation in the early 1950s of carcinomas in laboratory animals (mice) skin painted with a solution of the mainstream "tar" from commercial cigarettes (4306a) led to numerous studies to identify the possible causative agent(s) in the "tar." Since much more tumorigenicity data and knowledge were available on PAHs than on any other class of compounds, most of the effort was concentrated on identifying PAHs in cigarette smoke condensate (CSC) as the possible cause of the tumorigenicity. Because of its demonstrated potency as an initiator of carcinomas on skin painting and the wealth of information on it, B[*a*]P became the target of much research on CSC. In 1951, Hartwell (1544) listed nearly 350 studies on the tumorigenicity of B[*a*]P administered in various ways to various species. The other previously studied PAHs were dibenz[*a,h*]anthracene (DB[*a,h*]A) and 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) with 240 and 303 reported biological studies, respectively. Benz[*a*]anthracene (B[*a*]A) and 7,12-dimethylbenz[*a*]anthracene (DMB[*a*]A) were listed with 20 and 32 studies, respectively. In the 20 studies reported by Hartwell (1544), a malignant tumor was noted in only one instance with B[*a*]A.

Although B[*a*]P was reported as a CSC component in the mid-1950s by several American (55–57, 592–594) and British investigators (820) on the basis of spectral evidence, Fieser, as late as 1957 (1181), considered the published evidence to be

inadequate as proof of the presence of B[*a*]P in CSC. Obviously, in 1957, Fieser was unaware of the report by Rodgman in 1956 (3240) on the isolation of crystalline B[*a*]P from MSS or the reports by Falk and Kotin in 1955 and 1956 (1172) on the determination of the per cigarette yields of B[*a*]P (plus B[*a*]A and dibenzo[*def,p*]chrysene) in MSS and sidestream smoke (SSS). Shortly thereafter, in 1959, Wynder and Hoffmann reported the isolation of B[*a*]P in crystalline form from CSC (4307), thus ending the controversy about its presence in cigarette smoke.

In 1954, knowledge of cigarette MSS composition was extremely limited. As mentioned earlier, Kosak (2170) listed fewer than 100 components reported in tobacco smoke, and many of those listed were incorrect. Some of the early research on cigarette MSS composition, particularly the PAHs, was conducted at RJRT.* Complete details of the experimental procedures and findings are available on the Internet at www.rjrtdocs.com.

The initial RJRT PAH investigation involved 11 PAHs in the MSS from nonfiltered cigarettes (3240, 3244) [see Table 1 in (3262)]. Naphthalene, anthracene, pyrene, fluoranthene, and B[*a*]P, isolated in crystalline form, were characterized by UV absorption spectral data as well as by classical chemical means (mixture melting point, IR spectra, derivatization, and derivative properties). The other six PAHs were identified on the basis of agreement of their UV absorption spectra with those of authentic samples or with published UV data.

The second RJRT investigation involved the MSS from filter-tipped cigarettes (3249, 3273, 5077) [see Table 1.15 in (3262)]. In that study, 43 PAHs, including the 11 PAHs found in the initial study, were identified (3240, 3244). Of the 43 PAHs, 14 were isolated (12 in crystalline form and 2 as liquids) and characterized by both UV spectral and classical chemical means [see Table 1 in (3262)]. B[*a*]P, B[*a*]A, DB[*a,h*]A, and several other PAHs were also isolated in crystalline form from the CSC (3240, 3244, 3273). The other 29 were identified from the agreement of their UV absorption spectra with those of authentic samples or with published spectra. B[*a*]P, B[*a*]A, and DB[*a,h*]A had been reported to be tumorigenic to mouse skin, although the bioassay data for B[*a*]A were contradictory (983, 1543, 1544).

Although much of the early research at RJRT R&D on the identification of PAHs in MSS and the effect of various tobacco blends and/or treatments on their MSS yields was summarized in several recent publications (3262, 3307), other members of the U.S. tobacco industry were also much involved in similar research in the 1960s and 1970s. The following paragraphs provide a few examples of their early efforts:

At Philip Morris in 1963, Robb et al. (3191) described the identification of 14 PAHs (naphthalene, fluorene, anthracene, 9-methylanthracene, phenanthrene, fluoranthene, pyrene, 1-methylpyrene, B[*a*]P, B[*e*]P), DB[*a,h*]A, benz[*e*]acephenanthrylene, perylene, benzo[*ghi*]perylene), biphenyl, and the aza-arene, carbazole, in cigarette MSS. Almost all the details in this 1963 Philip Morris in-house report were subsequently presented at the 1964 CORESTA meeting and published in 1965 (3191). Also at Philip Morris, Carpenter (606a) in 1964 described the per cigarette B[*a*]P yields from several commercial cigarettes; Oakley (2817a) in 1965 reported the per cigarette B[*a*]P yields from cigarettes fabricated from different tobacco types (flue-cured, burley, Oriental); Segura (3579a) in 1966 reported the contribution of cigarette paper to the per cigarette B[*a*]P yield; Johnson (1962b) in 1965 described the effect of a tobacco additive, aluminum chloride, on the MSS B[*a*]P yield; and Oakley (2817b) in 1966 determined the difference in per cigarette B[*a*]P yield in MSS and SSS.

At British American Tobacco Company (BAT) in 1966, Chakraborty and Thornton (646a) studied the effect of various additives on MSS PAHs. The changes in the per cigarette yields of a variety of PAHs were determined. They included anthracene, B[*a*]A, benzo[*ghi*]fluoranthene, benzo[*k*]fluoranthene, B[*a*]P, B[*e*]P, chrysene, fluoranthene, fluorene, methylfluorene, phenanthrene, several alkylphenanthrenes, dimethylphenanthrene, pyrene, and several benzofluorenes.†

Although studies on PAHs in MSS were conducted at RJRT and L&M in the 1960s, publications only dealt with analytical techniques. For example, in 1963, Mold et al. (2596a) at Liggett and Myers Tobacco Company (L&M) described the use of a compound, tetramethyluric acid, that complexes with polycyclic compounds. It was a procedure reminiscent of the finding of the water-soluble purine–PAH complex defined by Weil-Malherbe (4161a), a finding subsequently developed into an alternative analytical method for the determination of PAHs and aza-arenes in tobacco smoke and other media by Rothwell and Whiteheart (3337–3340). Although the study was not described as relating to tobacco smoke, Cundiff and Markunas (869) at RJRT in 1963 reported a titrimetric analysis of the nitro groups in numerous PAH–2,4,7-trinitrofluorenone complexes as a means to define the molecular weight of the PAH. All but one of the PAH–2,4,7-trinitrofluorenone complexes could be obtained from the PAH fraction of cigarette MSS. Of course, there were also methods developed for the in-house determination of specific PAHs, particularly B[*a*]P by Bell (239a) at Lorillard, Oakley and Stahr (2820a) at Philip Morris, and Walker (4110) and Stamey et al. (3787, 3789) at RJRT.

These and many other in-house reports on PAHs demonstrate that the early PAH research was not limited to academic or governmental laboratories or to laboratories at private institutions such as the Sloan-Kettering Institute,

* Numerous formal in-house reports and memoranda authored by RJRT R&D personnel are cited herein. Many have been published totally or in part in peer-reviewed journals and/or presented totally or in part at scientific conferences (Tobacco Chemists' Research Conferences, American Chemical Society Symposia on Tobacco and Smoke, CORESTA Conferences, etc.). Whether published, presented, or neither, copies of all RJRT reports cited are stored in various repositories such as the one in Minnesota. Their contents are available on the Internet address indicated. Experimental procedures used, data collected, and interpretations summarized here are described in detail in the reports cited.

† At the Internet address, http://legacy.library.ucsf.edu/cgi, by inserting the topic "aromatic polycyclic hydrocarbons," one may access over 20 BAT and Brown and Williamson (B&W) memoranda by Chakraborty, Thornton, and others on PAHs in tobacco smoke.

American Health Foundation, or Roswell Park Memorial Institute. Many of the previously mentioned tobacco industry reports on PAHs may now be accessed at the Internet addresses cited in the references.

Additional PAHs—both tumorigenic and nontumorigenic—were subsequently identified in CSC, but the level of B[*a*]P in CSC could account for very little (1056, 3310, 3311, 4354) or less than 2% of the observed skin-painting effect (4312, 4354) and the contribution of all the known tumorigenic PAHs in CSC could account for not much more than 3% of the observed effect. These findings led to the proposal by Wynder and Wright (4354) that CSC contained a PAH that either possessed the same specific tumorigenicity as B[*a*]P but was present at about 50 times the B[*a*]P level or present in MSS was an unknown PAH that was "supercarcinogenic" compared to B[*a*]P, i.e., its specific tumorigenicity to mouse skin was 40–50 times that of B[*a*]P. After an 18-month search, Wright, a colleague of Wynder from the early to the late 1950s, concluded that neither type PAH was present in CSC. Subsequently, the absence of a "supercarcinogen" in CSC was confirmed by the identification of hundreds of PAHs in the PAH fraction of CSC by Snook et al. (3756–3759). Detailed examination of their lists does not reveal the presence of a PAH structurally different from any of those previously classified with regard to their specific tumorigenicity on mouse-skin painting.

No other CSC fraction possessed specific tumorigenicity to mouse skin comparable to the PAH fraction. In the mid-1950s, the tumorigenicity of the *N*-nitrosamines in CSC was not an issue for several reasons: (1) the tumorigenicity of an *N*-nitrosamine was first defined in 1956 (2441a), (2) the presence of *N*-nitrosamines in MSS was not suggested until the early 1960s (422, 423, 1057), and (3) of more than 300 *N*-nitrosamines tested for tumorigenicity, only one type not found in tobacco smoke—the *N*-nitrosoalkylureas—was found to be tumorigenic to mouse skin [e.g., see Appendixes A through D in (2991)].

Consideration of all the tumorigenic PAHs and their levels in CSC could account for no more than 3% of the observed biological activity in mouse-skin-painting studies. In 1961, Wynder and Hoffmann (4312) stated:

> The polynuclear aromatic hydrocarbons are mainly formed during the combustion of tobacco. The tobacco of our standard cigarettes contains only very minute quantities of benzo(a)pyrene [*sic*] (0.02 ppm). A bioassay indicates that these polycyclic hydrocarbons of the condensate by themselves, however, can account for not more than 3 per cent of the total biological activity.

In 1967, they reiterated their 1961 comment (4340):

> Without belaboring the point as to whether B*a*P as such contributes to the carcinogenicity of tobacco smoke condensate, we can certainly agree that the concentration of B*a*P may be regarded as an 'indicator' of carcinogenic PAH in tobacco smoke condensate… While B*a*P and other carcinogenic PAH can by themselves account for only a small portion of the total tumorigenic activity of cigarette smoke condensate, probably less than 2%, they are, nevertheless, of obligatory importance as tumor initiators.

Hoffmann and Wynder (1800) reported that the major carcinogenicity of CSC resided in the CSC fraction containing the bulk of the PAHs. However, the levels in CSC of the nonalkylated carcinogenic PAHs could explain no more than 1%–3% of the observed activity. They also reported that the artificial doubling and tripling of the levels of the 17 known tumorigenic PAHs in CSC significantly increased the tumorigenicity of the CSC. However, their biological findings were contradicted by those of Roe (3310, 3311) and Lazar et al. (2320) who reported that increasing the level of B[*a*]P in CSC by a factor of 10 or 30, respectively, produced no increase in the specific carcinogenicity of the CSC. Roe (3310, 3311) also noted that the CSC level of B[*a*]P, despite its known tumorigenic potency, accounted for very little of the observed specific tumorigenicity of CSC to mouse skin. The opposite of these observations were the findings that potently tumorigenic PAHs such as DB[*a*,*h*]A on subcutaneous injection [Dobrovolskaia-Zavadskaia (1021)] and B[*a*]P on mouse-skin painting [Poel et al. (2970a)] exhibited a threshold value. Wynder et al. (4303) reported that mice skin painted with the equivalent of the B[*a*]P content of the CSC from over 500 current cigarettes developed no carcinomas. Rabbits were found to be even more resistant to higher dose levels of B[*a*]P.

Paralleling the research on the presence or absence of PAHs in cigarette MSS, their precursors in tobacco, their mechanism of formation, their contribution to laboratory animal tumorigenesis, and their possible involvement in the smoking-health issue was extensive research on ways to generate a "less hazardous" cigarette by removal of PAHs from or reduction of their per cigarette yields in MSS. To successfully resolve these questions, much pioneering research and development were initiated in late 1954 (3262). When the question of the presence of PAHs in MSS was resolved, with many PAHs identified, and their per cigarette MSS yields determined, much effort was expended to develop technologies to reduce their MSS yield, particularly the yields of those PAHs reported to be tumorigenic to CSC-painted mouse skin. In the early 1960s, a "less hazardous" cigarette was defined on the basis of three criteria [see p. iii in (1329); p. 372 in (4319); pp. 503, 531 in (4332)]: (1) the per cigarette yield of a specific toxicant has been lowered, (2) the ratio of the specific toxicant to MSS "tar" has been lowered, and (3) the specific tumorigenicity of the MSS "tar" as measured in the mouse-skin-painting bioassay has been lowered. With the advent of meaningful tests for mutagenicity and genotoxicity, criterion 3 has been modified to include them.

The tobacco industry and nonindustry scientists investigated many additional approaches in the attempt to design a "less hazardous" cigarette [see Table 5 in (3262), Table 14 in (3300)]. Two examples of technologies that appeared to be promising but presented other toxicant problems were (1) the organic solvent extraction of tobacco and (2) the use of oxidative additives.

The extraction concept was patterned after the findings of Roffo (3327) with one addition: the hexane extract of the tobacco was partitioned between hexane and aqueous ethanol to separate the flavorful compounds from those considered to be the PAH precursors, i.e., the phytosterols, the aliphatic hydrocarbons, and the long-chained terpenoids

(116, 121, 3189). When the extracted tobacco was smoked in cigarette form, its CSC showed much lower PAH levels than the control tobacco CSC (3241, 3246, 4356) and reduced tumorigenicity (4356). The flavorful components, when returned to the extracted tobacco and smoked in cigarette form, contributed little to the total PAHs or B[*a*]P in the MSS [see Figure 1, Table 3, and accompanying text in (3262)]. The solvent extraction removed from the tobacco not only many of the PAH precursors but also much of several potent anticarcinogens to such tumorigens as B[*a*]P and DB[*a,h*]A, e.g., long-chained aliphatic hydrocarbons, *d*-limonene, α-tocopherol, α- and β-1,5,9-trimethyl-12-(1-methylethyl)-4,8,13-cyclodecatriene-1,3-diol [see Table 11 in (3300)]. Thus, because of their removal from the tobacco, the anticarcinogens obviously could not be transferred to MSS during smoking. Before some of the problems were discovered, the investigation of the benefits supposedly derived from the organic solvent extraction of tobacco led to several patents on the technology (121, 2713, 2717, 3189). The earliest major nontobacco industry proponents of the contribution of the extraction technology to a "less hazardous" cigarette eventually dismissed it with the comment that the technology was "impractical both technically and economically" (4311) and "of academic interest only" (4306d). Most of the findings on tobacco components that were, and tobacco components that were not, significant precursors of MSS PAHs in this early study were confirmed some years later by Severson et al. (3616). The problems arising from the organic solvent extraction included the increased levels of nitrate and the biopolymers cellulose, starch, and pectin in the solvent-extracted tobacco. These consequences increased the yields of nitric oxide, *N*-nitrosamines, and phenols (3277) in the MSS.

Although nitrate addition reduced the per cigarette yields of FTC "tar," MSS PAHs, phenols, and CSC tumorigenicity to mouse skin (1797), it was subsequently shown, as predicted (1798), to significantly increase the yields of MSS *N*-nitrosamines and nitrogen oxides (480). Thus, the recommendation to add nitrate to tobacco to reduce MSS PAHs was eventually replaced by the recommendation to use low-nitrate tobacco in the cigarette blend and/or remove nitrate from the tobacco (480). This reversal of recommendations was paralleled by another concerning the level of long-chained hydrocarbons such as *n*-hentriacontane in tobacco: Originally, it was proposed to reduce MSS PAHs by selection of tobaccos with low levels of such components or remove the PAH precursors by organic solvent extraction. This was replaced by a proposal to select tobaccos with high levels of such components (480).

By the early 1960s, several cigarette design technologies developed by the tobacco industry and used in commercial products were categorized as significant in their contribution to the "less hazardous" cigarette (4310). Ultimately, the initial four design technologies (tobacco blend, effective and efficient filtration, reconstituted tobacco sheet (RTS), air dilution via cigarette paper porosity) were increased to eight (tobacco blend, filter tip, filter tip additives, RTS, paper additives, expanded tobacco, air dilution (paper porosity), air dilution (filter tip perforation)). Their significance was recognized in "less hazardous" cigarette design by the National Cancer Institute (NCI) (2683)* and the U.S. Surgeon General [see Table 6 in (3262), Table 15 in (3300)] (3999, 4005, 4009, 4010). It should be noted that the first two technologies considered significant were used before 1954. Tobacco or tobacco blend selection had been used since 1913, even before the first tumors were induced in a laboratory animal by skin painting with a solution of coal tar (4361). RTS was introduced into cigarette blends in 1953 when little was known about the chemical composition or biological properties of tobacco smoke (2170) or the effect of RTS inclusion in the blend on them. When knowledge of tumor induction with CSC and the presence of PAHs including B[*a*]P became available, it was shown that use of these two technologies resulted in a cigarette whose MSS was in compliance with that in the definition of a "less hazardous" cigarette (3300).

Of course, the initial thrust of this across-the-board reduction was aimed at reducing the MSS "tar" delivery because of extrapolation by Wynder et al. (4351) of their 1957 mouse-skin bioassay findings:

> Although it is difficult to estimate a comparable exposure level for man, the human data in line with the animal data indicate that a reduction in total tar exposure will be followed by a decrease in tumor formation. For this reason, measures directed toward this reduction are of utmost importance… The minimum dose of tar capable of producing papillomas in mice is about one third, of producing cancer one half, that of the optimum dose…The practical implications of these data and their relationship to the human cancer problem have been emphasized.

In his 1957 testimony during the filter-tipped cigarette hearings, Wynder reiterated this opinion that reducing "tar" exposure dose by 40%–50% would substantially reduce lung-cancer induction in smokers (4296):

Examination of the sales-weighted average "tar" delivery for U.S. commercial cigarettes reveals that the 40%–50% reduction in MSS "tar" delivery considered vital by Wynder in 1957 was achieved in the late 1960s, i.e., a reduction from 38–39 to 19–20 mg/cig. Further examination reveals that by the early 1980s, the sales-weighted average "tar" was reduced to about 12 mg/cig, i.e., an additional 40% reduction had been achieved [see Figure 3 in (3262)]. Corresponding reductions in the per cigarette yields of total PAHs in general, B[*a*]P in particular (4158), and nicotine were also observed. These reductions were also accompanied by a reduction in the specific tumorigenicity (mouse-skin painting) of the MSS CSC (4005).

* All eight cigarette design technologies eventually classified as significant by NCI, several U.S. Surgeons General, and other investigators on the basis of the 10-year NCI Smoking and Health Program on the "less hazardous" cigarette had been incorporated into one or more U.S. commercial cigarette products prior to the first meeting of the Tobacco Working Group formed in 1968 for the NCI program. In other words, from 1968 to 1978, no new design technology was generated in the NCI Smoking and Health Program on the "less hazardous" cigarette.

By year-end 1963, 91 of the 97 PAHs identified in MSS were reported in the published literature. Six PAHs, identified in MSS by Rodgman and Cook (3273), had not been reported publicly at that time. However, by 1970, identification in MSS of all but one (cholanthrene) of the 97 had been reported. Despite the availability of such information, only 18 MSS PAHs were discussed by the Advisory Committee in its 1964 Report to the U.S. Surgeon General, 13 as mainstream CSC components and five as carbon black components (3999). The detailed discussion of so few MSS PAHs and citation of so few publications were done despite the fact the committee had been provided with a detailed Philip Morris monograph on tobacco and smoke composition, a monograph that listed 61 PAHs identified in tobacco smoke plus many pertinent published references to them (2939, 3262). The Advisory Committee did note, however, that 27 other nontumorigenic PAHs—none specifically named—had been identified in tobacco smoke. The 27 unnamed PAHs had to include several of those PAHs, e.g., naphthalene, anthracene, phenanthrene, fluoranthene, and pyrene, which had been reported to significantly inhibit the action of potently tumorigenic PAHs such as B[*a*]P and DB[*a*,*h*]A in laboratory animal studies. Of the 97 PAHs known to him, Rodgman (3262) discussed the 43 PAHs identified at RJRT plus 34 other PAHs reported in the literature in numerous reports between 1954 and 1964 and in a summary 1964 report on 10-year research on cigarette MSS (3251). Interestingly, Chapter 6, in the Advisory Committee's report on cigarette smoke chemistry and the tumorigenic PAHs, was primarily authored by Fieser, one of the two eminent American PAH authorities at that time.

For over half a century, numerous theories have been advanced in attempts to explain the relationship between the tumorigenicity of PAHs in treated laboratory animals and a variety of their structural properties, including such properties as their K, L, and bay regions, electron distribution, bond orders, bond strengths, resonance, octanol–water partitioning, and the like (Figure 1.5).

Such studies were triggered by the discovery that certain PAHs when administered to laboratory animals via skin painting or subcutaneous injection induced carcinomas or sarcomas, respectively. DB[*a*,*h*]A, synthesized independently by Clar (760) and Fieser and Dietz (1184) in 1929, was shown to be a potent tumorigen to laboratory animals by Kennaway and Hieger (2078). Shortly thereafter, Cook et al. (797) isolated several PAHs from coal tar, characterized one of them as the previously unknown benzo[*a*]pyrene (B[*a*]P), and demonstrated that it too was a potent tumorigen to laboratory animals (194). Over the next two decades, the first demonstrations of the carcinogenicity of two pure compounds, DB[*a*,*h*]A and B[*a*]P, led to the synthesis and subsequent testing for tumorigenicity in laboratory animals of literally hundreds of PAHs and their alkyl derivatives plus other derivatives.

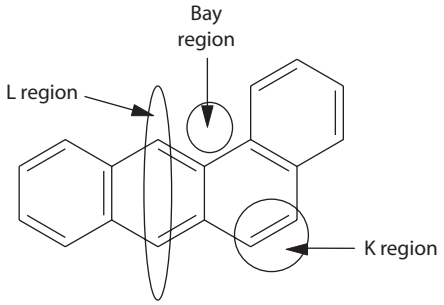


FIGURE 1.5 The L region, K region, and bay region of benz[*a*]anthracene.

During this time, the variation in biological responses observed with laboratory animals to individual PAHs eventually led to numerous unacceptable extrapolations of the results to PAH-exposed humans. To put the laboratory animal-to-human extrapolation in perspective, Shear and Leiter (3627) in 1941 issued a list of pertinent factors to be considered in such an extrapolation. Despite a diminution in PAH synthesis and tumorigenicity research during the World War II, the wealth of experimental data available in the late 1940s–early 1950s on the high-to-slight tumorigenic potency of some PAHs and the nontumorigenicity of other PAHs induced investigators to seek reasons for the observed differences in tumorigenicity and to attempt to develop explanations for them. Among those involved in the generation of the major early theories on the relationship between PAH structural properties and PAH tumorigenicity or lack of it were Coulson (829); Pullman and Pullman (3003); Daudel and Daudel (906a); Fieser et al. (1180a) and Fieser (1180b); and Lacassagne et al. (2247a). Much meaningful input to these theories was provided by other investigators such as Pauling (2910a) in the United States; Boyland, Weigert, and Mottram (423a) in the United Kingdom; and Buu-Hoï in France [see more than 30 Buu-Hoï references listed in (2247a)]. More recent studies include those by Herndon et al. (1623a, 2435a), Rubin (3365), Trosko (3966a), Zhang et al. (4410c), and Zhang, a graduate student under Herndon (4410d).

Because it was issued at the beginning of the extensive research on the composition of tobacco smoke with particular emphasis on the nature and levels of the PAHs in it, it is interesting to examine the lengthy 1955 review by Pullman and Pullman (3003) on the relationship between electronic structure and the tumorigenicity of a number of benzenoid hydrocarbons. Their publication was a detailed update of the 1953 review by Coulson (829) and included much data generated in the interim. The Pullmans used calculations based on three theoretical indexes of the K and L regions of the aromatic hydrocarbons. The indexes included Carbon Localization Energy (CLE), Bond Localization Energy (BLE), and *Para* Localization Energy (PLE) [see Table 1 in (3003)]. The Pullmans, by use of their CLE, BLE, and PLE calculations pertinent to the K and L regions in the PAHs, also attempted to relate the structures of various PAHs and their alkylated derivatives not only to their tumorigenicity but also to their rate of reaction in certain well-known reactions, e.g., Diels–Alder reaction with maleic anhydride, reaction with osmium tetroxide, reaction with lead tetraacetate, and photooxidation. Table 1.16 lists the hydrocarbons discussed by the Pullmans in

TABLE 1.16
Benzenoid Hydrocarbons Discussed by Pullman and Pullman (3003)

Aromatic Hydrocarbon Discussed	CAS No.	No. in Pullman and Pullman (3003)	Considered Tumorigenic[a] in 1955
Monocyclic			
Benzene[b]	71-43-2	I	No
Bicyclic			
Naphthalene	91-20-3	II	No
Tricyclic			
Anthracene	120-12-7	III	No
Phenanthrene	85-01-8	IV	No
Tetracyclic			
Naphthacene	92-24-0	VII	No
Benz[*a*]anthracene	56-55-3	VI	?
Benz[*a*]anthracene, 2,10-dimethyl-	—	XLIII	?
Benz[*a*]anthracene, 7,12-dimethyl-	57-97-6	XLII	Yes
Benz[*a*]anthracene, 7-methyl-	2541-69-7	XLIV	Yes
Benzo[*c*]phenanthrene	195-19-7	V	Yes
Benzo[*c*]phenanthrene, 1,2-dimethyl-	—	XLVIII	No
Chrysene	218-01-9	VIII	?
Chrysene, 2,3-dimethyl-[c]	—	XLIX	No
Triphenylene	217-59-4	X	No
Pyrene	129-00-0	IX	No
Pentacyclic			
Benzo[*b*]chrysene	214-17-5	XXIII	No
Benzo[*c*]chrysene	194-69-4	XIII	Yes
Benzo[*g*]chrysene	196-78-1	XIV	Yes
Pentacene	135-48-8	XVIII	No
Benzo[*a*]naphthacene	226-88-0	XVII	No
Dibenz[*a,h*]anthracene	53-70-3	XII	Yes
Dibenz[*a,j*]anthracene	224-41-9	XV	Yes
Pentaphene	222-93-5	XIX	No
Perylene	198-55-0	XXV	No
Picene	213-46-7	XXI	No
Benzo[*b*]triphenylene	215-58-7	XX	No
Benzo[*a*]pyrene	50-32-8	XI	Yes
Benzo[*a*]pyrene, 2-methyl-[d]	—	XLVII	Yes
Benzo[*a*]pyrene, 3-methyl-	—	XLVII	Yes
Benzo[*a*]pyrene, 5-methyl-	—	XLVII	Yes
Benzo[*a*]pyrene, 6-methyl-	2381-39-7	XLVII	Yes
Benzo[*a*]pyrene, 7-methyl-	63041-77-0	XLVII	Yes
Benzo[*a*]pyrene, 8-methyl-	63041-76-9	XLVII	No
Benzo[*a*]pyrene, 9-methyl-	—	XLVII	No
Benzo[*e*]pyrene	192-97-2	XVI	No
Dibenzo[*b,g*]phenanthrene	195-06-2	XXIV	No
Dibenzo[*c,g*]phenanthrene	188-52-3	XXII	No
Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl-[e]	56-49-5	XLV	Yes
Hexacyclic			
Anthra[1,2-*a*]anthracene	195-00-6	XXXV	No
Benzo[*c*]pentaphene	222-54-8	XXXVII	No
Benzo[*rst*]pentaphene	189-55-9	LIV	(Yes)[f]
Benzo[*pqr*]picene	189-96-8	LVII	No
Dibenzo[*b,def*]chrysene	189-64-0	XXVII	Yes
Dibenzo[*b,k*]chrysene	217-54-9	XXXVI	No
Dibenzo[*c,mno*]chrysene	196-28-1	LVI	No
Dibenzo[*def,mno*]chrysene	191-26-4	XXXI	No

TABLE 1.16 (continued)
Benzenoid Hydrocarbons Discussed by Pullman and Pullman (3003)

Aromatic Hydrocarbon Discussed	CAS No.	No. in Pullman and Pullman (3003)	Considered Tumorigenic[a] in 1955
Dibenzo[*def*,*p*]chrysene	191-30-0	XXVI	Yes
Dibenzo[*a*,*j*]naphthacene	227-04-3	XXXIII	No
Dibenzo[*a*,*l*]naphthacene	226-86-8	XXXIV	No
Dibenzo[*fg*,*op*]naphthacene	192-51-8	XXIX	No
Naphtho[1,2,3,4-*def*]chrysene	192-65-4	XXVIII	?
Naphtho[2,1,8-*qra*]naphthacene	196-42-9	XXX	No
Naphtho[1,2-*b*]triphenylene	215-26-9	XXXII	No
Heptacyclic			
Benzo[*a*]naphtho[8,1,2-*lmn*]naphthacene	190-01-2	LV	No
Dibenzo[*fg*,*qr*]pentacene	197-74-0	XL	No
Octacyclic			
Dinaphtho[1,2-*b*:1,2-*k*]chrysene	214-13-1	XXXIX	No
Naphthaceno[2,1,12,11-*opqra*]naphthacene	188-42-1	LVIII	?[g]
Phenanthro[1,10,9,8-*opqra*]perylene	190-39-6	XLI	No
Nanocyclic			
Dinaphtho[1,2-*b*:1,2-*n*] perylene	—	XXXVIII	No
Decacyclic			
Pentacenopentacene	—	LIX	?[g]

[a] Tumorigenic in mouse-skin-painting study.
[b] Benzene was reported as a component of the vapor phase of tobacco smoke in 1955 by Resnik and Holmes (3106) and Laurene (2293).
[c] A dimethylchrysene was subsequently reported in tobacco smoke, but the positions of the methyl groups were not defined.
[d] At least two methylB[*a*]Ps were subsequently reported in tobacco smoke, but the position of the methyl group in each case was not defined.
[e] This PAH is not totally benzenoid; its structure includes a cyclopentanoid ring.
[f] In 1955, the tumorigenicity of benzo[*rst*]pentaphene had not been determined; later, it was reported to be tumorigenic.
[g] Although no calculation was made on this PAH, Pullman and Pullman (3003) predicted it would be tumorigenic.

1955 with an indication of those, 34 in all, which were identified in tobacco smoke before and after 1955.

The Pullmans did introduce into their discussion various PAH metabolites, their diols and phenols, but not the epoxides which were unknown at that time. Even though it had been known since 1951 (3814), no explanation was offered for the inhibition of the activity of a potently tumorigenic PAH by coadministration of a weakly tumorigenic or nontumorigenic PAH. Lastly, of course, neither the Pullmans nor Coulson discussed the fact that a bioassay finding with a highly susceptible strain or species of laboratory animal administered an individual PAH in an excessive dose has little relationship to the situation where a human is exposed by a different administration route to a mixture of PAHs with various degrees of tumorigenicity plus other known antitumorigenic compounds.

By year-end 1955, very few of the PAHs considered by the Pullmans had been reported as tobacco smoke components. More had been identified in other sources such as air pollution. In the following discussion, the comments in the early 1950s about the inadequacy of the evidence indicating the presence of B[*a*]P in tobacco smoke (1181) are disregarded. Table 1.17 lists the PAHs reported in tobacco smoke at that time.

Of the 14 PAHs reported, only eight were included by the Pullmans in their assessment: naphthalene, anthracene, phenanthrene, B[*a*]A, B[*a*]P, B[*e*]P, dibenzo[*def,mno*]chrysene, and pyrene. Of course, only one of the eight, B[*a*]P, was considered at that time a significant and potent tumorigen to mouse skin. At that time, the tumorigenicity of B[*a*]A was questioned, and still was questioned in the mid-1980s (983).

As noted previously, Pullman and Pullman not only updated the electronic structure–tumorigenicity information generated after the Coulson 1953 review but also attempted to extend the theory to alkyl-PAHs. Examination of their review reveals that they discussed, in addition to 1,2-dihydro-3-methylbenz[*j*]aceanthrylene, a total of 12 alkyl-PAHs (see Table 1.16). It is obvious from their discussion that the prediction of tumorigenicity for most of these 12 PAHs was not calculated but derived from published biological data. However, examination of the biological data in Hartwell (1543, 1544) and Shubik and Hartwell (3664, 3665) indicates that at least

TABLE 1.17
Polycyclic Hydrocarbons Reported in Tobacco Smoke by Year-End 1955

	References Issued in the Year			
Hydrocarbon	**1947**	**1953**	**1954**	**1955**
Acenaphthylene[a]		818	819, 821	820, 2365
Azulene[a,b]	1857			2365
Anthracene		818	785, 819	820, 2352, 2365, 3578
Anthracene,2-methyl-				820
Benz[*a*]anthracene				2352, 2425, 2426
Benzo[*ghi*]perylene			819	820, 2365, 2425, 2426
Benzo[*a*]pyrene			785, 819, 821, 2335	55–57, 593, 1172, 2011, 2365, 3578, 4353
Benzo[*e*]pyrene				2352
Dibenzo[*def,mno*]chrysene			819	820, 2365
Fluoranthene[a]			819	820, 2365
Naphthalene				3578
Naphthalene,2-methyl-				820
Phenanthrene			819	820, 2365
Pyrene		818	785, 819	820, 2352, 2365, 2425, 2426

[a] Molecule has a cyclopentanoid ring; thus, it was not considered by Pullman and Pullman (3003).
[b] Molecule does not possess a benzenoid structure.

64 totally benzenoid alkyl-PAHs had been tested for tumorigenicity by 1955. Several 1,2-dihydromethylbenz[*j*]aceanthrylenes had been tested for tumorigenicity by 1955, but they were not included in our count of 64. This raises the question: Why was the prediction not calculated for more of the 64 alkyl-PAHs, the tumorigenicity of which was known at that time (1543, 1544, 3664, 3665)? Pullman and Pullman noted: "It must be acknowledged that the extension of the theory to substituted derivatives of polycyclic hydrocarbons is at present far from having achieved a completely consistent and satisfactory form."

Many of the more recent theories on the relationship between PAH structural properties and tumorigenicity suffer somewhat from this and other deficiencies [cf. Herndon et al. (1623a, 2435a), Rubin (3365), Trosko (3966a), Zhang et al. (4410c), and Zhang (4410d)]. Much studied in recent years has been the application of the quantitative structure–activity relationship (QSAR) method to PAHs.

Although many theories have involved the relationships between observed laboratory-derived biological data on individually administered PAHs and their structural elements, do they speak to the exposure situation experienced by humans? Whether the exposure is by inhalation of air pollutants or tobacco smoke, by ingestion of foodstuffs or beverages, by dermal contact, or by a combination of the exposures, very few of any human exposures involve exposure to a single PAH similar to the exposure of laboratory animals treated with a single PAH by skin painting or subcutaneous injection. One such example of human exposure to a single PAH was the past use of naphthalene as the major ingredient in mothballs.

Numerous PAHs have been either completely of partially characterized in many air pollutants, foodstuffs, beverages, and contact tars and dusts. Of all the products to which humans are exposed, none has been characterized to the extent of tobacco smoke. Over 5200 components have been identified in it, nearly twice as many as in the next consumer product, coffee, subjected to detailed compositional analysis. Of the identified tobacco smoke components, about 11% were either completely or partially identified as PAHs. It should also be noted that in the detailed examination of tobacco smoke, over 5200 identified components account for over 98% of the weight of cigarette MSS. It has been estimated, based on detailed gas chromatograms, that the number of actual components in cigarette MSS may be 12–20 times the number of identified ones (4103).

Of the more than 500 PAHs either completely or partially identified in cigarette MSS, relatively few PAHs, originally 13 in all, were repeatedly defined as significant tumorigens (1727, 1808, 1871). Eventually, the International Agency for Research on Cancer (IARC) redefined the tumorigenicity of chrysene. Thus, it was deleted from all subsequent lists (1740, 1741, 1743, 1744, 2825) except one (1217). MSS is not the only source of most of the 12 PAHs still considered as significant tumorigens in cigarette MSS. Except for 5-methylchrysene, most have also been identified as significant PAH components of gasoline and diesel engine exhaust gases (1406a, 4315) and many common foodstuffs and beverages (1345, 2438).

When one is dealing with a complex mixture, which in turn contains an assortment of PAHs ranging from bicyclic to decacyclic, one cannot extrapolate the biological effect observed by administration of an individual PAH to the biological effect of that PAH in such a complex mixture. It has long been known from laboratory studies that certain nontumorigenic or slightly tumorigenic PAHs when administered by skin painting or subcutaneous injection in an equimolar dose level with a highly tumorigenic PAH partially or totally inhibit its tumorigenicity. Few studies have been done to determine the effect of a non- or low-tumorigenic PAH on the tumorigenicity of a highly tumorigenic PAH when its level greatly exceeds that of the potent tumorigen. Also, there are differences in the classification of the potency of the tumorigenicity of some PAHs. For example, B[*a*]A is classified by some as a potent or significant tumorigen (1871) but by others as only slightly tumorigenic (983).

The list of either totally or partially identified PAHs in CSC gradually increased, but in the mid-1970s, the massive definitive PAH study by U.S. Department of Agriculture (USDA) personnel in Athens, GA, increased the number of known PAHs in CSC to well over 500 (3732, 3756–3759).

Although not isolated individually, their identifications, whether total or partial, have generally been accepted across the board.

Numerous authors, including Hoffmann and Hecht (1727), listed the PAH dibenzo[*a*,*l*]pyrene as a significant tumorigen in tobacco smoke. However, Hecht eventually stated (1557) that "the presence in cigarette smoke of dibenzo[*a*,*l*]pyrene, a highly carcinogenic PAH, had not been confirmed." One should weigh the comment by Hecht against the current status of defined MSS composition. Since the appreciable decline in detailed tobacco smoke composition studies after the late 1970s, no individual investigator or no research group has reported the confirmation of the identities of many of the PAHs (3756–3759), aza-arenes (3750, cf. 3414), nitrogen-containing components (1587), or ether- (2769) and water-soluble components (3553) reported in cigarette MSS in the 1970s. While many components have been confirmed by other investigators at the same institution as the authors, examination of the post-1980 literature indicates that the identities of nearly half the new components described in the previously mentioned studies have not been confirmed by investigators at other institutions. Because of such a situation, would Hecht also discount their presence in cigarette MSS in the same way as he discounted the presence of dibenzo[*a,l*]pyrene?

Although most of the past theories have attempted to define the relationship between structural properties of the PAHs and their specific tumorigenicity as measured individually in skin-painting studies, little has been done to explain the behavior of a PAH when it is present in a complex mixture which includes a host of PAHs, some of which are known antitumorigens as well as numerous known non-PAH antitumorigens (1174).

It has been known for over 60 years that coadministration of a potently tumorigenic PAH with an equimolar quantity of a nontumorigenic PAH often results in substantial reduction in % tumor-bearing animals (%TBA).

In 1953, Coulson noted [see p. 51 in (829)]:

> The action of inhibitors may be thought of as a competition between the carcinogenic and noncarcinogenic compounds for available sites on the enzyme. If sufficient noncarcinogenic molecules are able to occupy suitable sites, then the irreversible mutation cannot occur. We can see that inhibitors, in order to compete with the carcinogenic compounds, should themselves possess a K-region.

Some of the PAHs that substantially reduce or totally inhibit the tumorigenicity of several of the most potent tumorigens known are listed in Table 1.18. Obviously, neither naphthalene nor anthracene has a K region, a requirement proposed by Coulson for the inhibitory property.

Although many of the inhibition studies were conducted with the tumorigenic and inhibiting PAHs administered in equimolar quantities, it should be remembered that this is not the case in the PAH mixture in CSC. Table 1.19 is derived from CSC PAH data presented by Hoffmann and Wynder (1788, 1798) and Rodgman (3273). The per cigarette yield data in Table 1.19 were the averages of the data generated from two different commercial American cigarettes. One was unfiltered and yielded 36.8 mg/cig of total particulate matter (TPM) (1788); the other was a filtered cigarette that yielded 37.5 mg/cig of TPM (3273). The disparity between the relative yields in each category was less than 5%.

TABLE 1.18
Inhibition of Tumorigenicity of Potently Tumorigenic PAHs by Nontumorigenic or Weakly Tumorigenic PAHs

PAH[a]	CAS No.	Effective against	References
Naphthalene	91-20-3	B[*a*]P, DB[*a,h*]A	844
Anthracene	120-12-7	B[*a*]P, DB[*a,h*]A	844
Phenanthrene	85-01-8	DMB[*a*]A	976, 3685
Fluoranthene	206-44-0	B[*a*]P, DMB[*a*]A	976, 3685, 3686
Pyrene	129-00-0	DB[*a,h*]A, DMB[*a*]A	976, 3685, 3686
Benz[*a*] anthracene	56-55-3	B[*a*]P, DB[*a,h*]A	426, 4332
Benzo[*e*] pyrene	192-97-2	B[*a*]P, DB[*a,h*]A, DMB[*a*]A	976, 3685, 3686
Benzo[*b*] triphenylene	215-58-7	MC[b], DB[*a,h*]A, DMB[*a*]A	976, 3683, 3686

[a] Each PAH listed is a component of cigarette MSS.
[b] MC = 3-methylcholanthrene = 1,2-dihydro-3-methylbenz[*j*]aceanthrylene.

In the early structure–biological activity studies, PAHs with a pentacyclic ring were not included in the discussion of most theories, but pentacyclic compounds in which the pentacycle contained nitrogen were, i.e., benzacridines (829, 2247a). In the discussion of his theory, Coulson (829) did mention several cyclopentanoid compounds: six benzacridines and two PAHs, 2,3-dihydro-1*H*-benzo[*a*]cyclopent[*h*]anthracene, and 10,11-dihydro-9*H*-benzo[*a*]cyclopent[*i*]anthracene.

In her 1996 thesis, Zhang (4410d) noted the numerous sources of PAHs to which humans are exposed, e.g., air pollutants, foodstuffs and beverages, effluents from factories, vehicles, and heat and power sources. Zhang particularly stressed tobacco smoke, its complexity, and some of the PAHs contained therein:

> Tobacco smoke is a complex mixture which is estimated to contain at least 150 compounds in the gas phase and more than 2000 compounds have been identified in the particulate phase. Table 1* lists some PAHs that exist in the particulate phase of cigarette smoke.

Unfortunately, the inconsistent use of PAH nomenclature sometimes makes it difficult to follow the phases of the study by Zhang [cf. Table 7 and Appendix A in (4410d)].

* In her Table 1, Zhang (4410d) listed 19 MSS PAHs reported in 1978 by Hoffmann et al. (1781).

TABLE 1.19
Levels of PAH Classes in Cigarette MSS

PAH Category	Assumed Approximate mol. wt.	Mainstream Smoke Yield[a]		
		Yield, ng/cig	Approximate Nanomoles[b]	Nanomolar Ratio, PAH:B[*a*]P
Bicyclic	128[c]	4140 (77.1)[d]	32.3	293
Tricyclic	178[e]	720 (13.4)	4.0	36
Tetracyclic	228	420 (7.9)	1.8	16
Pentacyclic	278	72 (1.3)	0.26	2.4
B[*a*]P	252	27 (0.49)[f]	0.11	1.0
Non-B[*a*]P pentacyclic	278	45 (0.81)[f]	0.16	1.5
Hexacyclic	328	14 (0.3)	0.04	0.36
Totals		5366 (100.0)		

[a] Data reported by Hoffmann and Wynder (1788,1798) from a nonfiltered cigarette, TPM = 36.8 mg/cig, were averaged with data reported by Rodgman and Cook (3273) for a filtered commercial cigarette, TPM = 37.5 mg/cig.
[b] Nanomoles calculated with the approximate molecular weights in column 2.
[c] The molecular weight of naphthalene = 128, that of indene = 116. It is realized that the average molecular weight of the bicyclic PAH mixture will differ slightly from those of the parent PAH because of the presence of numerous homologs (methylnaphthalenes, dimethylnaphthalenes, etc.).
[d] Values in parentheses represent the fraction % of the PAH category in the total PAH fraction.
[e] The presence of tricyclic PAH homologs results in molecular weight slightly different from 178.
[f] The sum of the fraction % of B[*a*]P and the fraction % of non-B[*a*]P pentacyclic PAHs equals 1.3%.

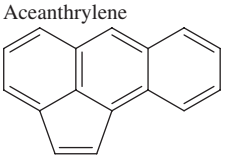
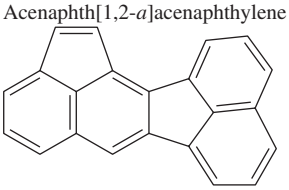
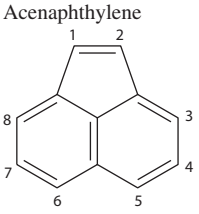
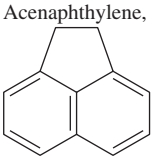
Another study, recently initiated by Martin et al. (2479), involved an attempt to develop a meaningful relationship between PAH structure, chemical properties, and biological properties, specifically the effect of PAHs on specific tumorigenicity in skin painting. Reported for naphthalene- and pyrene-related PAHs were the following molecular parameters: the measured and calculated log of the octanol–water partition coefficient (MlogP, ClogP), molecular volume (MgVol), calculated molar refractivity (CMR), and the number of valence electrons (NVE). The second phase of the study involved similar data for anthracenes, phenanthrenes, and indenes (3300a). All PAHs in the first two phases of this study (2479, 3300a) are reported components of cigarette MSS. The ultimate goal is to use these data to facilitate a QSAR on MSS PAHs. If such a meaningful relationship can be derived for the more than 500 MSS PAHs, then it probably can be applied to any PAH from any source.

As a prelude to this attempt to develop a possibly reasonable explanation for the PAH structure–tumorigenicity relationship, the PAHs completely or partially identified in cigarette smoke have been cataloged. For each PAH, the nomenclature used in Tables 1.14, 1.17, and 1.18 is the most recent proposed by the International Union of Pure and Applied Chemistry (IUPAC).

The tobacco smoke–PAH references cited in Table 1.20 are not necessarily all that are available, particularly for those PAHs such as B[*a*]P and DB[*a,h*]A, which have been the subject of much research and discussion for over half a century. In most cases, included is a reference to the publication or presentation by the investigator(s) who first reported a particular PAH in MSS. References of articles and/or presentations on specific PAHs that contained evidence later criticized are included plus references to the misinterpretations or errors. The criticism by Fieser (1181) in 1957 of the shortcomings of the evidence (55–57, 592–594, 820) supposedly indicating the presence of B[*a*]P in cigarette smoke has already been mentioned. Two other notable situations involved 1,2-dihydrobenz[*j*]aceanthrylene (cholanthrene) and dibenzo[*def,p*]chrysene (formerly named dibenzo[*a,l*]pyrene, initially 1,2,3,4-dibenzopyrene). These two PAH identifications, based solely on UV spectral data, were found to be incorrect. In their study, Rodgman and Cook (3273) incorrectly defined a PAH as 1,2-dihydrobenz[*j*]aceanthrylene (cholanthrene). In the massive study by USDA personnel on the identification of MSS PAHs, 1,2-dihydrobenz[*j*]aceanthrylene was not among the several benzocyclopentanthracenes reported (3756,3759). The other incorrectly characterized PAH was dibenzo[*def,p*]chrysene. For its identification, not only Rodgman and Cook (3273) but also Bonnet and Neukomm (397), Lyons and Johnson (2430), Lyons (2427), Wynder and Wright (4354), and Pyriki (3033) relied on published UV spectral data purportedly those of synthetic dibenzo[*def,p*]chrysene (dibenzo[*a,l*]pyrene). However, in 1966, Lavit-Lamy and Buu-Hoï (2314) determined that the published UV spectral data were not those of dibenzo[*a,l*]pyrene but of the isomeric dibenz[*a,e*]aceanthrylene (dibenzo[*a,e*]fluoranthene), generated during the supposed synthesis of dibenzo[*a,l*]pyrene. The authentic dibenzo[*def,p*]chrysene (dibenzo[*a,l*]pyrene) was identified in MSS in 1977 (3756), but its MSS level was not reported.

Some authorities insist that the B[*a*]P and 4-(methylnitrosoamino)-1-(3-pyridinyl)-1-butanone (NNK)

TABLE 1.20
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	202-03-9	Aceanthrylene 	2037a, 3615, 3618–3620, 4249, 5811b		
2.	641-48-5	Aceanthrylene, 1,2-dihydro-	5811, 5811a, 5811b		
3.	340-99-8	Acenaphth[1,2-*a*]acenaphthylene 	2328, 4249		
4.	71265-26-4	Acenaphth[1,2-*a*]acenaphthylene, methyl-	2328, 4249		
5.	208-96-8	Acenaphthylene 	48, 104, 141–143, 151, 394, 397, 583, 584, 603, 819–821, 966, 1139, 1172, 1211, 1287–1289, 1360, 1375, 1375a, 1375b, 1377, 1426, 1427, 1445, 1471, 1649, 1650, 1652, 1760, 2079, 2130, 2134, 2195, 2256, 2260, 2270, 2365–2367, 2425, 2427, 2428, 2438, 2510, 2543, 2557, 2570, 2731, 2735, 2765–2767, 2773, 2777, 2799a, 2939, 2961, 2962, 3149, 3176, 3240, 3245, 3249, 3251, 3262, 3273, 3292, 3300, 3302, 3307, 3308, 3370, 3410, 3452, 3465–3467, 3469, 3479, 3557, 3616, 3618–3620, 3729, 3732, 3757–3759, 3787, 3797, 3876, 3936, 3938, 4001, 4249, 4319, 4353–4355, 5010, 5034, 5077, 5539, 5811b	2339a, 4332, 4249, 5567, 5811b	1360, 1375a, 1377
6.	83-32-9	Acenaphthylene, 1,2-dihydro- {acenaphthene} 	104, 147, 394, 397, 603, 624, 726, 798, 869, 1139, 1287, 1288, 1426, 1427, 1471, 1650, 1652, 2013, 2079, 2113, 2134, 2194, 2195, 2256, 2260, 2438, 2570, 2731, 2735, 2767, 2799a, 2939, 2961, 2962, 3176, 3249, 3251, 3262, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3370, 3469, 3479, 3514, 3557, 3616, 3618–3620, 3732, 3757–3759, 3797, 4249, 4404, 5010, 5077, 5539, 5811b	903, 4249, 5567, 5811b	
7.	60684-29-9	Acenaphthylene, 1,2-dihydrodimethyl-	1650, 1652, 3615, 3618–3620, 3732, 3757–3759, 4249, 5811b		
8.	36541-21-6	Acenaphthylene, 1,2-dihydromethyl-	1650, 1652, 3479, 3618–3620, 3732, 3757–3759, 4249, 5811b		
9.	60826-72-4	Acenaphthylene, 1,2-dihydrotetramethyl-	1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 5811b		
10.	60826-69-9	Acenaphthylene, 1,2-dihydrotrimethyl-	1650, 1652, 3618–3620, 3757–3759, 5811b		
11.	60826-68-8	Acenaphthylene, dimethyl-	104, 2328, 3618–3620, 3732, 3757–3759, 4249, 5811b		
12.	19346-00-0	Acenaphthylene, 1,3-dimethyl-	3226, 4249, 5811b		
13.	19346-02-2	Acenaphthylene, 1,5-dimethyl-	5811, 5811a, 5811b		
14.	58548-40-6	Acenaphthylene, diphenyl-	2328, 4249		
15.	58548-38-2	Acenaphthylene, methyl-	104, 1650, 1652, 2438, 2570, 2731, 2735, 3616, 3618–3620, 3732, 3757–3759, 5811b		
16.	19345-99-4	Acenaphthylene, 1-methyl-	3615, 3618, 3758, 3759, 4249, 5811b		
17.	19345-94-9	Acenaphthylene, 3-methyl-	3615, 3617, 4249, 5811b		
18.	19345-97-2	Acenaphthylene, 4-methyl-	1145, 4249, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

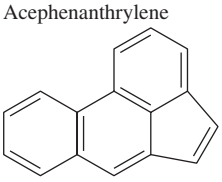
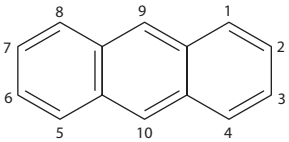
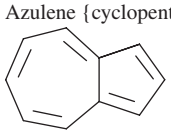
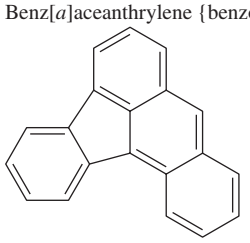
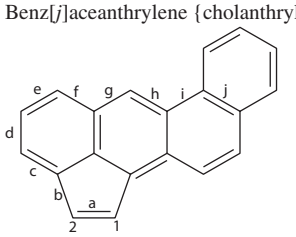
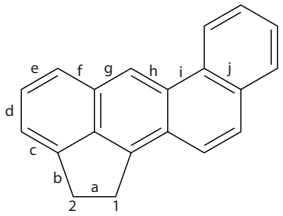
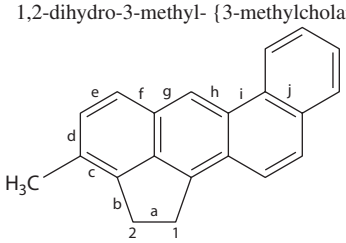
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
19.	19345-91-6	Acenaphthylene, 5-methyl-	1145, 4249, 5811b		
20.	60826-73-5	Acenaphthylene, tetramethyl-	1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 5811b		
21.	60826-70-2	Acenaphthylene, trimethyl-	104, 1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 5811b		
22.	201-06-9	Acephenanthrylene 	3437, 3616, 3618–3620, 3741, 3756, 4249, 5811b		
23.	6232-48-0	Acephenanthrylene, 4,5-dihydro-	1127a, 3617, 3618, 3756, 4249		
24.	120-12-7	Anthracene 	39, 49, 50, 84, 104, 126a, 128, 141–143, 147, 151, 172, 245, 290, 291, 329, 394, 397, 398, 443, 568b, 583, 584, 603, 624, 646a, 710, 726, 746a, 785, 818–820, 869, 878, 885, 966, 1099, 1100, 1136, 1139, 1172, 1211, 1287–1289, 1360, 1371, 1373, 1375a, 1378, 1388–1390, 1406, 1408, 1409, 1427, 1435a, 1445, 1462, 1471, 1485, 1649, 1767, 1842, 1870, 1871, 1873, 1933, 2013, 2037a, 2079, 2088, 2099, 2113, 2114, 2116, 2120, 2121, 2126, 2127, 2130, 2134, 2170, 2194–2196, 2200, 2203, 2210, 2255, 2256, 2270, 2313a, 2352, 2365–2367, 2370, 2425, 2501, 2543, 2557, 2570, 2596a, 2648–2650, 2710, 2713–2715, 2717, 2761, 2762, 2765–2767, 2773, 2777, 2799a, 2893, 2894, 2939, 2961, 2962, 2964, 3003, 3032, 3046, 3176, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3265, 3273–3275, 3286, 3291, 3292, 3300, 3302, 3307, 3308, 3323, 3324, 3340a, 3370, 3410, 3415, 3421–3424, 3437, 3452, 3465–3470, 3472, 3514, 3557, 3578, 3616, 3618–3620, 3741, 3758, 3759, 3787, 3788, 3797, 3863, 3876, 3973, 3999, 4001, 4248, 4249, 4282, 4284, 4296, 4300, 4311, 4342, 4352–4355, 4399, 4404, 5010, 5077, 5079, 5359, 5539, 5811b	84, 172, 568b, 903, 2079, 2939, 2995, 3059, 3194, 3547, 4249, 4332, 5567, 5811b	50, 1360, 1375a, 1378, 2210
25.		9-^{14}C-Anthracene {anthracene-9-^{14}C}	25A74	25A74	
26.		Anthracene, alkyl-	820, 1172, 1508, 2428, 2893, 2939, 3262, 3308, 3465–3467, 3469, 4249, 4284, 4355, 5077		
27.	613-31-0	Anthracene, 9,10-dihydro-	50, 1139, 2134, 2203, 2962, 3262, 3302, 3514, 3797, 4249, 5811b		50
28.	29063-00-1	Anthracene, dimethyl-	1650, 1652, 2438, 3437, 3514, 3618–3620, 3732, 3757–3759, 4249, 5811b	3615, 4249	
29.	781-43-1	Anthracene, 9,10-dimethyl-	139, 329, 3300, 3339, 3514, 4249, 5077, 5811b		
30.	41637-86-9	Anthracene, ethyl-	1508, 2767, 4249, 5077, 5811, 5811a, 5811b		
31.	605-83-4	Anthracene, 9-ethyl-	2767, 4249		
32.	71265-29-7	Anthracene, ethylmethyl-	2328, 4249, 5811b, 1D01, 1E01		
33.	26914-18-1	Anthracene, methyl-	104, 658, 966, 1649, 2550, 3262, 3273, 3286, 3437, 3470, 3472, 3514, 3876, 4248, 4249, 5077		§
34.	610-48-0	Anthracene, 1-methyl-	1471, 1650, 1652, 2037a, 3618–3620, 3732, 3757–3759, 4249, 5077, 5811b		
35.	613-12-7	Anthracene, 2-methyl-	245, 290, 291, 726, 820, 1139, 1462, 1471, 1650, 1652, 2037a, 2079, 2438, 2939, 3262, 3302, 3308, 3557, 3616, 3618–3620, 3732, 3757–3759, 3787, 3788, 3797, 4249, 5077, 5811b	5811b	

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
36.	779-02-2	Anthracene, 9-methyl-	50, 329, 869, 1462, 1650, 1652, 2037a, 2113, 2438, 3191, 3251, 3262, 3273, 3286, 3292, 3302, 3308, 3514, 3616, 3618–3620, 3732, 3757–3759, 3787, 3788, 3797, 4249, 5811b		50
37.	71265-30-0	Anthracene, propyl-	2328, 4249		
38.	27358-28-7	Anthracene, trimethyl-	1650, 1652, 2328, 3618–3620, 3732, 3757–3759, 4249, 5811b		
39.	275-51-4	Azulene {cyclopentacycloheptene} 	299, 814, 1139, 1287, 1288, 1857, 2079, 2170, 2171, 2270, 2365, 2425–2427, 2499, 2939, 3262, 3302, 3647, 3797, 4249, 5077, 5079, 5811b		
40.	529-05-5	Azulene, 1,4-dimethyl-7-ethyl-	2327c, 5077		
41.	203-33-8	Benz[*a*]aceanthrylene {benzo[*a*]fluoranthene} 	3616, 3618–3620, 3756, 3758, 3759, 5811b		
42.	202-33-5	Benz[*j*]aceanthrylene {cholanthrylene} 	1648, 4249		
43.	479-23-2	Benz[*j*]aceanthrylene, 1,2-dihydro- {cholanthrene} 	2037a, 2195, 2438, 3251, 3257, 3262, 3273, 3286, 3292, 3302, 3308, 5077		
44.	56-49-5	Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl- {3-methylcholanthrene} 	203, 139, 329, 869, 1373, 1425, 2037a, 2191, 2438, 2484a, 2939; 3257, 3262, 3302, 3365, 3685, 3787, 3788, 3814, 4249, 4335, 5077		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

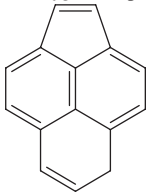
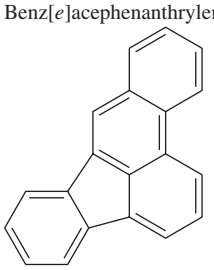
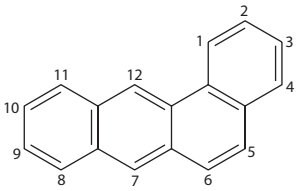
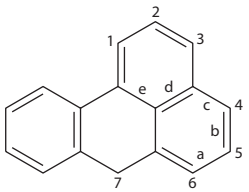
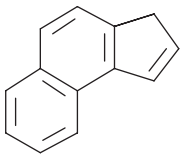
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
45.	76774-50-0	Benz[*fg*]acenaphthylene 	3327a, 4249, 5811b		
46.	205-99-2	Benz[*e*]acephenanthrylene {benzo[*b*]fluoranthene} 	50, 117, 126a, 128, 141–143, 147, 151, 216, 239, 290, 291, 603, 726, 804, 1019, 1139, 1148, 1217, 1237, 1373, 1375a, 1377, 1378, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1786–1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2013, 2079, 2099, 2116, 2428, 2438, 2473, 2474, 2501, 2524a, 2825, 2939, 3259, 3149, 3176, 3191, 3255, 3257, 3262, 3265, 3286, 3292, 3300, 3302, 3308, 3370, 3437, 3616, 3618–3620, 3714, 3756, 3758, 3759, 3787, 3788, 3797, 4005–4007, 4009–4011, 4037, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 4323, 4324, 4332, 4353, 4354, 5010, 5077, 5512, 5539, 5811b	1127a, 4037, 4249, 5567, 5811b	50, 1375a, 1377, 1378
47.	41637-94-9	Benz[*e*]acephenanthrylene, methyl-	1648, 3618–3620, 3756, 3758, 3759, 4249, 5811a		
48.	149021-93-2	Benz[*e*]acephenanthrylene, 10-methyl-	4249		
49.		Benzanthracene	642, 4249		
50.	63194-18-3	Benzanthracene, methyl-	1650, 1652, 2328, 3732, 3757, 4249		
51.	56-55-3	Benz[*a*]anthracene {B*a*A or B[*a*]A} 	39, 104, 126, 126a, 126b, 128, 139, 141–143, 147, 151, 203, 216, 237, 239, 290, 291, 329, 394, 397–399, 603, 624, 646a, 726, 746a, 797, 869, 1025, 1136, 1139, 1148, 1211, 1217, 1287–1289, 1329, 1330, 1332, 1333, 1373, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1471, 1492, 1674, 1709, 1727, 1740, 1741, 1743, 1744, 1760, 1767a, 1773, 1781, 1787, 1788, 1792, 1798, 1800, 1802, 1803, 1808, 1842, 1870, 1871, 1873, 1933b, 1971, 2013, 2037a, 2078, 2079, 2099, 2113, 2116, 2121, 2126, 2127, 2130, 2133, 2134, 2142, 2195, 2199, 2215, 2238, 2256, 2313a, 2352, 2366, 2367, 2425, 2426, 2430, 2438, 2524a, 2537, 2596a, 2710, 2799a, 2825, 2893, 2939, 2960–2962, 2964, 3003, 3007, 3024, 3030, 3032, 3033, 3047, 3049, 3081, 3082, 3087, 3088, 3131, 3158, 3162, 3176, 3190, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3264, 3265, 3272–3275, 3286, 3292, 3300, 3302, 3307, 3308, 3370, 3437, 3470, 3472, 3493, 3616, 3618–3620, 3713, 3741, 3756–3759, 3878, 3788, 3797, 3814, 3847, 3952, 3973, 3975, 3984, 3992, 4001, 4005–4007, 4009–4011, 4248, 4249, 4282, 4300, 4307, 4308, 4311, 4315, 4316, 4319, 4322, 4324, 4332, 4355, 5010, 5077, 5512, 5531, 5539, 5732, 5811b, 5869a	903, 3205, 4249, 4332, 5567, 5811b	1330, 1332, 1375a, 1377, 1378
52.		Benz[*a*]anthracene, alkyl-	4315		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
53.	43178-07-0	Benz[*a*]anthracene, dimethyl-	2328, 3307, 3618–3620, 3756–3759, 4249, 5811b		
54.	57-97-6	Benz[*a*]anthracene, 7,12-dimethyl- {DMBA}	139, 203, 329, 351–353, 356, 358, 359, 414, 869, 1139, 1373, 2112, 2191, 2195, 2438, 2939, 2961, 2962, 2964, 3257, 3262, 3300, 3302, 3308, 3365, 3683, 3685, 3686, 3688, 3787, 3788, 3797, 4037, 4249, 4311, 4318, 4319, 4325, 4330, 4335, 5077, 5811b		
		Benz[*a*]anthracene, 9,10-dimethyl-	This compound is misnamed in Stedman [see p. 159 in (3797)] and in Ishiguro and Sugawara (1884). It is 9,10-dimethyl-1,2-benzanthracene (obsolete nomenclature) or 7,12-dimethylbenz[*a*]anthracene (current nomenclature), reported by Pietzsch (2962) and Kröller (2191).		
55.	31632-62-9	Benz[*a*]anthracene, ethyl-	2328, 3300, 4249		
56.	71265-32-2	Benz[*a*]anthracene, ethylmethyl-	3226, 4249		
57.	43178-22-9	Benz[*a*]anthracene, methyl-	1781, 1802, 2550, 3616, 3619, 3620, 3756, 3758, 3759, 5811b		
58.	2498-77-3	Benz[*a*]anthracene, 1-methyl-	2037a, 2328, 3618; 3756–3759, 4249, 5811b, 1E02		
59.	2498-76-2	Benz[*a*]anthracene, 2-methyl-	39, 726, 2037a, 2113, 4249		
60.	2498-75-1	Benz[*a*]anthracene, 3-methyl-	1139, 2037a, 2328, 2939, 4249		
61.	316-49-4	Benz[*a*]anthracene, 4-methyl-	2037a, 2113, 2328, 4249		
62.	2319-96-2	Benz[*a*]anthracene, 5-methyl-	394, 1139, 2037a, 2710, 3033, 3251, 3262, 3273, 3286, 3292, 3300, 3302, 3797, 4249, 5077, 5811b		
63.	316-14-3	Benz[*a*]anthracene, 6-methyl-	2037a, 2113, 2328; 3300, 4249		
64.	2381-31-9	Benz[*a*]anthracene, 8-methyl-	2037a, 2328; 3300, 4249		
65.	2381-16-0	Benz[*a*]anthracene, 9-methyl-	2037a, 2328, 4249		
66.	2381-15-9	Benz[a]anthracene, 10-methyl-	2037a, 2113, 2328, 4249		
67.	2422-79-9	Benz[*a*]anthracene, 12-methyl-	2037a, 2113, 5811b, 1E02		
68.		Benz[*a*]anthracene, methylene-	3756		
69.	71265-33-3	Benz[*a*]anthracene, propyl-	2328, 4249		
70.		Benz[*a*]anthracene, tetramethyl-	1650, 1652, 3732, 3757		
71.	60826-78-0	Benz[*a*]anthracene, trimethyl-	1650, 1652, 2328, 3300, 3618–3620, 3732, 3757–3759, 4249, 5811b		
72.	199-94-0	7*H*-Benz[*de*]anthracene 	278, 2037a, 4249		
73.	2 32-54-2	1*H*-Benz[*e*]indene 	3615		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

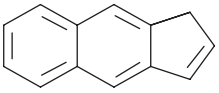
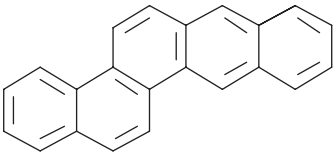
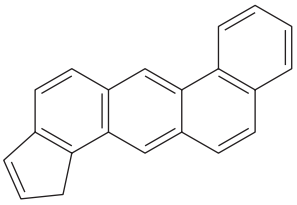
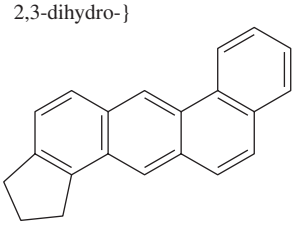
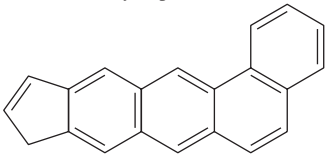
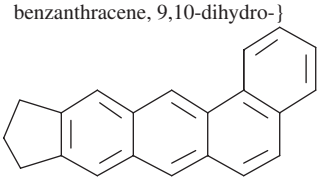
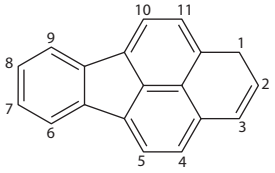
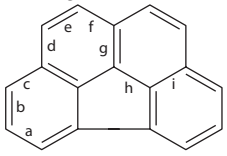
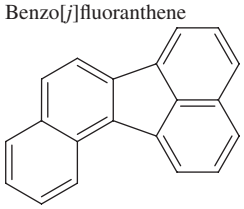
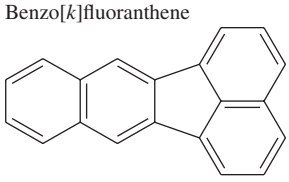
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
74.		1*H*-Benz[*e*]indene, dimethyl-	1650, 1652, 3732, 3757, 4249		
75.		1*H*-Benz[*e*]indene, ethylmethyl-	1650, 1652, 3732, 3757, 4249		
76.	64031-90-9	1*H*-Benz[*e*]indene, methyl-	3615, 4249		
77.	268-40-6	1*H*-Benz[*f*]indene 	3615, 3616, 3618–3620, 3758, 3759, 4249, 5811b		
78.	60826-71-3	1*H*-Benz[*f*]indene, dimethyl-	1650, 1652, 3615, 3618–3620, 3732, 3757–3759, 4249, 5811b		
79.	71265-34-4	1*H*-Benz[*f*]indene, ethylmethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
80.	60826-63-3	1*H*-Benz[*f*]indene, methyl-	3618–3620, 3758, 3759, 4249, 5811b		
81.	57827-84-6	Benzochrysene	5811		
82.	214-17-5	Benzo[*b*]chrysene {dibenzo[*b*,*h*]phenanthrene} 	141–143, 2037a, 2939, 3003, 3302, 5811b, 1E02		
83.	146506-80-1	Benzo[*g*]chrysene, methyl-	3327a, 5811b		
84.	240-44-8	1*H*-Benzo[*a*]cyclopent[*h*]anthracene 	5811, 5811a		
85.	7099-43-6	1*H*-Benzo[*a*]cyclopent[*h*]anthracene, 2,3-dihydro-{5,6-cyclopentano-1,2-benzanthracene, 2,3-dihydro-} 	392, 394, 397–399, 432, 1139, 2079, 2430, 2710, 2711, 2939, 3033, 3251, 3262, 3273, 3292, 3302, 3307, 4249, 5077, 5732, 5811b		
86.	226-78-8	9*H* Benzo[*a*]cyclopenta[*i*]anthracene 	5811, 5811a		
87.	7099-42-5	9*H*-Benzo[*a*]cyclopent[*i*]anthracene, 10,11-dihydro-{6,7-cyclopentano-1,2-benzanthracene, 9,10-dihydro-} 	39, 392, 394, 397–399, 1139, 2079, 2430, 2440, 2710, 2711, 2939, 3033, 3251, 3262, 3273, 3292, 3297, 3302, 3797, 4249, 5077, 5732		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
88.	56832-73-6	Benzofluoranthene	50, 2313a, 2328, 3741, 4249, 5811b		50
89.		Benzofluoranthene, dimethyl-	1650, 1652, 3732, 3757		
90.		Benzofluoranthene, ethyl-	2328, 4249		
91.	61089-87-0	Benzofluoranthene, methyl-	1650, 1652, 3732, 3757		
92.	16135-81-2 42126-84-1	11*H*-Benzo[*cd*]fluoranthene 	282, 603, 1971, 2939, 3262, 3370, 4249, 4300, 4353, 5077		
93.	203-12-3	Benzo[*ghi*]fluoranthene 	126a, 126b, 143, 151, 603, 624, 646a, 1139, 1397, 1409, 1462, 1781, 1787, 1788, 1800, 2037a, 2134, 2426, 2939, 3251, 3262, 3273, 3286, 3292, 3302, 3308, 3370, 3437, 3616, 3618–3620, 3756, 3758, 3759, 3787, 3788, 3797, 4018, 4019, 4031, 4037, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 4355, 5811b		
94.	64760-14-1	Benzo[*ghi*]fluoranthene, dimethyl-	2328, 3756, 4249, 5811b		
95.	71265-35-5	Benzo[*ghi*]fluoranthene, ethyl-	4249		
96.	51001-44-6	Benzo[*ghi*]fluoranthene, methyl-	3615, 3619, 3620, 3756, 3758, 3759, 4249, 4525, 5811b		
97.	71265-21-9	Benzo[*ghi*]fluoranthene, 1-methyl-	2328, 4249		
98.	71265-22-0	Benzo[*ghi*]fluoranthene, 2-methyl-	2328, 4249		
99.	71265-23-1	Benzo[*ghi*]fluoranthene, 3-methyl-	2328, 4249		
100.	71265-24-2	Benzo[*ghi*]fluoranthene, 4-methyl- {also reported as 7-methylbenzo[*ghi*]fluoranthene}	2328, 4249		
101.	205-82-3	Benzo[*j*]fluoranthene 	128, 141–144, 147, 151, 216, 239, 290, 291, 603, 1139, 1148, 1217, 1373, 1397, 1405, 1406, 1408, 1409, 1471, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1787, 1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2037a, 2134, 2438, 2524a, 2939, 3251, 3255, 3257, 3262, 3265, 3273, 3292, 3300, 3302, 3308, 3370, 3437, 3714, 3756, 3758, 3759, 3787, 3797, 3999, 4005, 4009–4011, 4031, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 4323, 4324, 4332, 5077, 5512, 5811b, 5869a		
102.	60826-67-7	Benzo[*j*]fluoranthene, methyl-	3756, 3758, 3759, 5811b		
103.	207-08-9	Benzo[*k*]fluoranthene 	49, 141–144, 147, 151, 216, 239, 290, 291, 432, 603, 646a, 726, 746a, 1139, 1148, 1217, 1375a, 1377, 1378, 1397, 1405, 1406, 1408, 1409, 1445, 1471, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1787, 1788, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2013, 2037a, 2099, 2116, 2134, 2238, 2327, 2427, 2430, 2438, 2524a, 2825, 2939, 3176, 3251, 3255, 3257, 3262, 3265, 3273, 3286, 3292, 3300, 3302, 3308, 3370, 3437, 3514, 3616, 3618–3620, 3714, 3756, 3758, 3759, 3787, 3788, 3797, 4018, 4019, 4031, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 5010, 5077, 5512, 5539, 5732, 5811b	5567, 5811b	1375a, 1377, 1378

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

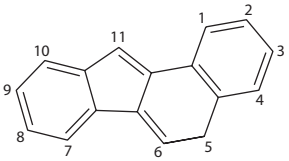
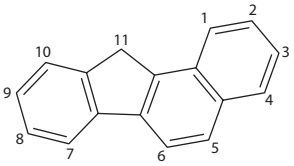
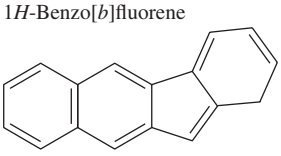
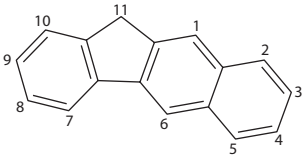
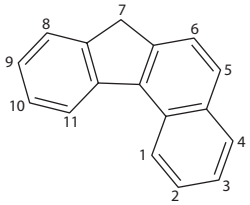
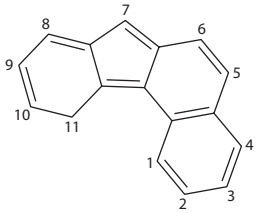
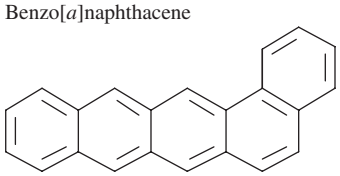
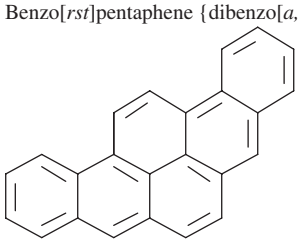
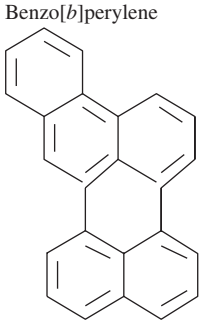
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
104.	41637-93-8	Benzo[*k*]fluoranthene, methyl-	3758, 3759, 4249, 5811b		
105.	61089-87-0	Benzofluorene	646a, 1560, 2195, 2313a, 3616, 4249		
106.		Benzofluorene, alkyl-	646, 1560, 4249		
107.	77271-50-2	Benzofluorene, dimethyl- {at least three isomers in MSS}	642, 3756–3759, 4249, 5811b		
108.	60918-47-0	Benzofluorene, methyl- {at least four isomers in MSS}	3615, 3618–3620, 3756–3759, 4249		
109.	77271-51-3	Benzofluorene, tetramethyl- {at least two isomers in MSS}	1650, 1652, 3732, 3757, 5811b		
110.	77271-52-4	Benzofluorene, trimethyl-	3619, 3620, 5811b		
111.	30777-18-5	Benzo[*a*]fluorene	126, 1870, 1871, 1873, 3262, 4248, 5811b, 1E02		
112.	238-82-4	1*H*-Benzo[*a*]fluorene	5811, 5811a, 5811b		
113.	238-79-9	5*H*-Benzo[*a*]fluorene 	1139, 1397, 1471, 1870, 1871, 1873, 2438, 2596a, 3262, 3797, 4249, 5077		
114.	238-84-6	11*H*-Benzo[*a*]fluorene 	39, 50, 126, 126a, 126b, 128, 142, 143, 394, 397, 1139, 1650, 1652, 1781, 1870, 1871, 1873, 2037a, 2710, 2939, 3262, 3302, 3308, 3618–3620, 3732, 3757–3759, 3788, 3797, 4018–4020, 4031, 4249, 4315, 4355, 5077, 5811b, 1E02		50
115.		11*H*-Benzo[*a*]fluorene, dimethyl-	3618, 3758, 3759		
116.	60826-64-4	11*H*-Benzo[*a*]fluorene, methyl-	128, 3618–3620, 3756, 3758, 3759, 4249, 5811b		
117.	54811-53-9	11*H*-Benzo[*a*]fluorene, 9-methyl-	5811		
118.	71265-25-3	11*H*-Benzo[*a*]fluorene, 11-methyl-	39, 128, 394, 1139, 2037a, 2710, 2939, 3262, 3302, 3308, 3797, 4249, 5077		
119.	71607-85-7	11*H*-Benzo[*a*]fluorene, trimethyl- {at least three isomers in MSS}	1650, 1652, 3618; 3619, 3732, 3757, 4249		
120.	243-18-5 30777-19-6	5*H*-Benzo[*b*]fluorene	1139, 1397, 1870, 1871, 1873, 2596a, 2893, 2939, 3262, 3797, 5811b		
121.	14458-76-5	1*H*-Benzo[*b*]fluorene 	5811, 5811a, 5811b		
122.	243-17-4	11*H*-Benzo[*b*]fluorene 	39, 50, 141, 143, 147, 726, 1139, 1781, 1788, 1870, 1871, 1873, 2037a, 2134, 2596a, 2939, 3302, 3308, 3619, 3620, 3756, 3758, 3759, 3788, 3797, 4300, 4315, 5077, 5811b	5811b	50

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
123.	60826-65-5	11*H*-Benzo[*b*]fluorene, methyl-	3618–3620, 3756, 3758, 3759, 4249, 5811b		
124.		11*H*-Benzo[*b*]fluorene, 9-methyl-	3756		
125.	77271-81-0	Benzo[*c*]fluorene, methyl-	1650, 1652, 3732, 3757, 5811, 5811a, 5811b		
126.	205-12-9	7*H*-Benzo[*c*]fluorene 	143, 1139, 1397, 1781, 1870, 1871, 1873, 2037a, 3262, 3302, 3618–3620, 3756, 3758, 3759, 3797, 4249, 4355, 5077, 5811b		
127.	60826-66-6	7*H*-Benzo[*c*]fluorene, methyl-	1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 5811b		
128.	73492-01-0	11*H*-Benzo[*c*]fluorene 	1870, 1871, 1873, 3479, 5811		
129.	226-88-0	Benzo[*a*]naphthacene 	1139, 2037a, 2079, 2939, 3003, 3262, 3302, 3797, 4249, 4282, 4354, 5077, 5811b		
130.	189-55-9	Benzo[*rst*]pentaphene {dibenzo[*a,i*]pyrene} 	126a, 141–143, 151, 239, 392, 394, 397–399, 726, 793, 794, 1139, 1148, 1157b, 1217, 1286, 1373, 1557, 1727, 1740, 1773, 1798, 1824, 1842, 1870, 1871, 1873, 2037a, 2079, 2438, 2708–2711, 2825, 3033, 3251, 3255, 3257, 3260, 3262, 3265, 3273, 3286, 3292, 3300, 3302, 3308, 3365, 3377, 3520, 3714, 3756, 3787, 3788, 3797, 3999, 4005, 4009–4011, 4249, 4296, 4319, 4332, 4355, 5077, 5811b, 5869a		
131.	11057-45-7	Benzoperylene	1800, 2313a, 4249		
132.	197-70-6	Benzo[*b*]perylene 	3756, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

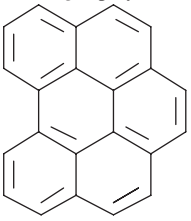
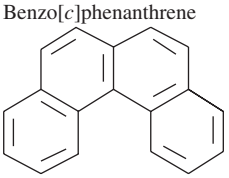
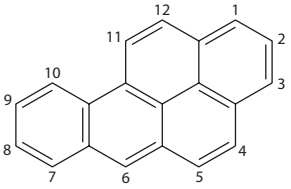
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
133.	191-24-2	Benzo[*ghi*]perylene 	39, 104, 126, 141–143, 151, 216, 290, 291, 432, 603, 726, 746a, 819, 820, 1025, 1099, 1100, 1136, 1139, 1172, 1211, 1375a, 1377, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1781, 1787, 1788, 1800, 1870, 1871, 1873, 2013, 2037a, 2079, 2116, 2130, 2134, 2238, 2270, 2365, 2425, 2430, 2438, 2601b, 2799a, 2893, 2696a, 2939, 2961, 2962, 3033, 3176, 3191, 3240–3242, 3249, 3255, 3257, 3262, 3273–3275, 3286, 3292, 3300, 3302, 3308, 3370, 3616, 3756, 3787, 3788, 3797, 4005, 4009–4011, 4019, 4031, 4079, 4110, 4249, 4296, 4300, 4307, 4308, 4309, 4315, 4319, 4355, 5010, 5077, 5539, 5732, 5811b	5567	1375a, 1377
134.	64760-22-1	Benzo[*ghi*]perylene, dimethyl- {at least three isomers in MSS}	3756, 4249, 5811b		
135.	41699-09-6	Benzo[*ghi*]perylene, methyl- {at least two isomers in MSS}	104, 2799a, 3615, 3618, 3756, 4249, 5811b		
136.	64760-23-2	Benzo[*ghi*]perylene, trimethyl- {at least two isomers in MSS}	3756, 4249, 5811b		
137.	65777-08-4	Benzophenanthrene	5811		
138.	195-19-7	Benzo[*c*]phenanthrene 	147, 432, 1139, 1375a, 1377, 1406, 1408, 1409, 1650, 1652, 1767a, 1781, 1798, 1802, 1870, 1871, 1873, 2037a, 2113, 2134, 2438, 2939, 3003, 3251, 3257, 3262, 3273, 3286, 3292, 3300, 3302, 3514, 3732, 3756, 3757, 3787, 3788, 3999, 4005–4007, 4009–4011, 4018, 4019, 4020, 4031, 4248, 4249, 4319, 4332, 4355, 5027, 5077, 5811b		1375a, 1377
139.	78328-47-9	Benzo[*c*]phenanthrene, methyl-	476, 1781, 1802, 3300, 4249		
140.	73467-76-2	Benzopyrene	3263		
141.	65357-69-9	Benzopyrene, methyl-	5811, 5811a		
142.	50-32-8	Benzo[*a*]pyrene {B[*a*]P} 	28, 30, 31, 39, 40, 48–50, 55–57, 83, 83a, 104, 116, 117, 126, 126a, 126b, 128, 132, 139–144, 147, 151, 158a, 167, 172, 174b, 174c, 174e, 179, 180, 183, 194, 203, 215, 216, 237, 239, 239a, 274, 276, 278, 284–286, 290, 291, 329, 351–354, 392–394, 397–399, 402, 433, 488, 489, 520, 521, 527, 532, 583, 584, 588, 589, 592–594, 603, 606a, 624, 636, 646, 646a, 658, 688, 694, 695, 704, 710, 722, 726, 765–767, 784, 785, 796a, 797, 804–808, 814, 817, 819–821, 830, 869, 875–878, 882, 885, 913, 916, 933, 934, 949, 953, 964, 966, 977–981, 988a, 1001, 1006a, 1007, 1015, 1016, 1016a, 1019, 1025, 1051, 1056, 1060, 1060a, 1061, 1076, 1091, 1098–1100, 1136, 1139, 1148, 1172, 1181, 1182, 1211, 1217, 1236, 1237, 1246, 1272, 1286–1289, 1329, 1330, 1332, 1333, 1348–1350, 1354, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1396, 1397, 1403–1406, 1406a, 1406b, 1407, 1408, 1409, 1410a, 1435, 1435a, 1437, 1442, 1443, 1445, 1462, 1471, 1473, 1475, 1492, 1502, 1537, 1538, 1551, 1557, 1572, 1573, 1589, 1592–1594, 1674, 1709, 1727, 1740, 1741, 1743, 1744, 1754, 1755, 1760, 1764, 1766, 1767a, 1773, 1781, 1786–1788, 1792, 1793, 1797, 1798, 1800, 1802, 1803, 1807a, 1808,		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
142.	50-32-8	Benzo[*a*]pyrene {B[*a*]P} (cont.)	1826, 1842–1846, 1870, 1871, 1873, 1933a, 1937, 1962b, 1966, 2011, 2013, 2037a, 2060, 2071, 2072, 2079, 2099, 2114–2116, 2119, 2121, 2126, 2127, 2130, 2133, 2134, 2134a, 2142, 2156, 2170, 2184–2192, 2194–2197, 2199, 2200, 2210, 2237, 2238, 2254–2258, 2260, 2268, 2270, 2313a, 2313e, 2319, 2320, 2327, 2335, 2352–2354, 2365–2368, 2370, 2374, 2426, 2430, 2438, 2457b, 2465, 2473, 2474, 2479, 2480, 2484a, 2518, 2524a, 2537, 2543, 2545, 2557, 2570, 2589, 2596a, 2614, 2648–2650, 2651, 2654, 2683, 2707, 2710, 2713–2715, 2717, 2719, 2737, 2738, 2744, 2761, 2762, 2767, 2775, 2777, 2799a, 2817a, 2817b, 2819, 2820a, 2825, 2856, 2865, 2881, 2893, 2894, 2899, 2906, 2911, 2918, 2927, 2939, 2935, 2960–2962, 2964, 3003, 3007, 3024, 3030, 3032, 3033, 3046, 3047, 3049, 3059, 3076, 3077, 3081, 3082, 3084, 3085, 3087, 3088, 3116, 3131, 3135–3137, 3141, 3148a, 3158, 3162, 3176, 3190, 3191, 3224, 3232, 3235, 3239–3243, 3245, 3246, 3249–3251, 3254, 3255, 3257, 3259, 3262, 3264, 3265, 3269, 3273–3275, 3286, 3291, 3292, 3299a, 3300–3304, 3307, 3308, 3310, 3311, 3316, 3323–3327, 3340a, 3365, 3370, 3377, 3378, 3415, 3419, 3421–3424, 3437, 3440, 3441a, 3452, 3465–3467, 3469, 3470, 3472, 3482, 3493, 3497, 3503, 3505, 3514, 3557, 3572, 3578, 3579a, 3610, 3615–3620, 3625, 3638, 3644, 3685, 3686, 3713, 3741, 3756, 3758, 3759, 3787–3789, 3797, 3811a, 3830, 3831, 3840, 3844, 3847, 3863, 3876, 3877, 3878, 3889, 3924, 3952, 3973, 3975, 3976, 3984, 3992, 3999–4001, 4005–4007, 4009–4011, 4018, 4019, 4020, 4031, 4037, 4106, 4110, 4114, 4117, 4232, 4241, 4248, 4249, 4281, 4282–4284, 4293–4296, 4300, 4301, 4303, 4307, 4309–4311, 4315, 4317–4319, 4322–4326, 4328, 4330, 4338, 4339–4341, 4342, 4351–4356, 4365, 4404, 4410, 4581, 5010, 5049, 5067, 5077, 5079, 5080, 5088, 5092, 5359, 5508, 5512, 5531, 5532, 5539, 5546, 5556, 5558, 5602, 5630, 5679, 5692, 5707, 5732, 5811b, 5836, 5869a	903, 1077b, 1722, 2079, 2484a, 2939, 3974b, 4098a, 4249, 4332, 4623, 5001, 5018, 5053, 5533, 5567, 5811b	50, 1330, 1332, 1354, 1375a, 1377, 1378, 2210, 3192
143.		7,10-Benzo[*a*]pyrene-^{14}C {benzo[*a*]pyrene-7,10-^{14}C}	25A74	25A74	
144.		Benzo[*a*]pyrene, alkyl-	142, 143, 966, 1139, 1172, 2939, 3251, 3262, 3269, 3273, 3286, 3308, 3876, 4249, 4284, 4315, 4355, 5077		
145.		Benzo[*a*]pyrene, dihydro-	5732		
146.	110081-38-4	Benzo[*a*]pyrene, 3,4-dihydro-	39, 1139, 2479, 2939, 3797, 4249, 5811, 5811a		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

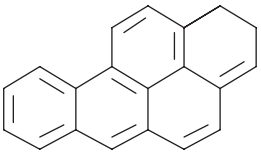
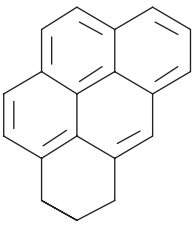
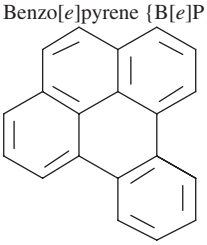
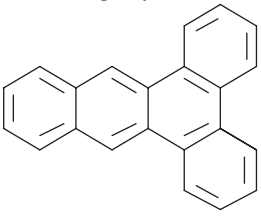
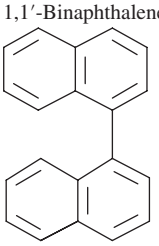
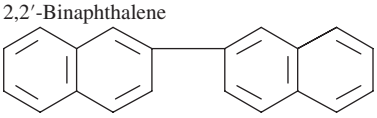
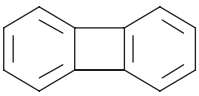
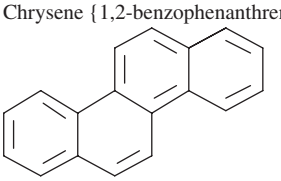
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
147.	17573-23-8	Benzo[*a*]pyrene, 7,8-dihydro- 	104, 2939, 3262, 3302, 3797, 4249, 5077		
148.	25167-90-2	Benzo[*a*]pyrene, dimethyl- {at least two isomers in MSS}	765, 2479, 3262, 3615, 3618, 3756, 3758, 3759, 4249, 5077, 5811b		
149.		Benzo[*a*]pyrene, ethyl-	2328, 4249		
150.	25167-89-9	Benzo[*a*]pyrene, methyl- {at least two isomers in MSS}	1471, 1781, 1802, 2479, 2939, 3251, 3262, 3265, 3273, 3286, 3292, 3302, 3470, 3472, 3616, 3618–3620, 3756, 3758, 3759, 3797, 4031, 4249, 4319, 4332, 5077, 5811b		
151.	7130-15-6	3*H*-Benzo[*cd*]pyrene, 4,5-dihydro- 	726, 2479, 3618, 3756, 3758, 3759, 5811b		
152.	192-97-2	Benzo[*e*]pyrene {B[*e*]P} 	39, 50, 104, 126a, 126b, 141–143, 151, 216, 290, 291, 329, 432, 646a, 726, 797, 1025, 1099, 1136, 1139, 1172, 1211, 1289, 1373, 1388–1390, 1397, 1406–1409, 1445, 1462, 1471, 1475, 1781, 1786, 1787, 1788, 1800, 1870, 1871, 1873, 2013, 2037a, 2060, 2099, 2116, 2130, 2134, 2210, 2238, 2255, 2256, 2260, 2313a, 2327, 2352, 2374, 2426, 2438, 2479, 2557, 2596a, 2744, 2799a, 2865, 2893, 2939, 2961, 2962, 2964, 3003, 3033, 3176, 3191, 3251, 3255, 3257, 3262, 3265, 3273, 3286, 3292, 3300, 3302, 3308, 3365, 3437, 3470, 3472, 3514, 3572, 3610, 3616, 3618–3620, 3685, 3686, 3741, 3756, 3758, 3759, 3787, 3788, 3797, 3952, 4005–4007, 4009–4011, 4018, 4019, 4031, 4036, 4110, 4249, 4300, 4307, 4308, 4315, 4317, 4319, 4323, 4324, 4332, 4355, 5010, 5077, 5732, 5811b	903, 3205, 4249, 5567, 5811b	50, 2210
153.	41699-06-3	Benzo[*e*]pyrene, dimethyl- {at least two isomers in MSS}	2479, 3618, 3756, 3758, 3759, 4249, 5811b		
154.	41699-04-1	Benzo[*e*]pyrene, methyl- {at least two isomers in MSS}	1471, 2479, 3470, 3472, 3616, 3618–3620, 3756, 3758, 3759, 4249, 5811b		
155.	64760-21-0	Benzo[*e*]pyrene, trimethyl-	1870, 1871, 2479, 3756, 4005, 4009–4011, 4249, 5811b		
156.	215-58-7	Benzo[*b*]triphenylene {dibenz[*a,c*]anthracene} 	1373, 1781, 2037a, 2438, 3003, 3255, 3257, 3265, 3300, 3365, 3683, 3685, 3686, 3688, 3756, 3787, 3788, 4005–4007, 4010, 4011, 4036, 4249, 5811b		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
157.	64760-20-9	Benzo[*b*]triphenylene, methyl-	3756, 4249, 5811b		
158.	604-53-5	1,1′-Binaphthalene 	144, 147, 726, 2037a, 2113, 2479, 4249		
159.	71265-39-9	1,1′-Binaphthalene, dimethyl-	2328, 4249		
160.	71277-81-1	1,1′-Binaphthalene, ethyl-	2328, 4249		
161.	59615-45-5	1,1′-Binaphthalene, methyl-	2328, 2479, 4249		
162.	4325-74-0	1,2′-Binaphthalene	144		
163.	612-78-2	2,2′-Binaphthalene 	142–144, 147, 151, 1900, 2037a, 3219, 3262, 3308, 4249, 5077		
164.	71294-43-4	2,2′-Binaphthalene, dimethyl-	2328, 4249		
165.	71277-82-2	2,2′-Binaphthalene, ethyl-	2328, 4249		
166.	41637-91-6	2,2′-Binaphthalene, methyl-	2328, 4249		
167.	259-79-0	Biphenylene 	430, 790, 4249		
168.	218-01-9	Chrysene {1,2-benzophenanthrene} 	39, 104, 126a, 128, 141–143, 147, 151, 216, 290, 291, 329, 432, 603, 646a, 710, 726, 746a, 966, 1136, 1139, 1148, 1172, 1148, 1211, 1217, 1373, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1471, 1475, 1560, 1573, 1649, 1712, 1727, 1740, 1743, 1773, 1781, 1787, 1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 1933b, 2013, 2037a, 2079, 2099, 2113, 2121, 2130, 2195, 2134, 2238, 2256, 2313a, 2430, 2438, 2524a, 2537, 2557, 2799a, 2825, 2893, 2939, 2961, 2962, 2964, 3003, 3033, 3162, 3176, 3191, 3240–3243, 3246, 3249, 3251, 3255, 3257, 3262, 3263, 3265, 3269, 3273–3275, 3286, 3291, 3292, 3300, 3302, 3308, 3370, 3377, 3437, 3452, 3470, 3472, 3493, 3514, 3610, 3616, 3618–3620, 3741, 3756, 3758, 3759, 3787, 3788, 3797, 3814, 3876, 3924, 3927, 3952, 4005–4007, 4009–4011, 4031, 4037, 4110, 4248, 4249, 4282, 4284, 4300, 4307, 4308, 4315, 4317, 4319, 4323, 4324, 4354, 4355, 5010, 5077, 5539, 5732, 5811b, 5869a	903, 3205, 5567, 5811b	
169.		Chrysene, alkyl-	128, 142, 143, 1139, 1172, 1787, 1788, 2893, 2939, 3251, 3269, 3273, 3286, 3308, 4284, 4300, 4307, 4308, 4309, 4315, 4319, 5077		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

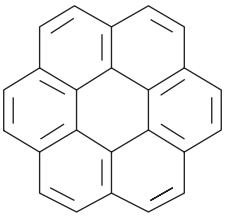
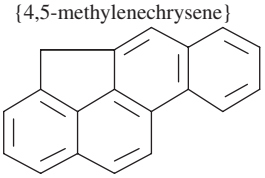
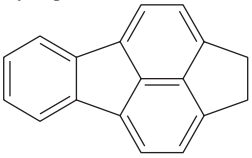
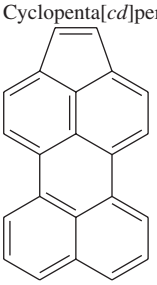
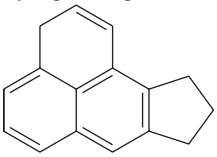
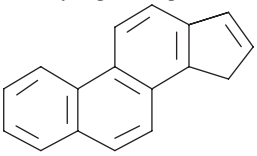
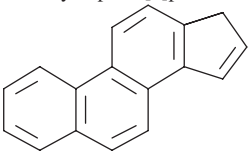
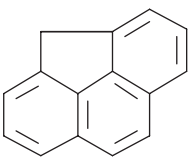
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
170.	41637-92-7	Chrysene, dimethyl- {at least three isomers in MSS}	39, 128, 1139, 1781, 2134, 2939, 3033, 3262, 3302, 3618–3620, 3756–3759, 3797, 5077, 5811b		
171.	71277-86-6	Chrysene, ethyl-	1781, 1800, 3479		
172.	71277-87-7	Chrysene, ethylmethyl-	2328		
173.	41637-90-5	Chrysene, methyl-	128, 657, 1471, 1788, 1802, 2134, 2550, 3251, 3273, 3286, 3292, 3308, 3437, 3616, 4031, 4248, 5811b		
174.	3351-28-8	Chrysene, 1-methyl-	39, 1139, 1397, 1560, 1781, 1870, 1871, 1873, 2037a, 2939, 3262, 3302, 3618–3620, 3756–3759, 3797, 4005–4007, 4009 4011, 4031, 4249, 5077, 5811b	5567	
175.	3351-32-4	Chrysene, 2-methyl-	290, 291, 1397, 1560, 1781, 1800, 1870, 1871, 1873, 2037a, 3618–3620, 3756–3759, 4005–4007, 4009–4011, 4249, 5811b		
176.	3351-31-3	Chrysene, 3-methyl-	290, 291, 1397, 1560, 1781, 1800, 1870, 1871, 1873, 2037a, 3618–3620, 3756–3759, 4005–4007, 4009–4011, 4249, 5811b	5567	
177.	3351-30-2	Chrysene, 4-methyl-	291, 1560, 1573, 1800, 1870, 1871, 1873, 3618–3620, 3756–3759, 4249, 5811b	5567	
178.	3697-24-3	Chrysene, 5-methyl-	126a, 237, 290, 291, 603, 1148, 1217, 1373, 1557, 1560, 1573, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1800, 1808, 1842, 1870, 1871, 1873, 2527e, 2825, 3255, 3257, 3260, 3265, 3300, 3370, 3618–3620, 3714, 4005–4007, 4009–4011, 4249, 4319, 4332, 5512, 5869a	5567	
179.	1705-85-7	Chrysene, 6-methyl-	290, 291, 1397, 1560, 1781, 1800, 1870, 1871, 1873, 2037a, 3618, 3756–3759, 4005–4007, 4009–4011, 4249, 5811b	5567	
180.	71277-88-8	Chrysene, pentamethyl-	1650, 1652, 2328, 3732, 3757, 4249, 5811b		
181.	71277-89-9	Chrysene, propyl-	2328, 4249		
182.	71277-90-2	Chrysene, tetramethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
183.	60826-77-9	Chrysene, trimethyl-	1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 5811b		
184.	191-07-1	Coronene 	104, 126, 126a, 126b, 151, 172, 216, 726, 933, 1136, 1139, 1211, 1287–1289, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1870, 1871, 1873, 2037a, 2079, 2115, 2116, 2130, 2134, 2194–2196, 2366, 2438, 2799a, 2939, 2961, 2962, 3255, 3257, 3262, 3269, 3273, 3286, 3292, 3302, 3308, 3616, 3756, 3787, 3788, 3797, 4036, 4249, 4296, 4315, 4319, 4355, 5077, 5811b	903, 5811b	
185.	64760-15-2	Coronene, dimethyl-	3620, 3756, 4249, 5811b		
186.	13119-86-3	Coronene, methyl-	3756, 4249, 5811b		
187.	98791-40-3	1*H*-Cyclopent[*d*]acenaphthylene, 2,7-dihydro-	5811, 5811a, 5811b		
188.	219-86-3	7*H*-Cyclopent[*d*]acenaphthylene	5811, 5811a, 5811b		
189.	202-98-2	4*H*-Cyclopenta[*def*]chrysene {4,5-methylenechrysene} 	2037a, 3756, 4249, 5811b		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
190.	193-54-4	Cyclopenta[*cd*]fluoranthene 	2328, 4249		
191.	189-01-5	Cyclopenta[*cd*]perylene 	2328, 4249		
192.		Cyclopenta[*cd*]perylene, methyl-	2328, 4249		
193.	211-95-0	Cyclopenta[*a*]phenalene 	2328, 4249		
194.	80455-52-3	Cyclopentaphenanthrene {at least two isomers in MSS}	1650, 1652, 3616, 3618–3620, 3732, 3757–3759		
195.	61261-04-9	Cyclopentaphenanthrene	5811, 5811a, 5811b		
196.		Cyclopentaphenanthrene, methyl- {at least two isomers in MSS}	3618–3620, 3758, 3759		
197.	219-07-8	15*H*-Cyclopenta[*a*]phenanthrene, 	1139, 3262, 4355, 5077		
198.	482-66-6	15*H*-Cyclopenta[*a*]phenanthrene, 16,17-dihydro-	966, 2939, 3262, 3302, 3618, 3797, 4249, 4355, 5077, 5811b		
199.	219-08-9	17*H*-Cyclopenta[*a*]phenanthrene 	1560, 1712, 1781, 1800, 1808, 4249		
200.	71277-92-4	17*H*-Cyclopenta[*a*]phenanthrene, ethyl-	1560, 1781, 1800, 1808, 4249		
201.	71277-93-5	17*H*-Cyclopenta[*a*]phenanthrene, methyl-	1560, 1781, 1800, 1808, 4249		
202.	203-64-5	4*H*-Cyclopenta[*def*]phenanthrene {4,5-methylenephenanthrene} 	1981, 2037a, 2191, 2194, 2195, 2200, 2939, 3262, 3308, 3616, 3756, 4249, 5077, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

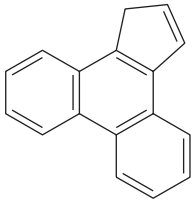
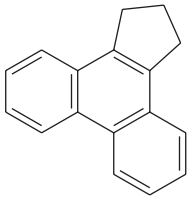
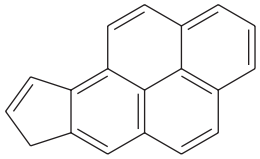
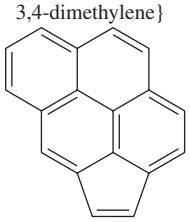
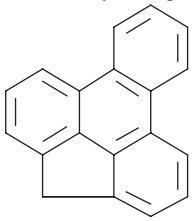
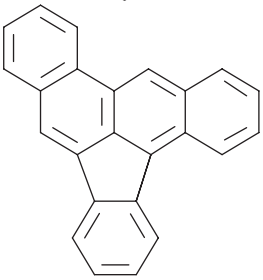
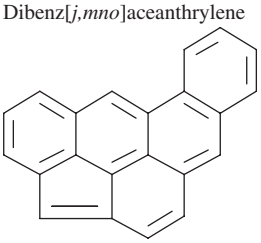
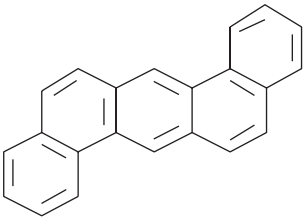
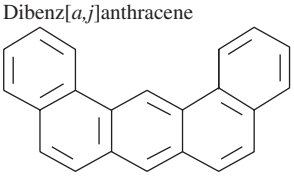
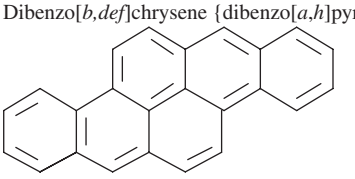
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
203.	71277-91-3	4*H*-Cyclopenta[*def*]phenanthrene, dimethyl-	2328, 4249		
204.	65319-51-9	4*H*-Cyclopenta[*def*]phenanthrene, ethyl-	2328, 4249		
205.	58548-39-3	4*H*-Cyclopenta[*def*]phenanthrene, methyl-	4249		
206.	235-92-7	1*H*-Cyclopenta[*l*]phenanthrene 	5811, 5811a, 5811b		
207.	723-98-8	1*H*-Cyclopenta[*l*]phenanthrene, 2,3-dihydro- 	3756, 5811		
208.	42315-22-0	Cyclopenta[*a*]pyrene 	3618–3620, 3756		
209.		Cyclopenta[*a*]pyrene, 3,4-dihydro- {sometimes listed as 3,4-trimethylenepyrene}	3437, 3618–3620, 3756, 3758, 3759		
210.		Cyclopenta[*a*]pyrene, 3,4-dihydromethyl-	3756, 4249		
211.	27208-37-3	Cyclopenta[*cd*]pyrene {pyrene, 3,4-dimethylene} 	1405, 1406, 1408, 1409, 2260, 2479, 3756, 4249, 5811b		
212.	25732-74-5	Cyclopenta[*cd*]pyrene, 3,4-dihydro-	2260, 2479, 3615, 3618–3620, 3756, 3758, 3759, 4249		
213.		Cyclopenta[*cd*]pyrene, 3,4-dihydrodimethyl-	3756		
214.	64760-18-5	Cyclopenta[*cd*]pyrene, 3,4-dihydromethyl- = Pyrene, 3,4-dimethylene, methyl-	3756, 4249, 4279, 5811b		
215.	23992-32-7	4*H*-Cyclopenta[*def*]triphenylene {4,5-methylenetriphenylene} 	3756, 4249, 5811b		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
216.	5385-75-1	Dibenz[*a,e*]aceanthrylene {dibenzo[*a,e*]fluoranthene} 	399, 1798, 1870, 1871, 1873, 2314, 2427, 2430, 2939, 3033, 3251, 3265, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3756, 4249, 4319, 4353, 4354, 4355, 5811b		
217.	189-75-3	Dibenz[*j,mno*]aceanthrylene 	2328, 4249		
218.	71630-69-8	Dibenz[*j,mno*]aceanthrylene, methyl-	2328, 4249		
219.	414-29-9 67775-07-9	Dibenzanthracene	2518		
220.	53-70-3	Dibenz[*a,h*]anthracene {DB[*a,h*]A} 	126a, 126b, 139–143, 174e, 239, 291, 329, 351, 726, 760, 869, 1021, 1136, 1139, 1148, 1184, 1211, 1217, 1373, 1397, 1405, 1406, 1406a, 1408, 1409, 1425, 1445, 1462, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1787, 1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2013, 2079, 2134, 2191, 2313a, 2438, 2465, 2518, 2601b, 2825, 2939, 2961, 2962, 2964, 3003, 3024, 3176, 3191, 3251, 3255, 3257, 3260, 3262, 3263, 3265, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3365, 3685, 3713, 3714, 3741, 3756, 3787, 3788, 3797, 3814, 3847, 3952, 3999, 4005, 4009–4011, 4024, 4031, 4110, 4232, 4249, 4296, 4300, 4307, 4308, 4311, 4315, 4317, 4319, 4323, 4324, 4332, 4355, 5010, 5077, 5512, 5539, 5811b, 5869a	5567, 5811b	
221.	224-41-9	Dibenz[*a,j*]anthracene 	126, 603, 1397, 1870, 1871, 1873, 2037a, 2134, 2438, 3003, 3257, 3370, 3300, 3756, 3787, 3788, 3788, 4249, 5811b		
222.	189-64-0	Dibenzo[*b,def*]chrysene {dibenzo[*a,h*]pyrene} 	139, 142, 143, 290, 291, 432, 1025, 1139, 1781, 1870, 1871, 1873, 2037a, 2114, 2430, 2438, 2825, 2939, 3003, 3033, 3243, 3244, 3251, 3257, 3262, 3265, 3273, 3292, 3300, 3302, 3308, 3520, 3714, 3741, 3756, 3787, 3788, 3797, 3973, 4005–4007, 4009–4011, 4249, 4282, 4296, 4319, 4332, 4354, 4355, 5077, 5732, 5811b, 5869a		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

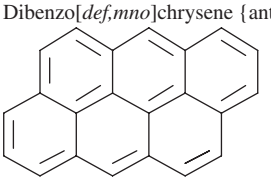
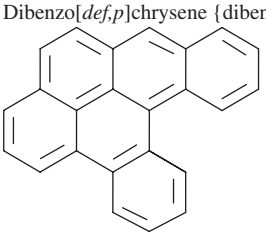
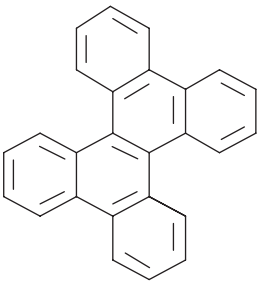
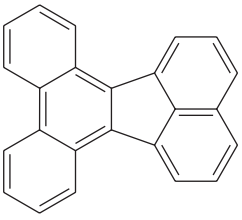
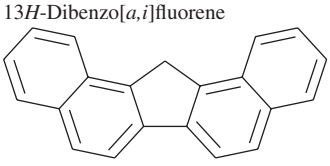
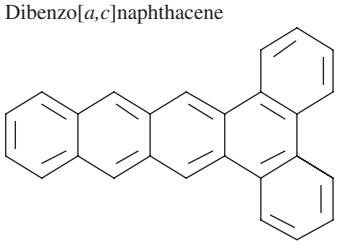
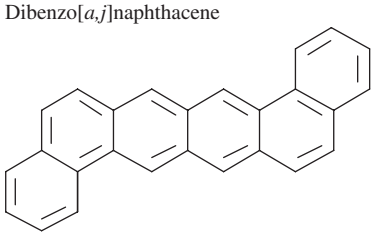
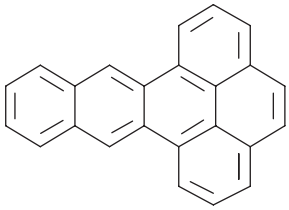
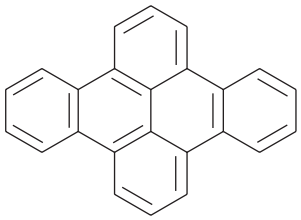
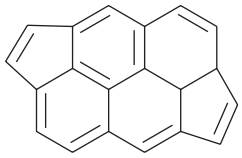
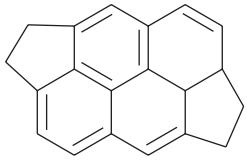
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
223.	191-26-4	Dibenzo[*def,mno*]chrysene {anthanthrene} 	104, 126a, 126b, 141–144, 151, 172, 624, 726, 819, 820, 869, 1136, 1148, 1172, 1287–1289, 1397, 1406, 1408, 1409, 1781, 1787, 1788, 1870, 1871, 1873, 2037a, 2079, 2256, 2270, 2365, 2366, 2430, 2438, 2596a, 2799a, 2939, 2961, 2962, 3003, 3240, 3241, 3251, 3255, 3262, 3273, 3286, 3292, 3302, 3308, 3424, 3756, 3787, 3788, 3797, 4036, 4249, 4282, 4315, 5077, 5811b	5811b	
224.	64760-24-3	Dibenzo[*def,mno*]chrysene, dimethyl- {at least two isomers in MSS}	3756, 4249, 5811b		
225.	41699-10-9	Dibenzo[*def,mno*]chrysene, methyl- {at least two, possibly three, isomers in MSS}	3307, 3756, 5811b		
226.	31927-64-7	Dibenzo[*def,mno*]chrysene, 6-methyl-	4036		
227.	191-30-0	Dibenzo[*def,p*]chrysene {dibenzo[*a,l*]pyrene} 	126a, 141, 143, 151, 399, 726, 1139, 1148, 1211, 1217, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1798, 1808, 1842, 1870, 1871, 1873, 2079, 2134, 2250, 2427, 2430, 2825, 2939, 3003, 3251, 3255, 3257, 3260, 3262, 3265, 3273, 3286, 3300, 3307, 3714, 3756, 3787, 3788, 3999, 4249, 4317, 4319, 4324, 4332, 4353, 4354, 4355, 5077, 5512, 5811b, 5869a	5811b	
228.	191-68-4	Dibenzo[*g,p*]chrysene 	278, 4249		
229.	60382-88-9	Dibenzofluoranthene {at least two isomers in MSS}	279, 4249		
230.	203-18-9	Dibenzo[*j,l*]fluoranthene 	1650, 1652, 3732, 3757		
231.	239-60-1	13*H*-Dibenzo[*a,i*]fluorene 	432, 1025, 1139, 2037a, 2426, 2430, 2939, 3033, 3262, 3300, 3302, 3308, 3797, 4249, 5077, 5732, 5811b		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
232.	216-00-2	Dibenzo[*a,c*]naphthacene 	432, 1139, 2037a, 2430, 2939, 3262, 3302, 3797, 4249, 5077, 5732, 5811b		
233.	227-04-3	Dibenzo[*a,j*]naphthacene 	1139, 2079, 2939, 3003, 3262, 3302, 3797, 3877, 4249, 4282, 4296, 4307, 4308, 4354, 4355, 5077, 5811b		
234.	193-09-9	Dibenzo[*de,qr*]naphthacene {naphtho[2,3-*d*]pyrene} 	2037a, 2249, 2939, 3251, 3262, 3273, 3286, 3302, 4249, 5077		
235.	192-51-8	Dibenzo[*fg,op*]naphthacene {dibenzo[*e,l*]pyrene} 	2438, 2479, 3003, 3756, 5811b		
236.	58615-36-4	Dibenzopyrene	399, 1796, 2479, 3262, 5077		
237.	98791-43-6	Dicyclopenta[*cd,jk*]pyrene 	5811, 5811a, 5811b		
238.	98791-44-7	Dicyclopenta[*cd,jk*]pyrene, 1,2-dihydro-	5811, 5811a, 5811b		
239.	98791-45-8	Dicyclopenta[*cd,jk*]pyrene, 1,2,3,4-tetrahydro- 	5811, 5811a, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

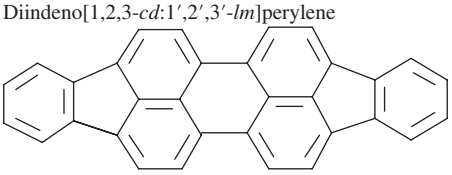
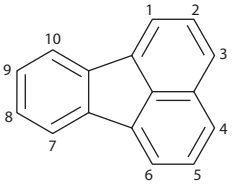
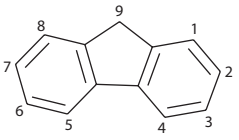
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
240.	188-94-3	Diindeno[1,2,3-*cd*:1′,2′,3′-*lm*]perylene 	3337–3340, 4249		
241.		Fluoraninene, ethylmethyl-	2328, 4249		
242.	206-44-0	Fluoranthene 	39, 49, 50, 104, 117, 126a, 126b, 128, 141–143, 151, 172, 216, 239, 244, 291, 329, 583, 584, 603, 646a, 726, 746a, 798, 804, 818–820, 966, 869, 1019, 1099, 1100, 1136, 1139, 1172, 1235, 1236, 1287–1289, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408, 1409, 1437, 1445, 1462, 1471, 1649, 1712, 1763, 1781, 1787, 1788, 1800, 1842, 1870, 1871, 1873, 1971, 2013, 2037a, 2079, 2099, 2130, 2134, 2191, 2196, 2200, 2203, 2210, 2238, 2256, 2270, 2313a, 2365–2367, 2430, 2438, 2473, 2474, 2501, 2557, 2596a, 2722, 2777, 2799a, 2893, 2939, 2961, 2962, 2964, 3083, 3141, 3149, 3176, 3191, 3240–3243, 3246, 3249–3251, 3255, 3257, 3262, 3265, 3273–3275, 3286, 3291, 3292, 3300, 3302, 3307, 3308, 3370, 3421–3424, 3437, 3452, 3465–3467, 3469, 3493, 3514, 3610, 3616, 3618, 3685, 3686, 3756, 3758–3759, 3787, 3788, 3797, 3820, 3876, 3952, 4005, 4009–4011, 4018, 4019, 4020, 4022, 4031, 4110, 4249, 4282, 4284, 4300, 4307, 4308, 4311, 4315, 4319, 4323, 4324, 4354, 4355, 4404, 5077, 5539, 5732, 5811b	903, 2079, 2939, 3059, 3194, 3205, 4249, 5567, 5811b	50, 1375a, 1377, 1378, 2210
243.		Fluoranthene, alkyl-	142, 143, 1139, 1172, 1560, 1787, 1788, 1971, 2893, 3251, 3262, 3273, 3286, 3308, 4031, 4284, 4300, 4307, 4308, 4315, 4319, 5077		
244.	41593-24-2	Fluoranthene, dihydro-	1508, 4249		
245.	71278-25-6	Fluoranthene, dihydromethyl-	1508, 4249		
246.	60826-74-6	Fluoranthene, dimethyl- {at least four isomers in MSS}	478, 1763, 1781, 2939, 3083, 3092, 3262, 3437, 3616, 3618–3620, 3756–3759, 4031, 4249, 5077, 5811b		
247.	23339-04-0	Fluoranthene, 2,3-dimethyl-	5811, 5811a, 5811b		
248.	38048-87-2	Fluoranthene, 7,8-dimethyl-	5811, 5811a, 5811b		
249.	22271-04-1	Fluoranthene, 7,10-dimethyl-	5811, 5811a, 5811b		
250.	25889-63-8	Fluoranthene, 8,9-dimethyl-	726, 2939, 3262, 3302, 3797, 4031, 4249, 5077, 5811b		
251.	55220-72-9	Fluoranthene, ethyl-	1781, 2767, 4249		
252.	20496-16-6	Fluoranthene, 3-ethyl-	5811, 5811a, 5811b		
253.	46864-87-3	Fluoranthene, 8-ethyl-	5811, 5811a, 5811b		
254.	71277-96-8	Fluoranthene, ethylmethyl-	1650, 1652, 3732, 3757, 5811b		
255.	71277-97-9	Fluoranthene, hexamethyl-	1650, 1652, 3732, 3757, 4249		
256.	30997-39-8	Fluoranthene, methyl-	1802, 3292, 3437, 3616, 4009–4011, 4249, 5811b		
257.	25889-60-5	Fluoranthene, 1-methyl-	1471, 1763, 1781, 2037a, 2767, 3083, 3618–3620, 3756, 3758–3759, 4249, 5811b		
258.	33543-31-6	Fluoranthene, 2-methyl-	1471, 1781, 1870, 1871, 2037a, 2767, 3083, 3618–3620, 3756, 3758–3759, 4005, 4009–4011, 4249, 5811b	2389, 2544	
259.	1706-01-0	Fluoranthene, 3-methyl-	1763, 1781, 1870, 1871, 2037a, 2767, 3083, 4005, 4009–4011, 4249, 5811b		
260.	23339-05-1	Fluoranthene, 7-methyl-	1781, 2037a, 2767, 4249		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
261.	20485-57-8	Fluoranthene, 8-methyl-	1139, 1471, 1781, 2939, 3083, 3262, 3302, 3618–3620, 3756–3759, 3797, 4018, 4019, 4031, 4249, 5077, 5811b		
262.	71277-98-0	Fluoranthene, pentamethyl- {at least two isomers in MSS}	1650, 1652, 3732, 3757, 4249		
263.	55220-69-4	Fluoranthene, propyl-	2328, 4249		
264.	71277-99-1	Fluoranthene, tetramethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
265.	41637-87-0	Fluoranthene, trimethyl-	1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 4746, 5811b		
266.	86-73-7	9*H*-Fluorene 	39, 50, 104, 142, 143, 151, 172, 245, 291, 394, 397, 603, 646a, 658, 746a, 869, 1139, 1287–1289, 1360, 1371, 1375, 1375a, 1375b, 1377, 1378, 1427, 1435a, 1437, 1462, 1649, 1650, 1652, 1759, 1842, 1870, 1871, 1873, 1981, 2013, 2079, 2113, 2116, 2130, 2134, 2195, 2200, 2313a, 2438, 2537, 2543, 2550, 2557, 2570, 2710, 2731, 2735, 2596a, 2761, 2762, 2765–2767, 2773, 2777, 2799a, 2822, 2939, 2961, 2962, 2964, 3083, 3149, 3176, 3191, 3251, 3262, 3263, 3273, 3286, 3292, 3300, 3302, 3308, 3370, 3410, 3452, 3465–3467, 3469, 3470, 3472, 3493, 3514, 3553, 3557, 3616, 3618–3620, 3729, 3732, 3741, 3757–3759, 3787, 3797, 3999, 4249, 4342, 4409, 5010, 5077, 5539, 5811b	172, 3547, 5567, 5811b	50, 1360, 1375a, 1377, 1378
267.	30582-01-5	9*H*-Fluorene, dimethyl- {at least five isomers in MSS}	245, 1650, 1652, 1759, 2570, 2767, 3083, 3557, 3618–3620, 3732, 3757–3759, 5811b	3547	
268.		9*H*-Fluorene, ?,9-dimethyl-	1650, 1652, 3732, 3757		
269.	17057-98-6	9*H*-Fluorene, 1,9-dimethyl-	1650, 1652, 1759, 2767, 3084, 3557, 4249, 5811b		
270.	4612-63-9	9*H*-Fluorene, 2,3-dimethyl-	1759, 2767, 3084, 4249, 5811b	3547	
271.	4569-45-3	9*H*-Fluorene, 9,9-dimethyl-	1759, 2767, 4249, 5811b		
272.	71278-00-7	9*H*-Fluorene, dimethylethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
273.	65319-49-5	9*H*-Fluorene, ethyl- {at least two isomers in MSS}	1508, 1650, 1652, 2767, 3732, 3757, 4249, 5811b		
274.	1207-20-1	9*H*-Fluorene, 2-ethyl-	1759, 2767, 5811b		
275.	2294-82-8	9*H*-Fluorene, 9-ethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
276.	71278-01-8	9*H*-Fluorene, ethylmethyl- {at least two isomers in MSS}	1650, 1652, 3732, 3757, 4249, 5811b		
277.	26914-17-0	9*H*-Fluorene, methyl-	245, 646a, 1360, 1371, 1375a, 1649, 2134, 2438, 2543, 2570, 2761, 2762, 2765, 2766, 2773, 2777, 3514, 5811b	3547	1360, 1375a
278.	1730-37-6	9*H*-Fluorene, 1-methyl-	50, 104, 1139, 1650, 1652, 1759, 2761, 2762, 2765–2767, 2939, 3083, 3262, 3616, 3618–3620, 3732, 3757–3759, 3797, 4019, 4249, 5077, 5811b	2093, 4249	45
279.	1430-97-3	9*H*-Fluorene, 2-methyl-	104, 1375, 1375b, 1378, 1650, 1652, 1759, 2767, 3083, 3514, 3553, 3557, 3618, 3616, 3619, 3620, 3732, 3757–3759, 4249, 5811b	1248, 3547, 4249, 5811b	1378
280.	2523-39-9	9*H*-Fluorene, 3-methyl-	104, 1650, 1652, 1759, 3083, 3557, 3618, 3619, 3620, 3732, 3757–3759, 4249, 5811b	3547, 4249, 5811b	
281.	1556-99-6	9*H*-Fluorene, 4-methyl-	104, 1378, 1650, 1652, 1759, 2767, 3083, 3557, 3618–3620, 3732, 3757–3759, 4249, 5811b	1248, 3547, 4249, 5811b	1378
282.	2523-37-7	9*H*-Fluorene, 9-methyl-	104, 245, 394, 1139, 1650, 1652, 1759, 2710, 2767, 2939, 3262, 3302, 3616, 3619, 3620, 3732, 3757–3759, 3797, 4019, 4249, 5077, 5811b	1248, 3547, 4249, 5811b	

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

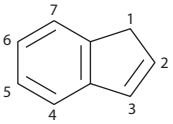
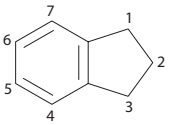
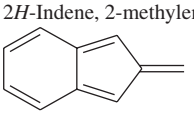
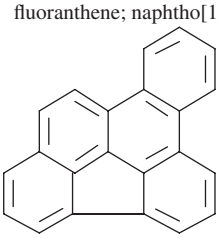
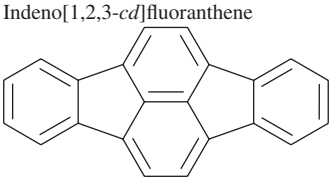
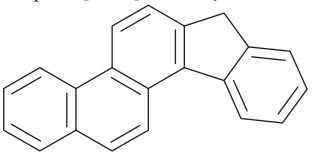
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
283.	4425-82-5	9*H*-Fluorene, 9-methylene-	1562, 1767, 3084, 4249		
284.	63372-50-9	9*H*-Fluorene, tetramethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
285.	30582-02-6	9*H*-Fluorene, trimethyl-	1650, 1652, 3732, 3757, 5811b		
286.	95-13-6	1*H*-Indene 	37, 104, 142, 143, 147, 151, 156, 157, 172, 216, 568b, 798, 1313, 1338, 1339, 1375, 1375b, 1426–1428, 1472, 1649, 1650, 1652, 1981, 2134, 2438, 2506, 2507, 2508, 2543, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2799a, 3262, 3308, 3465–3467, 3469, 3530, 3557, 3616, 3647, 3729, 3732, 3757–3759, 3797, 4249, 4570a, 5034, 5077, 5811b	38, 568b, 4249, 4425, 5811b	2506, 2507, 3401
287.	71278-05-2	1*H*-Indene, diethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
288.	496-11-7	1*H*-Indene, 2,3-dihydro- {indane} 	172, 299, 568b, 1426, 1427, 1444, 1881, 1959, 2508, 2545, 2570, 2742, 2743, 3530, 3557, 4249, 4570a, 5034, 5770, 5811b	5811b	3401
289.	53563-67-0	1*H*-Indene, 2,3-dihydrodimethyl- {four isomers detected}	2506, 2507, 2570, 2731, 2735, 2742, 2743, 3557, 4248, 4249		2506(0), 2507(0)
290.	17057-82-8	1*H*-Indene, 2,3-dihydro-1,2-dimethyl-	2767, 2769, 3557, 4249		
291.	71278-02-9	1*H*-Indene, 2,3-dihydroethyl-	2742, 2743, 2769, 3557, 4249		
292.	27133-93-3	1*H*-Indene, 2,3-dihydromethyl- {four isomers detected}	157, 1371, 1375, 1375b, 2506, 2507, 2543, 2545, 2570, 2628, 2629, 2636, 2731, 2735, 2742, 2743, 2773, 2799a, 3410, 4249, 5811b		2506 (0), 2507 (0)
293.	767-58-8	1*H*-Indene, 2,3-dihydro-1-methyl-	1375, 1375b, 1822, 2743, 5811b		
294.	824-63-5	1*H*-Indene, 2,3-dihydro-2-methyl-	2742, 2743, 4249, 5811b		
295.	824-22-6	1*H*-Indene, 2,3-dihydro-4-methyl-	1375, 1959, 4249		
296.	874-35-1	1*H*-Indene, 2,3-dihydro-5-methyl-	1959, 2769, 3557, 4249		
297.	16204-57-2	1*H*-Indene, 2,3-dihydro 1,1,4,5-tetramethyl-		2917a	
298.	942-43-8	1*H*-Indene, 2,3-dihydro 1,1,5,6-tetramethyl-		2917a	
299.	36541-18-1	1*H*-Indene, 2,3-dihydrotrimethyl-	2570, 2731, 2735, 2769, 3557, 4249, 5811b		
300.	29348-63-8	1*H*-Indene, dimethyl-	104, 1650, 1652, 2506, 2507, 2731, 2735, 2761, 2762, 2765, 2766, 3557, 3618–3620, 3732, 3757–3759, 4249, 5811b		2506, 2507
301.	71278-06-3	1*H*-Indene, dimethylethyl-	104, 1650, 1652, 3732, 3757, 4249, 5811b		
302.		1*H*-Indene, 5,6-dimethyl-2-phenyl-	245		
303.		1*H*-Indene, 2-(3′,4′-dimethylphenyl)-	245		
304.	58924-35-9	1*H*-Indene, ethyl-	104, 1650, 1652, 2438, 2731, 2735, 3732, 3757, 4249, 5811b		
305.	77227-01-1	1*H*-Indene, ethylmethyl-	1650, 1652, 3732, 3757, 4249, 5811, 5811a, 5811b		
306.	71278-07-4	1*H*-Indene, ethylpentamethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
307.	77242-77-4 86901-30-6	1*H*-Indene, heptamethyl-	1650, 1652, 3732, 3757, 5811, 5811a, 5811b		
308.	71278-08-5	1*H*-Indene, hexamethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
309.	29036-25-7	1*H*-Indene, methyl- {at least three isomers present in MSS}	104, 156, 157, 1360, 1375a, 1427, 1650, 1652, 2438, 2506, 2507, 2570, 2628, 2629, 2636, 2731, 2735, 2799a, 3557, 3616, 3619, 3620, 3732, 3757–3759, 4249, 5034, 5811b		1360, 1375a, 2506, 2507, 3401
310.	767-59-9	1*H*-Indene, 1-methyl-	1650, 1652, 3618–3620, 3732, 3757–3759, 4249, 5811b		
311.	2177-47-1	1*H*-Indene, 2-methyl-	638, 1650, 1652, 3618–3620, 3732, 3757, 4249		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
312.	767-60-2	1*H*-Indene, 3-methyl-	1650, 1652, 2767, 3557, 3618, 3732, 3757–3759, 4249, 5811b		
313.	2471-84-3	1*H*-Indene, 1-methylene-	3557, 4249		
314.	6596-86-7	2*H*-Indene, 2-methylene- {benzofulvene} 	3557		
315.		1*H*-Indene, 4-methyl-2-(2′-methylphenyl)-	245		
316.		1*H*-Indene, 5-methyl-2-(4-methylphenyl)-	245		
317.		1*H*-Indene, 6-methyl-2-(4-methylphenyl)-	245		
318.		1*H*-Indene, 7-methyl-2-(2′-methylphenyl)-	245		
319.		1*H*-Indene, 7-(4′-methylphenyl)-	245		
320.	71278-09-6	1*H*-Indene, pentamethyl-	3732, 3757, 4249, 5811b		
321.	38638-41-4	1*H*-Indene, phenyl-	1800, 3732, 3757, 4249, 5811b		
322.		1*H*-Indene, 2-phenyl-	278		
323.		1*H*-Indene, phenyltrimethyl-	245		
324.	27135-78-0	1*H*-Indene, tetramethyl- {at least four isomers present in MSS}	104, 1650, 1652, 2731, 2735, 3732, 3757, 4249, 5811b		
325.	60826-61-1	1*H*-Indene, trimethyl- {at least three isomers present in MSS}	104, 1650, 1652, 2506, 2507, 2731, 2735, 3618–3620, 3732, 3757–3759, 4249, 5811b		2506, 2507
326.	668-30-4	Indeno[1,2,3,4-*defg*]chrysene {also reported as indeno[3,2,1,7-*defg*]chrysene; dibenzo[*b,mno*]fluoranthene; naphtho[1,2,3,4-*ghi*]fluoranthene} 	2328, 4249		
327.	71277-94-6	Indeno[1,2,3,4-*defg*]chrysene, methyl- {indeno[3,2,1,7-*defg*]chrysene, methyl-; dibenzo[*b,mno*]fluoranthene, methyl-; naphtho[1,2,3,4-*ghi*]fluoranthene, methyl-}	2328		
328.	193-43-1	Indeno[1,2,3-*cd*]fluoranthene 	128, 142, 143, 1099, 1100, 1139, 1217, 1409, 1445, 1727, 1740, 1741, 1743, 1744, 1773, 1788, 1798, 1808, 1870, 1871, 2825, 3262, 3265, 3714, 3756, 3797, 4005, 4009, 4010, 4249, 4315, 4319, 4332, 5077, 5512		
329.	41699-07-4	Indeno[1,2,3-*cd*]fluoranthene, methyl-	2328, 4249		
330.	98791-41-4	1*H*-Indeno[1,7-*ab*]fluorene	5811, 5811a, 5811b		
331.	98791-42-5	1*H*-Indeno[1,7-*ab*]fluorene 2,11-dihydro-	5811, 5811a, 5811b		
332.	220-97-3	11*H*-Indeno[2,1-*a*]phenanthrene{11*H*-naphtho[2,1-*a*]fluorene} 	39, 1139, 2037a, 2939, 3262, 3302, 3308, 3337, 3339, 3797, 4249, 5077, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

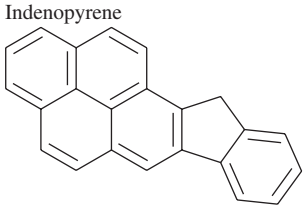
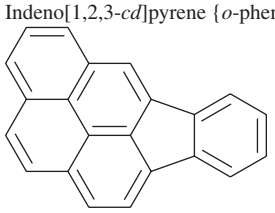
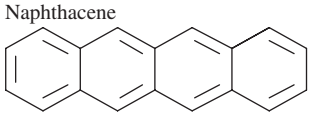
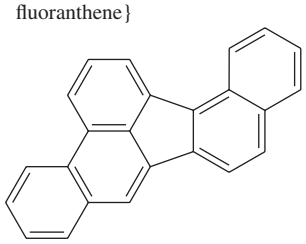
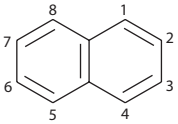
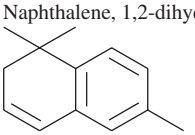
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
333.	72254-06-9	Indenopyrene 	5811, 5811a		
334.	193-39-5	Indeno[1,2,3-*cd*]pyrene {*o*-phenylenepyrene} 	104, 126a, 128, 141, 142, 151, 239, 290, 291, 603, 1099, 1139, 1217, 1397, 1405, 1406, 1408, 1409, 1445, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1788, 1798, 1800, 1802, 1808, 1870, 1871, 2013, 2134, 2438, 2479, 2524a, 2601b, 2799a, 2825, 3176, 3255, 3257, 3262, 3265, 3300, 3302, 3308, 3370, 3616, 3714, 3756, 3758–3759, 3797, 4005, 4010, 4011, 4249, 4311, 4315, 4317, 4319, 4324, 4325, 4332, 5010, 5077, 5512, 5539, 5811b, 5869a	5567	
335.	64158-99-2	Indeno[1,2,3-*cd*]pyrene, dimethyl- {at least two isomers present in MSS}	3615, 3756, 4249, 5811b		
336.	64158-98-1	Indeno[1,2,3-*cd*]pyrene, methyl- {at least two isomers present in MSS}	2328, 3756, 4249, 5811b		
337.		Indeno[1,2,3-*cd*]pyrene, trimethyl- {at least two isomers present in MSS}	3756		
338.	92-24-0	Naphthacene 	624, 658, 798, 1139, 1211, 2113, 2114, 2249, 2550, 2799a, 2963, 3003, 3191, 3262, 3797, 4249, 5077, 5811b		
339.	5385-22-8	Naphth[1,2-*e*]acephenanthrylene {dibenzo[*b,j*] fluoranthene} 	3615, 3756, 4249, 5811b		
340.	91-20-3	Naphthalene 	84, 104, 141–144, 147, 151, 156, 157, 167, 172, 174e, 239, 291, 299, 329, 394, 397, 568b, 603, 624, 710, 746a, 798, 869, 966, 1094, 1099, 1100, 1135, 1139, 1287, 1288, 1313, 1360, 1371, 1375, 1375a, 1375b, 1377, 1378, 1427, 1435a, 1437, 1442, 1445, 1447, 1462, 1472, 1485, 1649, 1650, 1652, 1760, 1767, 1781, 1842, 1959, 1972, 1981, 2013, 2079, 2113, 2114, 2133, 2134, 2142, 2195, 2255, 2270, 2313a, 2428, 2438, 2479, 2506, 2507, 2508, 2543, 2545, 2557, 2570, 2722, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2784, 2939, 2961, 2962, 3003, 3081, 3082, 3176, 3191, 3240, 3241, 3249, 3251, 3255, 3257, 3262, 3263, 3265, 3269, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3370, 3397, 3410, 3441a, 3452, 3464–3470, 3472, 3492, 3498, 3509, 3557, 3559, 3578, 3616, 3618–3620, 3647, 3729, 3732, 3741, 3757–3759, 3787, 3797, 3847, 4009, 4010, 4249, 4282, 4319, 4325, 4342, 4355, 4570a, 4966, 5010, 5034, 5077, 5539, 5811b, 5869a	84, 172, 568b, 2339a, 2784, 4249, 5533, 5567, 5636, 5811b	1360, 1375a, 1377, 1378, 2506, 2507, 3401, 3402

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
341.		Naphthalene, alkyl-	2508, 2570, 3262, 3452, 3465–3470, 4319, 4325, 5077		
342.	31831-35-3	Naphthalene, diethyl-		84, 4249	
343.	29828-28-2	Naphthalene, dihydro-	2479, 2767, 4249		
344.	72692-88-7	Naphthalene, dihydrodimethyl- {at least four isomers in MSS}	1375, 1375b, 2570, 2767, 2777, 3557, 4249		
345.	39292-53-0	Naphthalene, dihydromethyl- {at least three isomers in MSS}	1360, 1375, 1375a, 1375b, 2570, 2761, 2762, 2765–2767, 3557, 4249, 5811b		1360, 1375a
346.	2717-44-4	Naphthalene, 1,2-dihydro-3-methyl-	2479, 5811b		
347.	4373-13-1	Naphthalene, 1,2-dihydro-4-methyl-	1378, 3251, 3262, 3273, 3286, 3302, 5077		1378
348.	67494-22-8	Naphthalene,1,2-dihydro-5-methyl-3-(1-methylethenyl)-		946, 1156, 4090, 4249	
349.	2717-47-7	Naphthalene, 1,2-dihydro-6-methyl-	5811, 5811a, 5811b		
350.		Naphthalene, dihydrotrimethyl- {at least two isomers in MSS}	3557	3547	
351.	30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl- 	1110, 2479, 3219, 3308, 4249	909, 1149, 1149a, 2093, 2248, 2917a, 4249, 4564, 5811b	
352.	4506-36-9	Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	1375, 1375b, 2479, 2769, 3557, 4249	984, 2389, 2544, 4249, 5811b	
353.	28804-88-8	Naphthalene, dimethyl-	1360, 1375, 1375a, 1375b, 1427, 2438, 2479, 2543, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 3492, 3509, 3618, 4249, 5034	2339a	1360, 1375a
354.	573-98-8	Naphthalene, 1,2-dimethyl-	104, 291, 568b, 1135, 1650, 1652, 2479, 2767, 2784, 3616, 3732, 3757, 4249, 5811b	84, 568b, 2784, 4249, 4564, 5811b	
355.	575-41-7	Naphthalene, 1,3-dimethyl-	84, 104, 291, 568b, 1135, 1650, 1652, 2479, 2767, 2784, 3557, 3616, 3618–3620, 3732, 3757–3759, 4249, 5811b	84, 568b, 2784, 4249, 5811b	
356.	571-58-4	Naphthalene, 1,4-dimethyl-	104, 568b, 1135, 1650, 1652, 2479, 2784, 3492, 3616, 3618–3620, 3732, 3757–3759, 4249, 5811b	84, 568b, 2784, 4249, 5811b	
357.	571-61-9	Naphthalene, 1,5-dimethyl-	104, 1133, 1650, 1652, 2479, 2784, 3492, 3616, 3618–3620, 3732, 3757–3759, 5811b	84, 2784, 4249, 5811b	
358.	575-43-9	Naphthalene, 1,6-dimethyl-	84, 104, 568b, 798, 1135, 1139, 1375, 1375b, 1378, 1426, 1427, 1650, 1652, 1972, 2479, 2722, 2767, 2784, 3255, 3262, 3302, 3308, 3557, 3616, 3618–3620, 3732, 3757–3759, 3797, 4249, 5077, 5811b	84, 568b, 2784, 3547, 4249, 5811b	1378

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

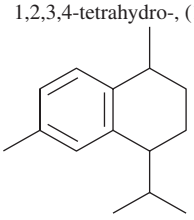
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
359.	575-37-1	Naphthalene, 1,7-dimethyl-	104, 1135, 1650, 1652, 2479, 2767, 2784, 3618–3620, 3732, 3757–3759, 4249, 5811b	84, 2784, 4249, 5811b	
360.	569-41-5	Naphthalene, 1,8-dimethyl-	104, 394, 568b, 798, 1135, 1139, 1650, 1652, 2479, 2784, 2939, 3262, 3302, 3308, 3557, 3616, 3618–3620, 3732, 3757–3759, 3787, 3797, 4249, 5077, 5811b	568b, 2784, 4249	
361.	581-40-8	Naphthalene, 2,3-dimethyl-	104, 1135, 1650, 1652, 2479, 2784, 3557, 3616, 3618–3620, 3732, 3757–3759, 4249, 5811b	84, 2784, 4249	
362.	581-42-0	Naphthalene, 2,6-dimethyl-	84, 104, 568b, 798, 1110, 1139, 1650, 1652, 1972, 2479, 2722, 3262, 3302, 3308, 3557, 3616, 3618–3620, 3732, 3741, 3757–3759, 3797, 4249, 5077, 5811b	84, 568b, 2784, 4249, 5811b	
363.	582-16-1	Naphthalene, 2,7-dimethyl-	84, 104, 568b, 798, 1135, 1139, 1650, 1652, 1972, 2479, 2722, 2784, 3262, 3308, 3557, 3618–3620, 3732, 3757–3759, 4249, 5077, 5811b	84, 568b, 2784, 4249, 5811b	
364.	71630-68-7	Naphthalene, dimethyl-2-ethenyl-	734, 2479, 4249, 5811b		
365.	65319-44-0	Naphthalene, dimethylethyl-	2479, 3557, 4249, 5811b		
366.	71607-89-1	Naphthalene, 1,4-dimethyl-2-ethyl-	2769, 3557, 4249		
367.	66309-90-8	Naphthalene, 1,4-dimethyl-5-ethyl-	1650, 1652, 3732, 3757, 4249		
368.	29350-19-3	Naphthalene, 1,6-dimethyl-1α,4α,4aα,6α,8α,8β-hexahydro-4-(1-methylethyl)- {cadinene}		1053, 3266	
369.	483-77-2	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-1,2,3,4-tetrahydro-, (1S-*Z*)- 		404, 1247, 1256, 4088, 4249, 5811b	
370.	71607-60-8	Naphthalene, dimethyl-2-phenyl-	1650, 1652, 2479, 3732, 3757, 4249, 5811b		
371.		Naphthalene, dimethyltetrahydro- {at least three isomers in MSS}	1375, 1375b, 2570, 2767, 3557, 4249		
372.	51855-29-9 65338-07-0	Naphthalene, dimethyl-1,2,3,4-tetrahydro- {at least five isomers in MSS}	2479, 2570, 2769		
373.		Naphthalene, ethenyl-	5034		
374.	826-74-4	Naphthalene, 1-ethenyl-	104, 2113, 2479, 2557, 3616, 3618–3620, 3758–3759, 4249, 5811b		
375.	827-54-3	Naphthalene, 2-ethenyl-	104, 1650, 1652, 2113, 2557, 3616, 3618–3620, 3732, 3757–3759, 4249, 5811b		
376.	64031-89-6	Naphthalene, 2-ethenylmethyl- {at least two isomers in MSS}	1650, 1652, 2479, 3615, 3732, 3757, 5811b		
377.	35737-86-1	Naphthalene, 2-ethenyl-1-methyl-	4249		
378.	27138-19-8	Naphthalene, ethyl-	1360, 1375a, 2328, 2438, 2506, 2507, 2761, 2762, 2765, 2766, 3410, 4249, 5811b		1360, 1375a, 2506, 2507
379.	1127-76-0	Naphthalene, 1-ethyl-	104, 1135, 1650, 1652, 1881, 2479, 2784, 3492, 3557, 3616, 3618–3620, 3732, 3757–3759, 4249, 5811b	84, 2339a, 2784, 4249, 5811b	
380.	939-27-5	Naphthalene, 2-ethyl-	104, 1135, 1650, 1652, 1881, 2479, 2767, 2784, 3492, 3557, 3616, 3618–3620, 3732, 3757–3759, 4249, 5811b	2339a, 2784, 4249	

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
381.	31391-42-1	Naphthalene, ethylmethyl-	104, 1135, 1650, 1652, 2784, 3226, 3732, 3757, 4249, 5811b		
382.	17057-94-2	Naphthalene, 1-ethyl-3-methyl-	1135, 2784	2784, 4249	
383.	17057-92-0	Naphthalene, 1-ethyl-5-methyl-	1135, 2784	2784, 4249	
384.	31032-91-4	Naphthalene, 1-ethyl-6-methyl-	1135, 2479, 2784	2784, 4249	
385.	31032-92-5	Naphthalene, 1-ethyl-7-methyl-	1135, 2479, 2784	2784, 4249	
386.	61886-71-3	Naphthalene, 1-ethyl-8-methyl-	1135, 2479, 2784	2784, 4249	
387.	31032-94-7	Naphthalene, 2-ethyl-3-methyl-	1135, 2479, 2784	2784, 4249	
388.	17179-41-8	Naphthalene, 2-ethyl-4-methyl- {= naphthalene, 3-ethyl-1-methyl-}	1135, 2784	2784, 4249	
389.	17059-53-9	Naphthalene, 2-ethyl-5-methyl- {= naphthalene, 6-ethyl-1-methyl-}	1135, 2784	2784, 4249	
390.	7372-86-3	Naphthalene, 2-ethyl-6-methyl-	1135, 2479, 2784	2784, 4249	
391.	17059-55-1	Naphthalene, 2-ethyl-7-methyl-	1135, 1375, 1375b, 1650, 1652, 2479, 2769, 2784, 4249	2784, 5811b	
392.	77242-78-5	Naphthalene, hexamethyl-	1650, 1652, 3732, 3757, 5811b		
393.	1321-94-4	Naphthalene, methyl-	222–224, 1649, 2438, 2506, 2507, 2767, 2777, 2799a, 3470, 3472, 4249, 5034, 5811b	3547	2506, 2507, 3401
394.	90-12-0	Naphthalene, 1-methyl-	84, 104, 141–143, 151, 291, 568b, 798, 1094, 1139, 1313, 1360, 1371, 1375, 1375a, 1375b, 1378, 1426, 1427, 1650, 1652, 1959, 1972, 2134, 2142, 2313a, 2479, 2722, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2784, 3240, 3251, 3255, 3262, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3410, 3492, 3509, 3557, 3559, 3616, 3618–3620, 3647, 3729, 3732, 3757–3759, 3787, 3797, 4010, 4011, 4249, 4570a, 5010, 5077, 5539, 5811b	84, 568b, 2339a, 2784, 4249, 5811b	1360, 1375a, 1378, 3402
395.	91-57-6	Naphthalene, 2-methyl-	84, 104, 141–143, 151, 291, 568b, 798, 820, 1094, 1139, 1287, 1288, 1313, 1360, 1371, 1375, 1375a, 1375b, 1377, 1378, 1426, 1427, 1650, 1652, 1822, 1959, 1972, 2079, 2134, 2142, 2313a, 2479, 2543, 2545, 2722, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2784, 2939, 3251, 3255, 3262, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3410, 3492, 3509, 3557, 3559, 3616, 3618–3620, 3647, 3729, 3732, 3741, 3757–3759, 3787, 3797, 4010, 4011, 4249, 4570a, 5010, 5077, 5539, 5811b	84, 568b, 1256, 2339a, 2784, 3186, 3188, 4249	1360, 1375a, 1377, 1378
396.	29253-36-9	Naphthalene, (1-methylethyl)-	104, 1650, 1652, 2479, 3226, 3732, 3757, 4249, 5811b	84	
397.	2027-17-0	Naphthalene, 2 (1-methylethyl)-		2339a, 5811b	
398.		Naphthalene, methylphenyl-	4249		
399.	71607-61-9	Naphthalene, methyl-2-phenyl-	1650, 1652, 2479, 3732, 3757, 4249, 5811b		
400.	34540-66-4	Naphthalene, methylpropyl-	4810a, 4249	84	
401.	1680-58-6	Naphthalene, 1-(1-methylpropyl)-	1135, 2479, 2767, 2769, 4249	84, 4249, 5811b	
402.	16727-91-6	Naphthalene, 1-(2-methylpropyl)-	1135, 2479		
403.	71607-57-3	Naphthalene, methyltetrahydro- {at least three isomers in MSS}	2761, 2762, 2765–2767, 3557, 4249		
404.	31291-71-1	Naphthalene, methyl-1,2,3,4-tetrahydro-	1822, 2479, 2767, 3557, 4249		
405.	1559-81-5	Naphthalene, 1-methyl-1,2,3,4-tetrahydro-	1884, 2485, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

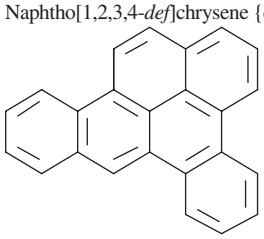
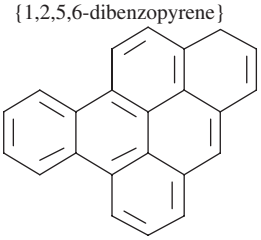
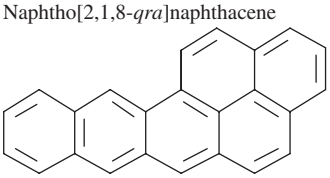
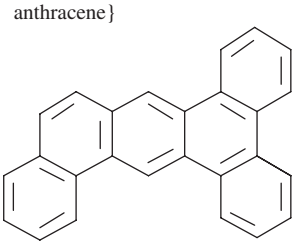
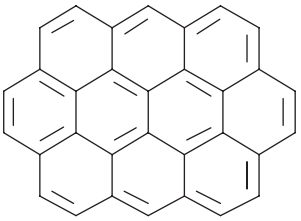
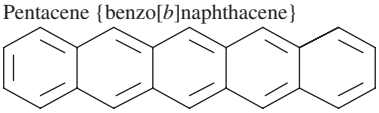
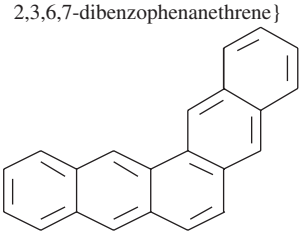
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
406.	3877-19-8	Naphthalene, 2-methyl-1,2,3,4-tetrahydro-	299, 2479, 2742, 2743, 4249, 5811b		
407.	2809-64-5	Naphthalene, 5-methyl-1,2,3,4-tetrahydro-	5811b	84, 4249, 5811b	
408.	1680-51-9	Naphthalene, 6-methyl-1,2,3,4-tetrahydro- = {naphthalene, 2-methyl-5,6,7,8-tetrahydro-}	39, 2742, 2743, 3618, 3758–3759, 4249	84, 4249	
409.	56908-81-7	Naphthalene, pentamethyl-	104, 1650, 1652, 2479, 3732, 3757, 4249, 5811b		
410.	605-02-7	Naphthalene, 1-phenyl-	39, 2037a, 2113, 2479, 3286, 3757, 4249, 5811b		
411.	612-94-2	Naphthalene, 2-phenyl-	143, 147, 151, 1650, 1652, 2037a, 2113, 2479, 3251, 3262, 3273, 3292, 3302, 3514, 3732, 3757, 3952, 4249, 5077, 5811b		
412.	71697-04-6	Naphthalene, phenyl-, monomethyl derivative	1508, 2479, 3797		
413.	27378-74-1	Naphthalene, propyl-		84	
414.	2765-18-6	Naphthalene, 1-propyl-	1135, 2479	1135, 4249	
415.	2027-19-2	Naphthalene, 2-propyl-	1135, 2479	1135, 4249	
416.	119-64-2	Naphthalene, 1,2,3,4-tetrahydro- {tetralin}	84, 142, 143, 151, 568b, 1426, 1427, 1959, 2479, 2743, 3219, 3308, 4249, 5811b	84, 568b, 4249, 5811b	
417.	121214-18-4	Naphthalene, tetrahydrotrimethyl- {at least three isomers in MSS}	1375, 1375b, 1650, 1652, 2570, 3557, 4249		
418.		Naphthalene, 1,2,3,4-tetrahydro-4,5,8-trimethyl-	568b, 4249		
419.		Naphthalene, 1,2,3,4-tetrahydro-4,5,8-trimethyl- (isomer)	568b, 4249		
420.	72843-02-8	Naphthalene, 1,2,3,4-tetrahydrotrimethyl-	4249		
421.	475-03-6	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl- {α-ionene}	1110, 2767, 3308, 3219, 3557, 3647, 3797, 4249, 5811b	2339a, 2917a	
422.	21693-51-6	Naphthalene, 1,2,3,4-tetrahydro-1,5,8-trimethyl-		2917a	
423.	30316-36-0	Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-		2917a	
424.	28652-74-6	Naphthalene, tetramethyl- {at least four isomers in MSS}	104, 1375, 1375b, 2479, 2570, 2731, 2735, 2767, 2769, 3618, 3732, 3757–3759, 4249, 5811b	84, 2784, 4249	
425.	28652-77-9	Naphthalene, trimethyl- {at least 10 isomers in MSS}	104, 1135, 1360, 1375, 1375a, 1375b, 1650, 1652, 2438, 2543, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2769, 2773, 2777, 3492, 3509, 3618–3620, 3732, 3757–3759, 4249, 5811b	84, 2339a, 3547, 4249, 5811b	1360, 1375a
426.	2717-42-2	Naphthalene, 1,2,4-trimethyl-	1135, 1375, 1375b, 2479, 2769, 2784, 3557, 4249	2784	
427.	3031-05-8	Naphthalene, 1,2,6-trimethyl-	1135, 2479, 2784, 4249	2784	
428.	486-34-0	Naphthalene, 1,2,7-trimethyl-	1135, 2784	2784, 4249	
429.	2131-39-7	Naphthalene, 1,3,5-trimethyl-	1135, 2479, 2784	2784, 4249	
430.	3031-08-1	Naphthalene, 1,3,6-trimethyl-	798, 1135, 1139, 1375, 1375b, 1972, 2722, 2784, 3262, 3302, 3308, 3557, 3797, 4249, 5077, 5811b	2784	
431.	2131-41-1	Naphthalene, 1,4,5-trimethyl-	2767, 2769, 3557, 4249		
432.	2131-42-2	Naphthalene, 1,4,6-trimethyl-	1135, 2784	2784, 3547, 4249	
433.	2245-38-7	Naphthalene, 1,6,7-trimethyl- {= naphthalene, 2,3,5-trimethyl-}	1135, 1378, 4249, 5811b	2784	1378
434.	829-26-5	Naphthalene, 2,3,6-trimethyl-	1135, 2479, 2784, 3402a, 3741, 4249, 5811b	2784	
435.	192-65-4	Naphtho[1,2,3,4-*def*]chrysene {dibenzo[*a,e*]pyrene} 	142, 151, 290, 291, 1741, 1743, 1744, 1870, 1871, 1873, 2037a, 2825, 3257, 3262, 3265, 3300, 3308, 3714, 3756, 3787, 3788, 4249, 5512, 5869a		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
436.	190-99-8	1*H*-Naphtho[3,2,1,8-*defg*]chrysene {1,2,5,6-dibenzopyrene} 	3262, 4249, 4296, 5077		
437.	196-42-9	Naphtho[2,1,8-*qra*]naphthacene 	1139, 1971, 2079, 2939, 3251, 3262, 3273, 3286, 3302, 3787, 4249, 4296, 4354, 4355, 5077, 5811b		
438.	215-26-9	Naphtho[1,2-*b*]triphenylene {tribenz[*a,c,h*]anthracene} 	432, 1139, 1971, 2037a, 2430, 2939, 3262, 3302, 3308, 3797, 4249, 5077, 5732, 5811b		
439.	190-26-1	Ovalene 	3337–3339, 4249		
440.	135-48-8	Pentacene {benzo[*b*]naphthacene} 	2114, 2194–2196, 3003, 3308, 4249		
441.	222-93-5	Pentaphene {dibenzo[*b,j*]phenanthrene; 2,3,6,7-dibenzophenanethrene} 	1139, 2037a, 2079, 2939, 3003, 3262, 3302, 4249, 4296, 4354, 5077, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

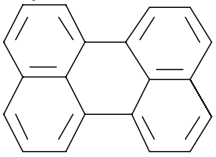
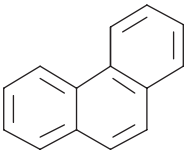
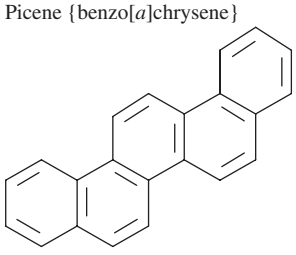
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
442.	198-55-0	Perylene 	50, 104, 126, 126a, 126b, 141–144, 147, 151, 172, 432, 726, 797, 966, 869, 1136, 1139, 1287, 1288, 1375a, 1377, 1397, 1405, 1406, 1408, 1409, 1462, 1781, 1787, 1788, 1800, 1870, 1871, 1873, 1873, 2037a, 2099, 2116, 2134, 2194, 2195, 2238, 2313a, 2327, 2428, 2430, 2438, 2596a, 2799a, 2939, 2961, 2962, 2964, 3003, 3176, 3191, 3242, 3249, 3251, 3255, 3257, 3262, 3273, 3292, 3302, 3308, 3616, 3618–3620, 3756, 3758, 3759, 3787, 3788, 3876, 3952, 4031, 4110, 4248, 4282, 4284, 4300, 4307, 4308, 4315, 4354, 4355, 5010, 5077, 5732, 5811b	903, 4249, 5811b	50, 1375a, 1377
443.		Perylene, alkyl-	4284		
444.	64760-19-6	Perylene, dimethyl-	3756, 4249, 5811b		
445.	64031-91-0	Perylene, methyl- {at least two isomers in MSS}	3615, 3756, 4249, 5811b		
446.	24471-47-4	Perylene, 3-methyl-	820, 2939, 4249		
447.	85-01-8	Phenanthrene 	39, 50, 84, 104, 126a, 128, 141–143, 151, 147, 172, 239, 291, 329, 394, 397, 443, 584, 603, 646a, 710, 726, 746a, 798, 819, 820, 869, 966, 1099, 1136, 1139, 1172, 1287, 1288, 1329, 1330, 1360, 1375, 1375a, 1375b, 1377, 1388–1390, 1406, 1408, 1409, 1427, 1435a, 1437, 1445, 1462, 1471, 1485, 1644, 1645, 1647–1649, 1767, 1842, 1981, 2013, 2037a, 2079, 2099, 2113, 2130, 2134, 2142, 2170, 2191, 2195, 2200, 2210, 2215, 2238, 2256, 2270, 2313a, 2365, 2438, 2537, 2543, 2557, 2596a, 2570, 2710, 2722, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2799a, 2822, 2858, 2894, 2939, 2961–2964, 3003, 3024, 3030, 3032, 3033, 3047, 3049, 3081, 3082, 3149, 3176, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3265, 3273, 3292, 3300, 3302, 3307, 3308, 3323–3325, 3370, 3410, 3421–3424, 3437, 3441a, 3452, 3465–3470, 3472, 3514, 3557, 3616, 3618–3620, 3685, 3729, 3741, 3758, 3759, 3787, 3797, 3876, 4248, 4249, 4282, 4284, 4300, 4311, 4342, 4355, 4400, 5010, 5027, 5077, 5079, 5359, 5510, 5539, 5811b	84, 172, 1660, 2339a, 2917a, 3059, 3194, 3205, 4249, 5567, 5811b	50, 1330, 1360, 1375a, 1375a, 1377, 2210
448.		Phenanthrene, alkyl-	142, 646a, 1172, 2195, 3308, 3465–3467, 3469, 4284		
449.		Phenanthrene, dihydro-	1375, 2195, 3219, 3308, 4249		
450.	776-35-2	Phenanthrene, 9,10-dihydro-	1375, 1375b, 3308		
451.	71607-56-2	Phenanthrene, dihydrobis(methylene)-	4249		
452.	29062-98-4	Phenanthrene, dimethyl-	394, 646a, 2134, 2438, 2570, 3251, 3262, 3273, 3286, 3292, 3437, 3514, 3618–3620, 3756, 3758, 3759, 4249, 5077, 5811b		
453.	20291-72-9	Phenanthrene, 1,2-dimethyl-	244, 1378, 2037a, 4249		1378
454.	22349-59-3	Phenanthrene, 1,4-dimethyl-	1870, 1871		
455.	20291-74-1	Phenanthrene, 1,6-dimethyl-	244, 2037a, 4249		

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
456.	483-87-4	Phenanthrene, 1,7-dimethyl-	244, 2037a, 4249		
457.	7372-87-4	Phenanthrene, 1,8-dimethyl-	5811b, 1E02		
458.	3674-66-6	Phenanthrene, 2,5-dimethyl-	39, 1971, 2939, 3262, 3302, 3308, 3797, 4249, 5077		
459.	17980-16-4	Phenanthrene, 2,6-dimethyl-	244		
460.	1576-69-8	Phenanthrene, 2,7-dimethyl-	244, 4249, 5811b		
461.	1576-67-6	Phenanthrene, 3,6-dimethyl-	49, 50, 3514, 4249, 5811b		50
462.	3674-69-9	Phenanthrene, 4,5-dimethyl-	2191, 3302, 4249		
463.	110053-52-6	Phenanthrene, dimethylene-	3756, 3758, 3759		
464.	71607-65-3	Phenanthrene, dimethylethyl-	3757, 4249, 5811b		
465.	30997-38-7	Phenanthrene, ethyl-	4249, 4249, 5811b		
466.	71607-66-4	Phenanthrene, ethylmethyl-	3757, 4249, 5811b		
467.	71607-67-5	Phenanthrene, hexamethyl-	3757, 4249, 5811b		
468.	31711-53-2	Phenanthrene, methyl-	104, 143, 1378, 1644, 1645, 1647–1649, 2134, 2195, 2438, 2543, 2570, 2773, 2777, 2799a, 3262, 3308, 3410, 3437, 3470, 3473, 3514, 3557, 3741, 4248, 4249, 5077, 5811b	1127a, 3547, 4249	1378
469.	832-69-9	Phenanthrene, 1-methyl-	50, 819, 1471, 1652, 1870, 1871, 1873, 2767, 3410, 3514, 3557, 3616, 3618–3620, 3732, 3757–3759, 3797, 4249, 5811b		50
470.	2531-84-2	Phenanthrene, 2-methyl-	50, 1471, 1652, 2210, 2767, 3557, 3616, 3618, 3732, 3757–3759, 4249, 5811b		50, 2210
471.	832-71-3	Phenanthrene, 3-methyl-	49, 50, 1471, 1652, 2767, 3514, 3616, 3618, 3732, 3757–3759, 4249, 5811b		50
472.	832-64-4	Phenanthrene, 4-methyl-	244, 3616, 3618–3620, 3758, 3759, 4249, 5811b		
473.	883-20-5	Phenanthrene, 9-methyl-	39, 392, 394, 1471, 1652, 2710, 2939, 3251, 3262, 3273, 3286, 3292, 3302, 3616, 3618–3620, 3732, 3757–3759, 3797, 4249, 5077, 5811b		
474.		Phenanthrene, 1-methyl-5-(1-methylethyl)-		4249, 4723	
475.	71607-68-6	Phenanthrene, pentamethyl-	1652, 2328, 3732, 3757, 4249, 5811b		
476.	71607-69-7	Phenanthrene, propyl-	2328, 4249		
477.	71607-70-0	Phenanthrene, tetramethyl- {at least five isomers in MSS}	1652, 3225, 3300, 3732, 3757, 4249, 5811b		
478.	30232-26-9	Phenanthrene, trimethyl- {at least three isomers in MSS}	642, 1652, 2570, 3615, 3618–3620, 3732, 3757–3759, 4249, 5811b		
479.	213-46-7	Picene {benzo[*a*]chrysene} 	142, 143, 726, 2037a, 2195, 2200, 3003, 3219, 3307, 3308, 3756, 3787, 3788, 4249, 5811b		
480.	30283-95-5	Picene, methyl-	3327a, 5811b		

(*continued*)

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

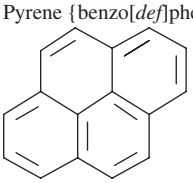
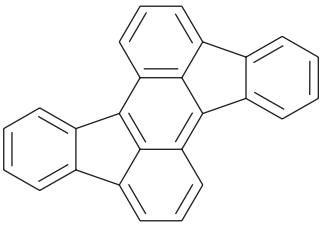
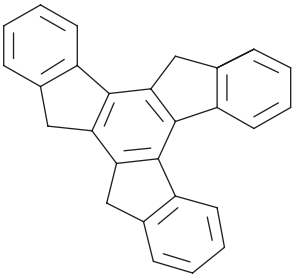
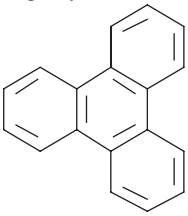
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
481.	129-00-0	Pyrene {benzo[*def*]phenanthrene} 	39, 49, 50, 104, 126a, 126b, 128, 141–143, 151, 154, 172, 239, 245, 290, 291, 329, 394, 397–399, 583, 584, 588, 589, 603, 646a, 710, 726, 746a, 785, 804, 818–820, 878, 885, 966, 869, 1019, 1099, 1100, 1136, 1139, 1172, 1211, 1287–1289, 1373, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408, 1409, 1437, 1445, 1462, 1471, 1475, 1644, 1645, 1647–1649, 1781, 1787, 1788, 1800, 1842, 1870, 1871, 1873, 2013, 2037a, 2099, 2113, 2116, 2130, 2134, 2142, 2195, 2203, 2238, 2255, 2256, 2270, 2313a, 2352, 2353, 2365–2367, 2425, 2426, 2428, 2430, 2438, 2473, 2479, 2501, 2557, 2596a, 2648–2650, 2709, 2710, 2713–2715, 2717, 2799a, 2865, 2893, 2894, 2939, 2960–2962, 2964, 3003, 3024, 3030, 3032, 3033, 3046, 3047, 3049, 3149, 3176, 3191, 3240–3243, 3246, 3249, 3251, 3255, 3257, 3262, 3265, 3269, 3273, 3286, 3291, 3292, 3300, 3302, 3307, 3308, 3370, 3415, 3421–3424, 3437, 3452, 3465–3467, 3469, 3470, 3472, 3514, 3610, 3616, 3618–3620, 3685, 3686, 3756, 3758, 3759, 3787, 3788, 3797, 3820, 3863, 3876, 3952, 3999–4001, 4005–4007, 4009–4011, 4018, 4019, 4020, 4031, 4110, 4248, 4249, 4282, 4284, 4300, 4307, 4308, 4311, 4315, 4319, 4354, 4355, 4399, 4404, 5010, 5027, 5077, 5079, 5486, 5539, 5811b	172, 903, 2079, 2939, 3059, 3194, 3205, 3973, 4249, 5567, 5811b	50, 1375a, 1377, 1378
482.		Pyrene, alkyl-	966, 1172, 1560, 1787, 1788, 2428, 2893, 2894, 2939, 3262, 3308, 3756, 3758, 3759, 3876, 4284, 4300, 4307, 4308, 4315, 4319, 5077		
483.	35980-18-8	Pyrene, 1-butyl-	3339, 4249		
484.	55682-90-1	Pyrene, 1-decyl-	3339, 4249		
485.	28779-32-0	Pyrene, dihydro-	2195, 2203, 2207, 2479, 3308, 4249		
486.	14927-67-4	Pyrene, 1,2-dihydro-	5811		
487.	30582-03-7	Pyrene, dimethyl- {at least three isomers in MSS}	1471, 1800, 1652, 2479, 3437, 3616, 3618–3620, 3756–3759, 5811b		
488.	64401-21-4	Pyrene, 1,3-dimethyl-	1800, 4249		642
489.		Pyrene, ethyl-	1172, 2939, 3262, 3302, 3339, 4249, 5077		
490.	56142-12-2	Pyrene, 1-ethyl-	2939, 3302, 3339		
491.	71607-74-4	Pyrene, ethylmethyl-	2328, 4249		
492.	71607-75-5	Pyrene, hexamethyl-	1652, 2479, 3732, 3757, 4249, 5811b		
493.	72692-89-8	Pyrene, 1-hexyl-	3339, 4249		
494.	27577-90-8	Pyrene, methyl- {several isomers in MSS}	39, 104, 143, 966, 1648, 1649, 2479, 2799a, 3046, 3251, 3262, 3273, 3286, 3308, 3470, 3472, 3876, 4005–4007, 4009–4011, 4018, 4019, 4020, 4031, 4248, 4249, 5077, 5811b		
495.	2381-21-7	Pyrene, 1-methyl-	394, 726, 820, 1139, 1287, 1288, 1378, 1462, 1471, 1781, 1800, 2037a, 2438, 2479, 2709, 2710, 2939, 3191, 3240, 3241, 3251, 3262, 3273, 3286, 3292, 3302, 3308, 3437, 3616, 3618–3620, 3756, 3758, 3759, 3787, 3788, 3797, 4037, 4249, 5077, 5811b	5811b	1378

TABLE 1.20 (continued)
PAHs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
496.	3442-78-2	Pyrene, 2-methyl-	1139, 1471, 1781, 1800, 2037a, 2479, 2939, 3251, 3262, 3273, 3286, 3292, 3302, 3308, 3437, 3616, 3618–3620, 3756, 3758, 3759, 3787, 3788, 3797, 4019, 4031, 4249, 4355, 4356, 5077, 5811b		
497.	3353-12-6	Pyrene, 4-methyl-	394, 966, 1139, 1289, 1378, 1462, 1471, 1475, 1781, 1788, 1800, 2037a, 2079, 2479, 2557, 2709, 2710, 2939, 2961, 3251, 3262, 3273, 3286, 3292, 3302, 3308, 3437, 3616, 3618–3620, 3756, 3758, 3759, 3797, 4018, 4019, 4031, 4249, 5077, 5811b		1378
498.	71608-00-9	Pyrene, 1-octyl-	3339, 4249		
499.	71607-76-6	Pyrene, pentamethyl- {at least three isomers in MSS}	1652, 2479, 3732, 3757, 4249, 5811b		
500.	56142-09-7	Pyrene, propyl-	2328, 4249		
501.	71630-71-2	Pyrene, 1-tetradecyl-	3339, 4249		
502.	66161-17-9	Pyrene, tetrahydro-	2195, 2203, 2205, 3308, 4249		
503.	57633-59-7	Pyrene, 1,2,6,7-tetrahydro-	5811		
504.	60826-75-7	Pyrene, tetramethyl- {at least four isomers in MSS}	1652, 2479, 3618–3620, 3756–3759, 4249, 5811b		
505.	41637-88-1	Pyrene, trimethyl- {at least three isomers in MSS}	1652, 2328, 2479, 3618–3620, 3756–3759, 4249, 5811b		
506.	197-61-5	Rubicene 	1900, 3262, 3337, 3339, 4249, 5077		
507.	27096-03-3 548-35-6	5*H*-Tribenzo[*a,f,l*]trindene, 10,15-dihydro- {5*H*-diindeno[1,2-*a*:1′,2′-*c*]fluorene; {truxene} 	3262, 3337–3339, 4249		
508.	217-59-4	Triphenylene {9,10-benzophenanthrene} 	104, 143, 151, 726, 1405, 1406, 1408, 1409, 1870, 1871, 1873, 1900, 2037a, 2113, 2557, 2799a, 3003, 3262, 3616, 3618–3620, 3756, 3758, 3759, 3787, 3788, 4249, 4315, 5077, 5811b		
509.	60826-76-8	Triphenylene, dimethyl-	3618–3620, 3756–3759, 4249, 5811b		
510.	41637-89-2	Triphenylene, methyl-	3618–3620, 3756, 3758, 3759, 4249		
511.	60826-79-1	Triphenylene, trimethyl-	3618–3620, 3758, 3759, 4249, 5811b		

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

in cigarette smoke are the major causes of lung cancer in cigarette smokers [Hecht (1557), Hecht and Hoffmann (1571a), Hoffmann and Hecht (1727), the World Health Organization (4279a)] despite the following:

1. Neither B[*a*]P nor any other PAH in CSC either individually or in combination with the other PAHs in CSC can explain more than a few percent of the biological response observed in skin painting with CSC [Druckrey (1056), Roe (3310, 3311), Wright and Wynder (4283), Wynder (4296), Wynder and Hoffmann (4307, 4312, 4343, 4343a, 4354)].
2. Neither B[*a*]P nor any other PAH in CSC either individually or in combination with the other PAHs and assorted promoters (phenols) in CSC can explain more than a few percent of the biological response observed in skin painting with CSC (4332).
3. In general, the *N*-nitrosamines in CSC are not tumorigenic to mouse skin but are organ-specific tumorigens [Preussmann and Stewart (2991)*], a point stressed in numerous reviews issued between the mid-1960s and the late 1990s on *N*-nitrosamines [Rodgman (3256)] and recognized by Hoffmann and Hecht [see p. 75 in (1727)].
4. NNK has never been shown to induce lung cancer in a laboratory animal by inhalation (1727).

While the minor contribution of B[*a*]P to the tumorigenicity of CSC to mouse skin has been recognized since the mid-1950s (4353, 4354), its presence in CSC has elicited continued interest since that time. Examination of the references to various smoke components reveals an interesting fact about B[*a*]P: When all the cigarette smoke components are tabulated with regard to similar selection of references across the board, very few tobacco smoke components exceed B[*a*]P in the number of pertinent references available. Obviously, the smoke component discussed most in publications and presentations between the mid-1950s and 2005 was nicotine. Next was acetaldehyde, followed by B[*a*]P.

Another interesting fact about B[*a*]P is that, despite its minimal contribution to mouse-skin tumorigenicity from CSC, almost every year since the mid-1950s there has been at least one publication on a new and/or improved method to quantitate the yield of B[*a*]P in MSS [see Table 1.21, a modified version of Table 6 in (3306b)].

In 2004, CORESTA published its recommended method for the determination of B[*a*]P in tobacco smoke (825a). Much emphasis has been placed on the determination of B[*a*]P in the MSS from fewer and fewer cigarettes. Before the advent of all the newly introduced and subsequently improved spectral and chromatographic systems, estimations of individual PAHs required the CSC from many cigarettes. For example, in their studies on the effect of various treatments of tobacco on the PAHs in MSS, Rodgman and Cook (3241, 3246, 3269, 3274, 3275) chemically analyzed the MSS from 3600 cigarettes for each control and treated sample. For the MSS PAH analyses in the 50 treated and control samples described in (3246), more than 183,000 cigarettes were smoked, the condensate collected, and processed. Nowadays, only a few cigarettes are needed for similar analyses. To permit comparison of the chemical data with the biological findings of Rodgman–Cook studies in the 1950s, i.e., the cigarettes on a manifold were machine smoked (35 mL puff volume, 2 s puff duration, 3 puffs/min) with a collection system that duplicated the one described by Wynder et al. (4306a). This smoking regime differed from the usual 35 mL puff volume, 2 s puff duration, and 1 puff/min described by Bradford et al. (423b) in 1936 and used by most investigators in smoke studies after that date.

Table 1.22 summarizes the PAHs identified in CSC that were included in earlier descriptions of proposed structure–tumorigenicity theories.

Examination of Table 1.22 indicates that most of the PAHs considered in the various theoretical systems designed to establish a relationship between molecular structure and tumorigenicity are totally benzenoid. Only a few PAHs with a combined benzenoid–cyclopentanoid structure were included in the early studies. Lacassagne et al. (2247a) in their discourse on structure–tumorigenicity relationship mentioned a few benzenoid PAHs, but their major emphasis was on the structure–tumorigenicity relationship of numerous angular benzacridines. While the number of aza-arenes, including the benzacridines, in CSC is less than the number of PAHs, nearly 200 have been identified, many by the USDA group at Athens, GA (3750). With the knowledge that CSC contains nontumorigenic PAHs that have been shown to substantially reduce the tumorigenicity of several potently tumorigenic PAHs, consideration of the study of Lacassagne et al. raises several interesting questions with regard to tobacco smoke composition. (1) Do any of the benzacridines or other aza-arenes in CSC partially or totally inhibit the tumorigenicity of the tumorigenic benzacridines or other aza-arenes? (2) Do any of the benzacridines inhibit the tumorigenicity of tumorigenic PAHs? (3) Do any of the PAHs reduce the tumorigenicity of the tumorigenic aza-arenes?

The mixture known as CSC is so complex that it is not possible to ascribe its biological activity to any individual component because of the known behavior of that component when administered individually.

The following situation pertinent to PAHs is an interesting one: The numerous studies conducted between the early 1930s and the mid-1950s on the tumorigenic PAHs in various air pollutants and the multitude of new and improved procedures reported periodically to define the levels of PAHs, particularly B[*a*]P, in the air pollutants parallel similar studies conducted after the mid-1950s on the tumorigenic PAHs in cigarette smoke and the multitude of new and/or improved analytically procedures reported periodically to define the levels of PAHs, particularly B[*a*]P, in cigarette smoke.

* Subsequent to the publication of the Preussmann and Stewart review (2991), Deutsch-Wenzel et al. (956a) reported that in a skin-painting study with *N′*-nitrosonornicotine (NNN), tumors were initiated at the site of application. The specific tumorigenic potency of NNN was estimated to be only 0.8% of that of B[*a*]P. However, no dose–response relationship was observed with NNN over a treatment range of 12.5–200 µg.

TABLE 1.21
Chronology of Analytical Methodology Used in the Determination of Benzo[*a*]pyrene in Cigarette Mainstream Smoke

Date	Title of Presentation or Publication	Methodology Described	Reference
1956/1958	Analysis of cigarette smoke condensate	Partitioning, complex formation (PA, TNF), LCC, UV, multiple crystallizations, derivatization, m.p., m.m.p.	3240, 3273
1957	Paper chromatography of carcinogenic hydrocarbons	PC	2960
1959	The role of higher polycyclic hydrocarbons in tobacco carcinogenesis	PC, sublimation, m.p., m.m.p.	4307
	Use of the fine structure of the fluorescence spectrum of 3:4-benzpyrene to increase the certainty of its detection	Fluorescence spectrophotometry	977
	Fluorescence spectral analysis of the products of tobacco smoke		978
1960	Characterization and level of 3,4-benzpyrene by luminescence spectrophotometry at −190°C	Spectrophotometry	2650
1961	A method for the estimation of 3,4-benzpyrene in tobacco smoke condensate	Partitioning, PC, LCC, UV	1396
1962	A new method for the determination of 3,4-benzpyrene in tobacco smoke condensate	Partitioning, LCC, PC, UV fluorescence	183
1963	A rapid analytical technique for routine determination of benzo[*a*]pyrene in cigarette smoke condensate	LCC, UV	3889
	A new method for the determination of 3,4-benzpyrene in tobacco smoke condensate	PC	3440
1964	Demonstration of carcinogenic hydrocarbons, with special reference to paper chromatography	PC	2964
	Improved method for the determination of benzo[*a*]pyrene in cigarette smoke condensate	TLC	3503
	Contribution to the determination of 3,4-benzpyrene in tobacco smoke condensate	LCC, PC	2918
1965	Determination of benzo[*a*]pyrene and related compounds in cigarette smoke	PC, TLC, GC, ^{14}C-B[*a*]P	128
	Improved methods for determination of benzo[*a*]pyrene in cigarette smoke	LCC, GC, TLC, fluorescence	3191
	Thin-layer chromatographic separation of benzo[*a*]pyrene from cigarette tar	TLC	2856
	Contribution to the determination of benzo[*a*]pyrene in tobacco smoke condensate	LCC, TLC, UV absorption and fluorescence	2881
1966	The fluorometric determination of benzo[*a*]pyrene in cigarette smoke condensate	Fluorometry	913
	The fluorometric determination of 3,4-benzpyrene in low-temperature carbonization and smoke condensates	Fluorometry	2199
1968/1970	Gas chromatography of polynuclear aromatic hydrocarbons	GC	2473, 2474
1971	Rapid thin-layer method for fluorometric determination of benzo[*a*]pyrene in cigarette smoke	LCC, TLC, fluorometry	3789
1971/1972	Determination of benzo[*a*]pyrene in smoke condensate by ultraviolet spectroscopy	UV	1593
	Modification of routine thin-layer method for determining benzo[*a*]pyrene in smoke	TLC	1594
1972	A rapid method for the determination of polycyclic hydrocarbons in cigarette smoke	LCC, PC or TLC, fluorescence	2819
1973	Separation analysis of polycyclic aromatic hydrocarbons by high pressure liquid chromatography; elective separation system for the quantitative estimation of isomeric benzpyrenes and coronene	HPLC	2115, 2116
1976	A rapid method for the determination of benzo[*a*]pyrene…in cigarette smoke; Quantitative determination of benzo[*a*]pyrene in cigarette smoke condensates by high pressure liquid chromatography	HPLC	2121 2119
	Analysis of benzo[*a*]pyrene in cigarette smoke	HPLC	3638, 3644
	Gas chromatographic quantitation of polynuclear aromatic hydrocarbons in tobacco smoke	GC	3612

(*continued*)

TABLE 1.21 (continued)
Chronology of Analytical Methodology Used in the Determination of Benzo[*a*]pyrene in Cigarette Mainstream Smoke

Date	Title of Presentation or Publication	Methodology Described	Reference
1976/1978	Polynuclear aromatic hydrocarbons in cigarette smoke condensate… …multialkylated polynuclear aromatic hydrocarbons in cigarette smoke condensate…	GelC, GC, HPLC, GC/MS	3756, 3758, 3757
1977	Analysis of polycyclic aromatic hydrocarbons (PAH) in the condensates of natural and synthetic smoking materials	GelC, TLC, ^{14}C-labeled B[*a*]P (and DB[*a,h*]A)	2465
1981	Analysis of benzo[*a*]pyrene in cigarette smoke by high-performance liquid chromatography	HPLC	3638
1986	Determination of benzo[*a*]pyrene… in the total particulate matter of cigarette smoke by high-performance liquid chromatography	HPLC	3158
1988/1990	The determination of benzo[*a*]pyrene in the total particulate matter of cigarette smoke	HPLC	3158, 3176
1989	An alternative isolation procedure for the subsequent determination of benzo[*a*]pyrene in total particulate matter of cigarette smoke	HPLC	1076
1998	The measurement of benzo[*a*]pyrene in mainstream cigarette smoke	HPLC, Sep-Pak® cartridge	1246
1999	Determination of benzo[*a*]pyrene in complex matrix by multidimensional high-performance liquid chromatography	HPLC	934
1999	Quantitation of benzo[*a*]pyrene from mainstream smoke by liquid chromatography tandem mass spectrometry	LCC/MSS	2614
2002	Determination of benzo[*a*]pyrene in cigarette smoke total particulate matter by two-dimensional chromatography	2-DimC	4410
2004	CORESTA issued its description of a GC/MS method for the quantitative determination of B[*a*]P in CSC	GC/MS	825a
2005	Microwave-assisted extraction: An efficient method for the determination of polycyclic hydrocarbons in particulate phase mainstream cigarette smoke		746a
	Precursors to the pyrosynthesis of PAHs in cigarette smoke. I. Experimental design, matrix preparation and analytical methods	GC/MS	1435a, 2931a
2006	Distribution of polycyclic aromatic hydrocarbons between the particulate and vapor phase of mainstream cigarette smoke	LC/FLD	3340a
2007	Development and validation of an improved GC/MS method for the determination of polycyclic aromatic hydrocarbons (PAHs) in mainstream tobacco smoke	GC/MS	4966
2008	Determination of PAHs in exhaled cigarette smoke		5010
2009	Analysis of cigarette smoke condensate	Partitioning, complex formation (PA, TNF), LCC, UV, multiple crystallizations, derivatization, m.p., m.m.p.	5077
	Routine analysis of B[*a*]P in cigarette MSS	Modified MDGC/MS	5080
2010	Determination of PAHs in smokeless tobacco	GC/MS	5533, 5567

TNF, 2,4,7-trinitrofluorenone; PA, picric acid; LCC, liquid column chromatography; PC, paper chromatography; TLC, thin-layer chromatography; GC, gas chromatography; HPLC, high pressure liquid chromatography; GelC, gel chromatography; 2-DimC, 2D chromatography; FLD, fluorescence determination; m.p., melting point; m.m.p., mixture melting point; MS, mass spectrometry.

After many decades of failure by numerous investigators who attempted to induce tumors in laboratory animals by treatment with various air pollutants, industrial tars, and pyrolysates, Yamagiwa and Ichikawa described in 1915–1918 the procedure whereby tumors could be successfully induced in laboratory animals by skin painting with a coal-tar solution (4361).

The 1915–1918 reports of the Yamagiwa–Ichikawa success triggered a significant number of studies on the tumorigenicity of a variety of tars produced by the pyrolysis of individual components, e.g., in the mid-1920s, Kennaway and his colleagues studied the tumorigenicity of the pyrolysates of isoprene, acetylene, cholesterol, and other compounds (2073–2080). In 1930, Kennaway and Hieger (2076, 2078) reported the induction of tumors in mice skin painted with solutions of the pentacyclic PAH DB[*a*,*h*]A, subsequently classified as an extremely potent tumorigen.

Shortly thereafter in the early 1930s, the colleagues of Kennaway—Cook, Hewett, and Hieger—isolated from 2 ton of coal tar a series of PAHs, one of which by synthesis was demonstrated to be what is now named benzo[*a*]pyrene (B[*a*]P) (796a, 797, 1631). It was demonstrated not only that

TABLE 1.22
Tobacco Smoke PAHs Discussed in Various Publications on the Relationship between PAH Structure and Tumorigenicity

PAH Discussed	Coulson (829)	Fieser et al. (1180a)	Herndon (1623a, 2435a)	Lacassagne et al. (2247a)	Martin et al. (2479)	Pullman and Pullman (3003)	Rubin (3365)	Trosko-Upham (3966a)	Zhang et al. (4410c)	Zhang (4410d)
Acenaphthylene	—	—	X	—	—	—	—	—	—	X
Acenaphthylene, 1,2-dihydro-	—	—	—	—	—	—	—	—	—	X
Anthracene	X	X	X	—	—	X	—	X	X	X
Anthracene, dimethyl-[a]	—	—	—	—	—	—	—	X [1]	—	X [5]
Anthracene, 9,10-dimethyl-	—	—	—	—	—	—	—	—	X	X
Anthracene, 1-methyl-	—	—	—	—	—	—	—	X	—	—
Anthracene, 2-methyl-	—	—	—	—	—	—	—	X	—	—
Anthracene, 9-methyl-	—	—	—	—	—	—	—	—	—	X
Anthracene, trimethyl-	—	—	—	—	—	—	—	—	—	X [1]
Azulene	—	—	X	—	—	X	—	—	—	—
Benz[*a*]aceanthrylene	—	—	X	—	—	—	—	—	—	X
Benz[*j*]aceanthrylene, 1,2-dihydro-	—	—	—	—	—	—	—	—	X	X
Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl-	—	—	—	X	—	X	X		X	X
Benz[*e*]acephenanthrylene	—	—	X	—	—	—	—	—	X	X
Benz[*e*]acephenanthrylene, methyl-	—	—	—	—	—	—	—	—	—	X [6]
Benz[*a*]anthracene	X	X	—	X	—	X	—	—	—	X
Benz[*a*]anthracene, dimethyl-[a]	X [8][b]	—	—	—	—	—	—	—	X [6]	X [23]
Benz[*a*]anthracene, 7,12-dimethyl-	X	—	—	X	—	X	X	X	X	X
Benz[*a*]anthracene, ethyl-	—	—	—	—	—	—	—	—	X [1]	—
Benz[*a*]anthracene, 1-methyl-	X	—	—	—	—	—	—	—	—	X
Benz[*a*]anthracene, 2-methyl-	X	—	—	—	—	—	—	—	—	X
Benz[*a*]anthracene, 3-methyl-	X	—	—	—	—	—	—	—	—	X
Benz[*a*]anthracene, 4-methyl-	X	—	—	—	—	—	—	—	—	X
Benz[*a*]anthracene, 5-methyl-	X	—	—	—	—	—	—	—	X	X
Benz[*a*]anthracene, 6-methyl-	X	—	—	—	—	—	—	—	X	—
Benz[*a*]anthracene, 8-methyl-	X	—	—	—	—	—	—	—	X	X
Benz[*a*]anthracene, 9-methyl-	X	—	—	X	—	—	—	—	X	X
Benz[*a*]anthracene, 10-methyl-	X	—	—	—	—	—	—	—	X	X
Benz[*a*]anthracene, 12-methyl-	X	—	—	—	—	—	—	—	X	X
Benz[*a*]anthracene, propyl-	—	—	—	—	—	—	—	—	X [1]	—
Benz[*a*]anthracene, tetramethyl-	X [1]	—	—	—	—	—	—	—	X [2]	—
Benz[*a*]anthracene, trimethyl-	X [3]	—	—	—	—	—	—	—	X [3]	X [13]
Benzo[*b*]chrysene	—	—	X	—	—	X	—	—	—	X
1*H*-Benzo[*a*]cyclopent[*h*]anthracene, 2,3-dihydro-	X	—	—	—	—	—	—	—	—	—
9*H*-Benzo[*a*]cyclopent[*i*]anthracene,10,11-dihydro-	X	—	—	—	—	—	—	—	—	X
Benzo[*ghi*]fluoranthene	—	—	—	—	—	—	—	—	—	X

(*continued*)

TABLE 1.22 (continued)
Tobacco Smoke PAHs Discussed in Various Publications on the Relationship between PAH Structure and Tumorigenicity

PAH Discussed	Coulson (829)	Fieser et al. (1180a)	Herndon (1623a, 2435a)	Lacassagne et al. (2247a)	Martin et al. (2479)	Pullman and Pullman (3003)	Rubin (3365)	Trosko-Upham (3966a)	Zhang et al. (4410c)	Zhang (4410d)
Benzo[*ghi*]fluoranthene, 2-methyl-	—	—	—	—	—	—	—	—	—	X
Benzo[*ghi*]fluoranthene, 3-methyl-	—	—	—	—	—	—	—	—	—	X
Benzo[*j*]fluoranthene	—	—	—	—	—	—	—	—	X	X
Benzo[*k*]fluoranthene	—	—	X	—	—	—	—	—	—	X
Benzo[*k*]fluoranthene, methyl-	—	—	—	—	—	—	—	—	—	X [3]
7*H*-Benzo[*c*]fluorine	—	—	—	—	—	—	—	—	—	X
Benzo[*a*]naphthacene	—	—	X	—	—	X	—	—	—	X
Benzo[*rst*]pentaphene	—	—	X	—	—	—	X	—	X	X
Benzoperylene	—	—	—	—	—	—	—	—	—	—
Benzo[*ghi*]perylene	—	—	X	—	—	—	—	—	X	X
Benzo[*c*]phenanthrene	X	—	X	—	—	X	—	—	X	X
Benzo[*c*]phenanthrene, methyl-	X [4]	—	—	—	—	—	—	—	X [6]	X [6]
Benzopyrene[c]	—	—	—	—	—	—	—	—	X	—
Benzo[*a*]pyrene	—	—	X	—	X	X	X	X	X	X
Benzo[*a*]pyrene, 7,8-dihydro-	—	—	—	—	X	—	—	—	—	—
Benzo[*a*]pyrene, dimethyl-[a]	—	—	—	—	X	—	—	—	—	X [9]
Benzo[*a*]pyrene, methyl-[d]	—	—	—	—	X	—	—	—	—	X [1]
3*H*-Benzo[*cd*]pyrene, 4,5-dihydro-	—	—	—	—	X	—	—	—	—	—
Benzo[*e*]pyrene	—	—	X	—	X	X	X	X	X	X
Benzo[*e*]pyrene, dimethyl-	—	—	—	—	X	—	—	—	—	—
Benzo[*e*]pyrene, methyl-	—	—	—	—	X	—	—	—	—	X [12]
Benzo[*e*]pyrene, trimethyl-	—	—	—	—	X	—	—	—	—	—
Benzo[*b*]triphenylene	—	—	X	—	—	X	X	—	X	X
1,1′-Binaphthalene	—	—	—	—	X	—	—	—	—	—
1,1′-Binaphthalene, methyl-	—	—	—	—	X	—	—	—	—	—
Chrysene	X	—	X	X	—	X	—	X	X	X
Chrysene, dimethyl-[a]	—	—	—	—	—	X [1]	—	—	X [1]	X [10]
Chrysene, 1-methyl-	—	—	—	—	—	—	—	—	—	X
Chrysene, 2-methyl-	—	—	—	—	—	—	—	—	X	X
Chrysene, 3-methyl-	—	—	—	—	—	—	—	—	X	X
Chrysene, 4-methyl-	—	—	—	—	—	—	—	—	X	X
Chrysene, 5-methyl-	—	—	—	—	—	—	—	—	X	X
Chrysene, 6-methyl-	—	—	—	—	—	—	—	—	X	X
Coronene	—	—	X	—	—	—	—	—	X	X
4*H*-Cyclopenta[*def*]chrysene	—	—	—	—	—	—	—	—	—	X
Cyclopenta[*cd*]pyrene	—	—	—	—	X	—	—	—	—	—
Dibenz[*a,e*]aceanthrylene	—	—	X	—	—	—	—	—	—	X

Dibenz[*a,h*]anthracene	X	X	X	X	—	X	X	—	X	X
Dibenz[*a,j*]anthracene	X	—	X	—	—	X	—	—	X	X
Dibenzo[*b,def*]chrysene	—	—	X	—	—	X	—	—	X	X
Dibenzo[*def,mno*]chrysene	—	—	X	—	—	X	—	—	—	X
Dibenzo[*def,p*]chrysene	—	—	X	—	—	X	—	—	X	X
13*H*-Dibenzo[*a,i*]fluorene	—	—	—	—	—	—	—	—	—	X
Dibenzo[*a,j*]naphthacene	—	—	—	—	—	X	—	—	—	—
Dibenzo[*de,qr*]naphthacene	—	—	X	—	—	—	—	—	—	—
Dibenzo[*fg,op*]naphthacene	—	—	X	—	X	X	—	—	—	X
Dibenzopyrene	—	—	—	—	X	—	—	—	—	—
Fluoranthene	—	—	X	—	—	—	—	—	—	X
Fluoranthene, 2-methyl-	—	—	—	—	—	—	—	—	—	X
Fluoranthene, 3-methyl-	—	—	—	—	—	—	—	—	—	X
Fluoranthene, 7-methyl-	—	—	—	—	—	—	—	—	—	X
Fluoranthene, 8-methyl-	—	—	—	—	—	—	—	—	—	X
9*H*-Fluorene	—	—	—	—	—	—	—	—	—	X
Indeno[1,2,3-*cd*]pyrene	—	—	—	—	X	—	—	—	X	X
Indeno[1,2,3-*cd*]pyrene, dimethyl-	—	—	—	—	X	—	—	—	—	—
Indeno[1,2,3-*cd*]pyrene, methyl-	—	—	—	—	X	—	—	—	—	—
Naphthacene	X	—	—	—	—	X	—	—	—	X
Naphthalene	X	X	X	X	X	X	—	—	—	X
Naphthalene, dihydro-	—	—	—	—	X	—	—	—	—	—
Naphthalene, dihydromethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2-dihydro-3-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,3-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,4-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,5-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,6-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,7-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,8-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2,3-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2,6-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2,7-dimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, dimethyl-2-ethenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, dimethylethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, dimethyl-2-phenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, dimethyl-1,2,3,4-tetrahydro-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-ethenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-ethenyl-	—	—	—	—	X	—	—	—	—	—

(*continued*)

TABLE 1.22 (continued)
Tobacco Smoke PAHs Discussed in Various Publications on the Relationship between PAH Structure and Tumorigenicity

PAH Discussed	Coulson (829)	Fieser et al. (1180a)	Herndon (1623a, 2435a)	Lacassagne et al. (2247a)	Martin et al. (2479)	Pullman and Pullman (3003)	Rubin (3365)	Trosko-Upham (3966a)	Zhang et al. (4410c)	Zhang (4410d)
Naphthalene, 2-ethenylmethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-ethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-ethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, ethylmethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-ethyl-3-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-ethyl-7-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-ethyl-8-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-ethyl-3-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-ethyl-6-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-ethyl-7-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, hexamethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-methyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, (1-methylethyl)-	—	—	—	—	X	—	—	—	—	—
Naphthalene, methylphenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, methyl-2-phenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-(1-methylpropyl)-	—	—	—	—	X	—	—	—	—	—
Naphthalene, methyl-1,2,3,4-tetrahydro-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-methyl-1,2,3,4-tetrahydro-	—	—	—	—	X	—	—	—	—	—
Naphthalene, pentamethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-phenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-phenyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1-propyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 2-propyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, tetramethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2,4-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,2,6-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,3,6-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,4,5-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphthalene, 1,6,7-trimethyl-	—	—	—	—	X	—	—	—	—	—

Naphthalene, 2,3,6-trimethyl-	—	—	—	—	X	—	—	—	—	—
Naphtho[1,2,3,4-*def*]chrysene	—	—	X	—	—	X	—	—	X	X
Naphtho[2,1,8-*qra*]naphthacene	—	—	X	—	—	X	—	—	—	X
Naphtho[1,2-*b*]triphenylene	—	—	X	—	—	X	—	—	—	X
Ovalene	—	—	X	—	—	—	—	—	X	—
Pentacene	—	—	X	—	—	X	—	—	X	X
Pentaphene	X	—	—	—	—	X	—	—	—	X
Perylene	—	—	X	—	—	X	—	—	—	X
Phenanthrene	X	X	X	X	—	X	—	X	X	X
Phenanthrene, dimethyl-	—	—	—	—	—	—	—	—	X [1]	—
Phenanthrene, methyl-	—	—	—	—	—	—	—	X	—	—
Phenanthrene, tetramethyl-	—	—	—	—	—	—	—	—	X [1]	—
Picene	—	—	—	—	—	X	—	—	—	—
Pyrene	X	—	X	—	X	X	—	X	—	X
Pyrene, dihydro-	—	—	—	—	X	—	—	—	—	—
Pyrene, dimethyl-	—	—	—	—	X	—	—	—	—	—
Pyrene, 3,4-dimethylene-	—	—	—	—	X	—	—	—	—	—
Pyrene, hexamethyl-	—	—	—	—	X	—	—	—	—	—
Pyrene, 1-hexyl-	—	—	—	—	X	—	—	—	—	—
Pyrene, methyl-	—	—	—	—	X	—	—	—	—	—
Pyrene, 1-methyl-	—	—	—	—	X	—	—	—	—	X
Pyrene, 2-methyl-	—	—	—	—	X	—	—	—	—	X
Pyrene, 4-methyl-	—	—	—	—	X	—	—	—	—	X
Pyrene, pentamethyl-	—	—	—	—	X	—	—	—	—	—
Pyrene, tetramethyl-	—	—	—	—	X	—	—	—	—	—
Pyrene, trimethyl-	—	—	—	—	X	—	—	—	—	—
5*H*-Tribenzo[*a,f,l*]trindene, 10,15-dihydro-	—	—	—	—	—	—	—	—	X	—
Triphenylene	X	—	X	—	—	X	—	X	X	X
Triphenylene, methyl-	—	—	—	—	—	—	—	—	—	X [1]

[a] The positions of the two methyl groups were not specified.

[b] Number in square brackets indicates the number of isomers included in the study.

[c] The nature of the benzopyrene was not specified.

[d] The position of the methyl group was not specified.

B[*a*]P was tumorigenic to laboratory animal skin but also that B[*a*]P was an extremely potent tumorigen [194; see pp. 197–232 in (1544)]. The significant tumorigenic potency of B[*a*]P was the reason it was studied for many years between the 1930s and mid-1950s as the marker component in many tumorigenic pollutants such as tars, oils, soots, etc. The B[*a*]P content of coal tar had already been defined by Cook and his colleagues (796a, 797, 1631). In 1937, Hieger described the level of B[*a*]P in pitch (5938). Between 1937 and 1939, Kling et al. (5946, 5947) described the level of B[*a*]P in tumorigenic asphalt road tars.

Surprisingly, during these same years, 1937 through 1939, A.H. Roffo (3323–3325) and his son A.E. Roffo (3316, 3318) described their identification of three PAHs—anthracene, phenanthrene, and B[*a*]P—in a destructive distillate of tobacco and the tumorigenicity of the destructive distillate. Their discoveries were subsequently either ignored because the three PAHs had not been identified at that time in tobacco smoke or much criticized with the claim that a destructive distillate of tobacco was obviously not equivalent to tobacco smoke. In 1942, Roffo also reported (3327) that the organic solvent extraction of tobacco prior to its destructive distillation yielded a destructive distillate with lower levels of the three PAHs and a much reduced tumorigenicity. The criticisms of the reports by the Roffos are discussed in more detail in Section 1.5.1.

In 1943 and 1944, Berenblum and Schoental (5912, 5913) defined the difference between the tumorigenicities of shale and shale oil and the relationship of the difference to their B[*a*]P contents. Later, the tumorigenicity and B[*a*]P content of coal tar was also studied in detail by Berenblum and Schoental (5911, 5914). In 1949, Goulden and Tipler described the identification and quantitation of B[*a*]P in domestic soot (5935). This was followed by the 1951 report from Falk et al. (5934) on the levels of tumorigenic PAHs, including B[*a*]P, in processed rubber such as that used in automobile tires and the 1952 report by Falk and Steiner (5933) on the PAHs in carbon black. Also in 1952, Hieger and Woodhouse (HIE2) described the tumorigenicity and B[*a*]P content of various petroleum fractions.

In 1955, Falk and Kotin reported the results of several of their studies (5930). One involved the fate of PAHs, including B[*a*]P, in soot emitted into the atmosphere and subsequently deposited in human lungs (5930); another involved the presence of PAHs in diesel exhaust and the tumorigenicity of diesel exhaust extracts (5949). A third study did not involve PAHs per se but involved the study of the tumorigenicity of aliphatic hydrocarbons extracted from atmospheric pollution (5956).

In 1957, Fieser, a U.S. PAH expert, criticized (1181) the inadequacy of the spectral data used by Cooper and Lindsey in the United Kingdom (818–821) and Alvord and Cardon in the United States (55–57, 592–594) to define the presence of B[*a*]P in cigarette smoke. Fieser's colleagues, unable to detect B[*a*]P in cigarette smoke, were successful in their identification of B[*a*]P in roast coffee. Obviously, Fieser was unaware of the 1955 and 1956 reports of B[*a*]P identified in cigarette smoke by Falk and Kotin (1172) or the 1956 isolation of B[*a*]P in crystalline form from a commercial cigarette by Rodgman (3240). After the published 1959 report by Wynder and Hoffmann (4307) on the isolation of crystalline B[*a*]P from cigarette smoke, Fieser accepted it as a cigarette smoke component. Later, Fieser served on the 1964 Advisory Committee that prepared the report on smoking and health for the U.S. Surgeon General (3999). Fieser was the Advisory Committee member responsible for the chapter on cigarette smoke composition and emphasized the tumorigenic components identified in it.

The next year, Kuratsune (2237) studied the B[*a*]P content of various pyrolysates, and Tebbens et al. (3874) reported the generation of PAHs during combustion. Commins et al. (5922) reported on the content of B[*a*]P and other PAHs in the atmosphere of a diesel engine bus garage.

In his 1955 review of the epidemiological and experimental data on exogenous respiratory tumorigen, Hueper (5944) concluded that it was unlikely that cigarette smoke was a major factor in lung cancer but that much of the available evidence implicated occupational and/or industry-related factors such as soot, coal tar and pitch, petroleum oils, and gasoline and diesel engine exhausts. Later in 1957, Hueper (5230) modified his view of cigarette smoke but retained his view on environmental pollutants.

Between the mid-1930s and mid-1960s, there were many studies conducted in many countries around the world in which the PAHs (and B[*a*]P) in the atmosphere above many cities and towns were determined.

The rise in lung-cancer rates began many years before cigarette smoking became widespread, and no consistent relation existed between cigarette consumption and lung-cancer rates in different countries. For example, the lung-cancer death rate in England and Wales was twice that in the United States. The per capita cigarette consumption was 30% higher in the United States and primarily involved a blended cigarette (flue-cured, burley, Oriental, Maryland tobaccos), whereas the U.K. cigarettes were primarily flue-cured. Other data indicated that the U.K. cigarette smokers smoked their cigarettes to a shorter butt length [Hammond (5936)]. Additional data were provided on PAHs in smoke (5958) and the cigarette butt lengths in Canada, the United Kingdom, and the United States (5937).

Between the mid-1930s and mid-1950s, a great number of reports were issued in which successively improved analytical procedures for the PAHs, particularly the highly tumorigenic B[*a*]P, in the significant air pollution over urban areas were published (Table 1.23). The air pollutants, particularly PAHs, were determined in the atmosphere over various cities in the United States and in other countries around the world, e.g., Los Angeles, Pittsburgh, New York, New Haven, Cincinnati, Geneva, Osaka, Tokyo, Sidney, Budapest, Copenhagen, Prague, Kiev, Liverpool, London, Genoa, Bologna, Milan, and Rome.

This series of events was subsequently paralleled between the mid-1950s and the years in the early twenty-first century by the history of the PAHs, and of course B[*a*]P,

TABLE 1.23
Studies Prior to 1966 on Carcinogenic Components in Cigarette Smoke *vs.* in Air Pollution and Other Sources

Investigator	Air Pollution Studies	Cigarette Smoke Studies
Yamagiwa and Ichikawa	For over a century, investigators attempted to induce tumors in laboratory animals by skin painting with various pollutant items. All such studies were unsuccessful until the mid-1910s when Yamagiwa and Ichikawa (4361) by significantly increasing the painting period with a coal-tar solution from just a few weeks	
Kennaway	In the mid-1920s and the early 1940s, Kennaway published numerous articles on the tumorigenicity of various commercial tars (140a, 194) and the generation of tumorigenic tars by pyrolysis of various compounds such as isoprene, acetylene, and cholesterol (2073–2080). He and his colleagues became interested in the tumorigenicity of arsenic in air pollutants (5239, 5240, 5264) and subsequently in tobacco and its smoke (159, 889, 889a, 5160)	Kennaway and his colleagues published several articles on the relationship between arsenic I tobacco and tobacco smoke and its effect on smokers (159, 889, 889a, 5160)
Cook, J.W., Hieger, Kennaway	In the early 1930s, Hieger conducted spectral analysis of tumorigen-producing oils and tars (1630, 1631) and in the early 1952 studied the tumorigenicity of petroleum fractions (5939). The spectral procedure was used in the following study by Cook et al. (796a, 797) who described and discussed the tumorigenic PAHs that they had isolated from coal tar. The most significant PAH isolated and identified was the previously unknown potent tumorigenic PAH benzo[*a*]pyrene (B[*a*]P). In many subsequent studies, B[*a*]P was used as a marker for tumorigenicity	Some 30 years later in the early 1960s, Cook published several articles on the tumorigenic PAHs in tobacco smoke (796. 798)
Waller	In 1952, Waller reported on the B[*a*]P content of town air (25A81). Later, he discussed air pollution as significant factor in lung-cancer incidence (5978)	In 1991, Waller coauthored a publication on the cigarette smoke "tar" and certain toxicants from U.K. cigarettes (2947)
Campbell, J.A.	In the 1930s, Campbell (579–581) demonstrated the tumorigenicity of a variety of air pollutants (tarred road dust, exhaust gases from internal combustion engines, atmospheric pollutants). His subsequent studies involved the tumorigenicity of anthracite coal dust and other city atmospheric pollutants (5915)	
Berenblum and Schoental	During the mid-1940s, Berenblum and Schoental studied the PAH content, particularly the B[*a*]P content, in such pollutants as coal tar, shale tar, and shale oil and the relationship to the tumorigenicity of the pollutant (5911–5913)	
Clemmesen	In the 1950s, Clemmesen and his colleagues published several papers on the relationship between respiratory cancer and air pollution in Denmark (5917–5919)	
Cooper	In the early 1950s, Cooper described the level of PAHs in town air (5923–5926)	In the mid-1950s, Cooper's studies moved from air pollution to cigarette-related research in which he and his colleagues determined the various tumorigenic PAHs in cigarette smoke (785, 817, 818, 820, 821), and the PAHs in the pyrolysis product of cigarette paper (819)
Clemo, G.R. et al.	In 1955, Clemo et al. described the carcinogenic action of the smoke issued into the atmosphere over a city (Newcastle-on-Tyne) (5920, 5921)	Between 1958 and 1960, Clemo published several articles on the toxicants in cigarette some (765–767)
Shubik	In 1955, Shubik and Saffiotti described the tumorigenicity and tumor-promoting activity of catalytically cracked oils (SH1). In the mid-1960s, Lijinsky and Shubik described the tumorigenic components identified in various cooked food (2364a, 2364b). Their findings added to those reported in the early 1940s by Steiner et al. (25A69)	
Dickens, F.	In the early 1940s, Dickens and Weil-Malherbe described the results of their study on the tumorigenicity of wood smoke (5928)	In the mid-1960s, Dickens and Black described the results of their chemical and biological studies on some components of tobacco smoke (961)

(*continued*)

TABLE 1.23 (continued)
Studies Prior to 1966 on Carcinogenic Components in Cigarette Smoke *vs.* in Air Pollution and Other Sources

Investigator	Air Pollution Studies	Cigarette Smoke Studies
Badger	Beginning in the 1940s and proceeding to the early 1960s, Badger and his colleagues studied the pyrolysis of a number of compounds and their generation of PAHs during pyrolysis (140, 141, 143, 144, 144a, 145–154). Many of the compounds studied were eventually shown to be tobacco and/or smoke components that were subjected to high temperatures during the tobacco smoking process, e.g., isoprene (143), naphthalene (144), indene (146), acetylene (149), *n*-decane (151), several alkylated benzene (153), and 1,3-butadiene (154). Tumorigenic PAHs such as B[*a*]P were generated in each case	In one particular 1965 study, Badger et al. (142) studied the generation by pyrolysis of PAHs from known tobacco components (142). The tobacco components studied were dotriacontane, typical of the many saturated aliphatic hydrocarbons in tobacco, and stigmasterol. Typical of the phytosterols in tobacco. On pyrolysis, both yielded PAHs subsequently identified in cigarette MSS: B[]A, B[a]P, dibenzo[*def,p*]chrysene, dibenzo[*b,def*]chrysene, naphtho91,2,3,4-*def*]chrysene, benzo[*rst*]pentaphene
Eby et al.	In 1954, Eby et al. described the means of reducing the tumorigenicity of high boiling petroleum products (5929)	Wynder et al. (4306a) did note that Eby (25A21), in his examination of the cigarette tar used in the Wynder et al. 1953 biological study (4306a), did not detect B[*a*]P. They made little comment about Eby's failure to identify B[*a*]P or any other tumorigenic PAH in the Wynder et al. cigarette tar
Kotin, Falk et al.	Between 1951 and 1963, Kotin, Falk, and their colleagues conducted numerous studies on the chemical and biological properties of components contributing to the adverse effect of air pollution (5931–5934, 5948–5957, 5977). Several of their publications dealt with the tumorigenesis of PAHs to humans (1173, 5932, 5952, 5954–5956), the inhibition of the tumorigenesis of some PAHs by other coadministered PAHs (1174), and the ciliastatic activity of air pollutants (5977)	In the mid-1950s, Falk and Kotin studied the generation of tumorigenic PAHs from tobacco during a simulated smoking process (1172). In the early 1960s, Kotin, Falk, and colleagues published their views on the ciliastasis of cigarette smoke (1173a, 1175) and on the biological effects of several of its components (methanol, formaldehyde) (2179, 2180). For some years in the 1950s and 1960s, Kotin served on the Industry Technical Committee, Council for Tobacco Research (United States)[a] but left it because of a controversy over his publication of articles on the ciliary activity of cigarette smoke (1173a, 1175).
Stocks	In 1953, Stocks reported on his study of lung-cancer incidence in England and Wales (5971). Later in 1957 and 1959, he described the results of his study on the comparison of the effect of air pollution and tobacco smoking (5972, 5973). In 1955, Stocks and Campbell compared the effect of tobacco smoking, nonsmoking, and exposure to air pollution by B[*a*]P and other compounds (5974)	In 1955, Stocks and Campbell compared the effect of tobacco smoking, nonsmoking, and exposure to air pollution by B[*a*]P and other compounds (5971). In 1957 and 1959, Stocks reported on his comparison of the effect of tobacco smoking and air pollution on respiratory tract problems (5972, 5973)
Commins	In 1956, Commins et al. (5922) described the composition of the air in a London Diesel bus garage with emphasis on the PAHS, including B[*a*]P	In the mid-1950s, Commins with Lindsey reported not only on the PAHs, including B[*a*]P, in cigarette smoke but also on a procedure to determine the levels of various phenols in cigarette smoke (785–789a)
Fieser	In 1957, Fieser, a U.S. PAH expert, criticized (1181) the inadequacy of the spectral data used by various U.K. (818–821) and U.S. investigators (55–57, 592–594) to define the presence of B[*a*]P in cigarette smoke. Fieser's colleagues, unable to detect B[*a*]P in cigarette smoke, successfully identified B[*a*]P in roast coffee	After the published 1959 report by Wynder and Hoffmann (4307) on the isolation of crystalline B[*a*]P from cigarette smoke, Fieser accepted it as a cigarette smoke component. Later, Fieser served on the 1964 Advisory Committee that prepared the report on smoking and health for the U.S. Surgeon General (3999). He was the Advisory Committee member responsible for the chapter on cigarette smoke composition and emphasized the tumorigenic components identified in it
Lyons	In 1957, Lyons and Johnson described the PAHs they identified in vehicular exhausts (5962). In 1959, Lyons (5961) described the results of his additional study on the PAHs in vehicular exhausts (5961). In 1962, Lyons reported on his comparison of the PAHs in gasoline engine and diesel engine exhausts, general atmospheric dust, and cigarette smoke condensate (2428)	Between 1955 and 1962, Lyons and his colleagues published numerous papers on components in cigarette smoke (2425–2435). Several involved the identification of free radicals in both cigarette smoke (2429, 2432) and air pollution (2435). In 1962, Lyons reported on his comparison of the PAHs in gasoline engine and diesel engine exhausts, general atmospheric dust, and CSC (2428)

TABLE 1.23 (continued)
Studies Prior to 1966 on Carcinogenic Components in Cigarette Smoke *vs.* in Air Pollution and Other Sources

Investigator	Air Pollution Studies	Cigarette Smoke Studies
Johne et al.	In 1957, several studies were reported on the tumorigenicity of and the B[*a*]P content of diesel engine exhaust; cf. Johne et al. (5945) and Marterstock and Reuter (5963)	
Bonnet, Neukomm	In 1962, Bonnet (393) described the level of B[*a*]P in melted "tar"	In the late 1950s, Bonnet and Neukomm published the results of their research on the composition of cigarette (394–398)
Wynder, Hoffmann et al.	For several years during the 1960s, Wynder, Hoffmann, and their colleagues not only studied various aspects of cigarette smoke but also studied the contribution of air pollutants to respiratory tract problems. The possible contribution of gasoline engine exhaust (1790, 4315, 4316, 5942, 5943, 26A59) and other pollutants (1799, 4331, 5980, 5981) were studied. In their comparison of gasoline engine exhaust and cigarette smoke, they reported that the levels of tumorigenic PAHs such as B[*a*]P in the gasoline engine exhaust were much higher than that in cigarette MSS and that the mouse-skin tumorigenicity of the "tar" derived from the gasoline engine exhaust was much great than that of cigarette MSS "tar." However, it should be noted that after the 1960s, Wynder, Hoffmann, and their colleagues did almost no further research on air pollutants [see the 1972 study (5941)] but devoted their subsequent research totally to tobacco and tobacco smoke. From the late 1960s to 2005 or so, they were involved in hundreds of scientific meeting presentations and scientific journal publications in which the results of their tobacco-related research were reported	Data generated by Wynder, Hoffmann, and their colleagues outlined many of the problems of tobacco smoke, and such data were presented at literally hundreds of scientific meeting and/or published in scientific journals. Those issued between the early 1950s and the mid-1960s, the date of issuance of the 1964 report to the U.S. Surgeon General (3999), dealt with epidemiology (4293, 4306b), tumorigenicity studies with laboratory animals (1795, 1797, 1798, 4301, 4306, 4306a, 4306c, 4309, 4311, 4312, 4317, 4330, 4351, 4352, 4355, 4356), ciliastasis studies (4304, 4305, 4350), tobacco and/or tobacco smoke components such as the PAHs (589, 1766, 1786–1788, 1796, 3085, 4284, 4303, 4307, 4308, 4353, 4354), aza-arenes (587, 1778), phenols (1789), acidic compounds (1785, 4280, 4313), nitrohydrocarbons (1755, 3086), pesticides, and agronomic compounds (1756, 1767, 2383). In the mid-1960s, Wynder and Hoffmann published a lengthy review article in 1964 (4319) and their noted 1967 book (4332) on the tumorigenicity of tobacco smoke and the suspected responsible components. Between the mid-1960s and his death, Hoffmann presented at scientific meetings and/or published in scientific journals over 500 articles on some aspect of tobacco and/or tobacco smoke
Pailer	In 1965, Pailer et al. (5965) described the results of their determination of B[*a*]P in the atmosphere over Vienna	For several years starting in 1965, Pailer and his colleagues reported on their studies of various components in tobacco smoke, e.g., B[*a*]P (2881), aromatic amines (2882), aliphatic amines (2883, 2889), NNAs (2884, 2885), nickel (2886), and carbonyl components (2887). They also studied the pyrolysates from tobacco additives (2888)
Strach	Shortly after the committee's smoking and health report to the U.S. Surgeon General, the results of comparison studies, e.g., Strach (3821), were issued in which cigarette smoke components and air pollutants were compared with regard to respiratory tract toxicity and exposure	

[a] From 1956 through 1962, one of us (AR) represented R.J. Reynolds on the Industry Technical Committee of the Council for Tobacco Research (United States).

in MSS. Green and Rodgman (1373) noted the interesting fact about B[*a*]P in MSS: Despite its extremely low level in MSS and its minimal contribution to mouse-skin tumorigenicity from CSC, almost every year since the mid-1950s there has been at least one journal publication or meeting presentation on a new and/or improved method to quantitate the yield of B[*a*]P in MSS [see Table 6 in (3306b)]. In 2004, CORESTA published its recommended method for the determination of B[*a*]P in tobacco smoke (825a). Much emphasis has been placed on the determination of B[*a*]P in the MSS from fewer and fewer cigarettes. Before the advent of all the newly introduced and subsequently improved spectral and chromatographic systems, estimations of individual PAHs required the CSC from many cigarettes. For example, in their studies on the effect of various treatments of tobacco on the PAHs in MSS, Rodgman and Cook (3241, 3246, 3269, 3274, 3275) chemically analyzed the MSS from 3600 cigarettes for each control and treated sample. For the MSS PAH analyses in the more than 50 treated and control samples described in (3246), more than 183,000 cigarettes were smoked, the condensates collected, and processed. Nowadays, only a few cigarettes are needed for similar analyses. To permit comparison of the Rodgman–Cook PAH data with the biological findings reported by Wynder et al.

TABLE 1.24
Distribution of Identified Hydrocarbons between Tobacco and Tobacco Smoke

		Number of Identified Hydrocarbons in Tobacco and Tobacco Smoke			
Hydrocarbon	**Table**	**Total**	**Smoke**	**Tobacco**	**Smoke and Tobacco**
Alkanes	Table 1.10	136	116	100	80
Alkenes and alkynes	Table 1.11	392	376	49	33
Alicyclics	Table 1.12	164	117	70	23
Monocyclic aromatic	Table 1.13	113	103	47	37
Polycyclic aromatic	Table 1.20	511	502	102	92
	Totals	1316	1214	368	265
Polycyclic aromatic	Table 1.20	618[a]	607[a]	91	80
	Totals[a]	1423[a]	1320[a]	368	265

[a] This number includes the various isomers of alkyl-PAHs reported in which the position of the alkyl group or groups has not been precisely defined.

in the 1950s, Genoa (401), i.e., the cigarettes on a manifold were machine smoked (35 mL puff volume, 2 s puff duration, 3 puffs/min) with a collection system that duplicated the one described by Wynder et al. (4306a). This smoking regime differed from the usual 35 mL puff volume, 2 s puff duration, and 1 puff/min described by Bradford et al. (423b) in 1936 and used by most investigators in smoke studies after that date.

1.6 SUMMARY

Detailed examination of the lists presented in the five subchapters on hydrocarbons indicates that over 1200 hydrocarbons have been identified to date in tobacco and tobacco smoke. The data are summarized in Table 1.24.

It is obvious from the tabulation that the PAHs represent nearly 44% of the hydrocarbons identified to date and a substantial number of them are smoke components. The one category in the PAHs that is found to an appreciable extent in a particular type of tobacco, Latakia tobacco, is the bicyclic aromatic hydrocarbon naphthalene and its homologs (1135, 2784). The few remaining PAHs present in both tobacco and its smoke include several tricyclic, tetracyclic, and pentacyclic PAHs, e.g., anthracene, phenanthrene, pyrene, and B[*a*]P. As a result of the study by Bentley and Burgan (285) in the early days of the concern about B[*a*]P in tobacco smoke and its origin, the presence of B[*a*]P and the other PAHs in tobacco is usually attributed to its contamination by pollutants during transportation, curing, etc.

2 Alcohols and Phytosterols

2.1 ALCOHOLS

Periodically, tobacco researchers have reported the progress on the identification of tobacco and smoke components. Review articles by Johnstone and Plimmer (1971) and Izawa (1900) detailed much of the tobacco and smoke research conducted over the preceding century. Izawa listed 440 identified smoke components by 1961. The next year, Quin (3059) published a review of components found in tobacco and smoke. Herrmann (1625) reviewed phenolic compounds in tobacco smoke. In 1963, Philip Morris (2939) published a monograph on tobacco and smoke composition, a copy of which was provided the Advisory Committee on smoking and health to the U.S. Surgeon General (3999). In 1964, Elmenhorst and Reckzeh (1139) tabulated the aromatic hydrocarbons identified in tobacco smoke. Kuhn (2228, 2229) published articles on alkaloids in tobacco and their pyrolysis products in smoke. In their 1967 book, Wynder and Hoffmann (4332) discussed tobacco and smoke chemistry and the results of animal studies with tobacco smoke. Elmenhorst and Schultz (1140) listed 250 low-boiling components and vapor-phase components identified in tobacco smoke. In his 1968 review, Stedman (3797) listed nearly 1200 identified tobacco and smoke components. The next year, Neurath (2724) reported on the presence of 180 *N*-containing compounds in smoke.

With the meaningful advancements in analytical methodology, the number of tobacco and smoke components increased dramatically (1373). In an in-house catalog assembled at R. J. Reynolds Tobacco Company (RJRT) in 1975, Roberts et al. (3224) listed 2783 identified components of tobacco and tobacco smoke. During the mid-1970s at RJRT, Schumacher et al. (3553), Heckman and Best (1587), and Newell et al. (2769) identified over 1540 compounds in the water-soluble and ether-soluble fractions of tobacco smoke. Of these, over 820 compounds were newly reported as tobacco smoke components. In 1977, Schmeltz and Hoffmann (3491) cataloged nearly 500 *N*-containing compounds identified in tobacco smoke, but their catalog did not include the more than 230 *N*-containing compounds newly identified in tobacco smoke by Heckman and Best (1587). Between 1974 and 1978, Snook et al. (3756–3758) published the results of their massive study of the PAHs and a number of benzofurans identified in tobacco smoke, a study that was followed by an equally definitive one on the identification of aza-arenes and monocyclic *N*-containing compounds in tobacco smoke (3750). In 1980, Ishiguro and Sugawara (1884) listed 1889 identified tobacco smoke components in their monograph. However, a tally of the tobacco smoke components reported at that time exceeded 2500. No additional catalogs of the total number of identified components of cigarette mainstream smoke (MSS) have been published since the 1980 Ishiguro and Sugawara (1884) publication. Smith et al. (3712) recently reported the chemical structures of the 253 identified phenols reported in cigarette MSS.

In the past, different authors had different views on the classification of alcohols in tobacco and tobacco smoke. In our catalog, we employ a system different from those used by our forerunners. In 1954, Kosak (2170) in his smoke component compilation listed seven "alcohols": four alcohols (methanol, glycerol, diethylene glycol, and ethylene glycol) and three phenols (phenol, "phenols," and catechol). He did not list either levoglucosan or a "phytosterol" as an alcohol but listed both as miscellaneous smoke components. In 1959, Johnstone and Plimmer (1971) listed 13 alcohols plus 5 phytosterols identified in tobacco and/or smoke.

In his 1968 review, Stedman (3797) divided the alcohols into three categories, namely, alcohols, sterols, and oxygenated isoprenoid constituents. The latter category contained constituents other than those with an alcoholic hydroxyl group, e.g., farnesyl acetone (a ketone), solanachromene (a phenol), the tocopherols (phenols), and the levantanolides and levantenolide (ether–lactone combinations). In the category usually considered alcohols, Stedman listed a total of 25 alcohols (15 aliphatic, 2 aromatic, 5 polyols, and 3 cyclic).

In our current catalog, compiled periodically since 1955, we have considered three types of components with hydroxyl groups: (1) the components with a carboxyl group and its hydroxyl group (discussed in Chapter 4), (2) the components with a hydroxyl group attached to a monocyclic or polycyclic benzenoid nucleus, i.e., a phenol (discussed in Chapter 9), and (3) a hydroxyl group attached to a saturated or unsaturated aliphatic, alicyclic, or nonbenzenoid nucleus which may or may not include another functional entity. An example of category (3) is the first item in Table 2.1, hydroxyacetaldehyde (glycolaldehyde) which is both an alcohol and aldehyde. The saturated aliphatic alcohols range from methanol to 1-triacontanol with alkyl homologs included in some cases, e.g., 1-butanol and 2-methyl-1-propanol. The unsaturated aliphatic alcohols include 2-propen-1-ol (allyl alcohol) and such terpenoid structures as the C_{10} alcohol 3,7-dimethyl-1,6-octadien-3-ol (linalool), the C_{20} alcohol 3,7,11,15-tetramethyl-2-hexadecen-1-ol (phytol), and the C_{45} alcohol 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaen-1-ol (solanesol). Examples of the alicyclic alcohols range from cyclopentanol to various carotenediols and triols to numerous cyclotetradecadienols, diols, and triols. Other alicyclic alcohols include a great variety of carbohydrates such as glucose and fructose plus the cases where such carbohydrates are linked to another component such as a phytosterol to form a glycoside.

TABLE 2.1
Tobacco and Tobacco Smoke Components Identified by Classical Chemical Methods

Year	Investigator (Reference)	Component(s) Identified	Smoke	Tobacco
1953	Sasaki (3413)	2,3-Butanedione	+	−
1956	Rowland et al. (3359)	Solanesol	−	+
1956	Rowland (3345)	Neophytadiene	−	+
1956	Rowland (3347)	α-Tocopherol, solanachromene	−	+
1957	Kosak et al. (2178)	Stigmasterol	+	−
1958	Kosak and Swinehart (2175)	Squalene	+	−
1958	Philippe and Hackney (2941)	Nitrous oxide, methyl nitrite	−	+
1958	Wender et al. (4164)	Scopoletin	+	−
1959	Dieterman et al. (969)	Esculetin	−	+
1959	Dymicky and Stedman (1082)	Campesterol	−	+
1959	Gladding et al. (1307)	Neophytadiene	+	+
1959	Rodgman and Cook (3271)	α-Tocopherol	+	−
1959	Kobashi and Sakaguchi (2145)	Glucose, fructose, arabinose, xylose	+	−
1960	Carruthers and Johnstone (614)	Docosanol, solanesol	−	+
1960	Schumacher (3535)	β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylpentanoate)	−	+
1960	Yang et al. (4376)	Caffeic acid	+	−
1962	Roberts and Rowland (3221)	α- and β-4,8,13-Duvatriene1,3-diol	−	+
1962	Cook and Rodgman (801)	α- and β-Levantenolide	+	−
1962	Rodgman and Cook (3280)	Eugenol, isoeugenol	+	−
1962	Yang and Wender (4378)	Protocatechuic acid, 5-hydroxymethylfurfural	+	−
1964	Philippe and Honeycutt (2943)	Methyl isocyanate	+	−
1965	Zane et al. (4402)	4-*O*-Caffeoylquinic acid	−	+

With our method of defining an alcohol in tobacco and/or smoke, the alcohols number over 1400. We realize that some readers may disagree with our classification of several hydroxypyridines as alcohols but the listed ones appear not only in this chapter, Section 2.1, but also appear in Section 17.2 in which monocyclic *N*-containing six-membered ring compounds are described and cataloged.

Present analytical technology to identify a component in a complex mixture such as tobacco smoke or a tobacco extract involves the generation of a variety of spectra from which the compound may be characterized. The spectra may include separation of the component from the mixture by glass capillary gas chromatography, its retention time, plus those generated by ultraviolet, infrared, nuclear magnetic resonance, and mass spectroscopy studies. Nowadays, seldom is the component in the complex isolated in a tangible amount. In the early days, the study of the composition of tobacco was accomplished by so-called classical chemical procedures. The following example illustrates how an isolated terpenoid alcohol was subsequently characterized: Ozonization of the compound followed by degradation of the ozonide and derivatization of the degradation products with 2,4-dinitrophenylhydrazine yielded the 2,4-dinitrophenylhydrazones of the compounds shown in Figure 2.1: glycolic aldehyde (hydroxyacetaldehyde) {II}, levulinaldehyde (4-oxopentanal) {III}, and acetone (2-propanone) {IV}. These findings led to the assignment in 1956 of the structure {I} in Figure 2.1 by Rowland et al. (3359) to the terpenoid alcohol they named solanesol.

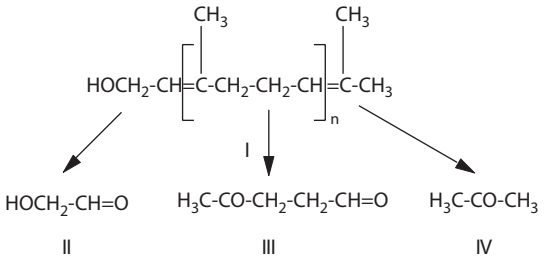


FIGURE 2.1 The degradation products from ozonized solanesol.

In the mid-1950s, the determination of the molecular weight of a compound with a molecular weight above 300–400 was difficult and often inaccurate. As a result, Rowland et al. were unable to precisely define the molecular weight of solanesol and therefore its structure. Originally, they had intended to report that solanesol was either a C_{45} compound (I, $n = 8$ in Figure 2.1) or a C_{50} compound (I, $n = 9$ in Figure 2.1) but were forced to choose one or the other. Because the majority of known isoprenoids at that time were terpenoids, i.e., multiples of C_{10}, and relatively few were sesquiterpenoids, i.e., multiples of C_{15}, Rowland et al. elected to report solanesol as a pentaterpenoid, i.e., a C_{50} compound. In 1957, Mold and Booth (2590) reported the identification of solanesol in cigarette mainstream smoke (MSS).

Subsequently, with more advanced analytical technology, Erickson et al. (2A01) and Shunk et al. (2A03) reported in back-to-back publications in 1959 that a more precise

molecular weight method indicated that solanesol was a C_{45} compound (I, $n = 8$ in Figure 2.1) with the formula $C_{45}H_{74}O$ (molecular weight, 630), 3,7,11,15,19,23,27,31,35-nonamethy l-2,6,10,14,18,22,26,30,34-hexatriacontanonaen-1-ol.

Since its characterization in 1956, solanesol has had an interesting history as a tobacco component. It is present in:

1. The different types of tobacco (flue-cured, burley, Oriental, Maryland) (3295)
2. In the smoke from each when smoked in cigarette form (2559, 3270, 3295)
3. As a variety of esters in tobacco [Rowland and Latimer (3358)] and tobacco smoke [Rodgman and Cook (3270), Rodgman et al. (3286)]

It generates isoprene [Gil-Av and Shabtai (1286); Grossman et al. (1431, 1432)], several solanesenes [Rodgman et al. (3297)], and numerous polycyclic aromatic hydrocarbons [Rodgman and Cook (3269), Severson et al. (3616)] during the smoking process. It was proposed by Wright (4282) as a more significant precursor in tobacco of polycyclic aromatic hydrocarbons (PAHs) in MSS than the aliphatic long-chained hydrocarbons and eventually was found to be such by Rodgman and Cook (3269) and Severson et al. (3616). More recently solanesol was studied as an indicator of environmental tobacco smoke (ETS) in room space [Ogden (2829), Ogden and Maiola (2833, 2834), Robinson et al. (3230), Tang et al. (3868)].

In the early tobacco and tobacco smoke studies, the chemical nature of one or two components was defined by means of classical chemical procedures and described in an appropriate publication, e.g., the identification of the previously discussed terpenoid alcohol solanesol in flue-cured tobacco (3359), the phenols eugenol and isoeugenol identified in the mainstream smoke (MSS) from Oriental tobacco (3280), and maltol identified in the MSS from an ingredient-free German tobacco blend (1131). A random selection of several of these early studies is presented in Table 2.1.

However, as analytical methodology became more sophisticated and precise, many more components—sometimes several hundred newly identified in tobacco or smoke—were reported in a single publication. In his pioneer research on glass capillary gas chromatography in 1965, Grob (1416) in his study of the MSS from cigarettes containing additive-free tobacco identified 63 components, a number of which were polar components. Later, some of the polar components in MSS identified by Grob are also listed in the Doull et al. catalog of cigarette flavor ingredients (1053).

In the 1950s, the organic solvent extraction of tobacco was studied extensively with the purpose of removing PAH precursors from the tobacco. Incorporated into one process was an aqueous alcohol–hexane partition to separate the polar, more flavorful tobacco components from the lipophilic PAH precursors. At that time, almost nothing was known about the nature of the polar tobacco components, although it was apparent they made a considerable positive contribution to the flavor and aroma of cigarette MSS. Despite the lack of knowledge about the precise nature of the polar components, it was demonstrated they were not significant PAH precursors (3262). Our inability at that time to separate highly polar compounds in a complex mixture contributed to our lack of knowledge of the nature of the polar components in tobacco and/or tobacco smoke. This situation continued during years of intensive effort on cigarette MSS composition but was finally resolved and utilized by Schumacher et al. (3553) in the 1970s. Of the total of 1545 MSS components identified by Schumacher et al. (3553), by Newell et al. (2769), and by Heckman and Best (1587), 828 (53.6%) were new to the tobacco smoke literature at the time of the publication and a great number of them were highly polar compounds (see Table 2.2).

TABLE 2.2
Tobacco and Tobacco Smoke Studies in Which Components Were Identified by a Combination of Spectral Technologies

Year	Investigator (Reference)	No. of Identified Components	Smoke	Tobacco	New[a]
1965	Grob (1416)	63	+	–	27
1973/1974	Schumacher and Vestal (3561)	118	–	+	25
1974/1976[b]	Lloyd et al. (2389)	323	–	+	132
1974/1977	Schumacher et al. (3553)	479	+	–	387
1975	Newell et al. (2769)	643	+	–	173
1976	Snook et al. (3758)	115	+	–	NI[c]
1977	Snook et al. (3756)	157	+	–	NI
1978	Snook et al. (3757)	536	+	–	NI
1978	Heckman and Best (1587)	423	+	–	268
1982/1982	Schumacher (3550)	97	–	+	1
2004	Peng et al. (2917a)	408	–	+	NI
2005	Leffingwell and Alford (2339a)	334	–	+	49

[a] Newly reported components to tobacco and/or smoke at the date of the publication.
[b] The first date is that of a scientific conference presentation; the second is that of a publication in a peer-reviewed scientific journal.
[c] NI, not indicated was the number of components not previously identified in tobacco or tobacco smoke.

With regard to tobacco components, Lloyd et al. (2389) identified 275 previously unidentified components of additive-free flue-cured tobacco, 132 new to all additive-free tobacco types. Many of these compounds were highly polar and considered significant contributors to MSS flavor and aroma. Similar detailed studies were conducted on the composition of burley tobacco by Roberts and Rohde (3219), Oriental tobacco by Schumacher and Vestal (3561), and Maryland tobacco by Schumacher (3550). Years later, it became apparent that many of the highly polar components of tobacco and tobacco smoke were identical with or similar to many of the components used in the flavor formulations, i.e., the "top dressing," added to a specific tobacco blend to impart its unique smoking characteristics (1053). Randomly selected publications on the identification of many additive-free tobacco and/or tobacco smoke components are listed in Table 2.2.

The description of the isolation and/or identification of a great number of tobacco and/or smoke components was not always the case even after the development of sophisticated analytical technologies that generated informative spectral data. Between the early 1970s and the late 1980s, the research group at the Swedish Tobacco Company in Stockholm, Sweden, generated a great number of publications on flue-cured and Oriental tobacco composition in many of which only a single component or a few newly identified tobacco components were described. Admittedly, much attention was paid to the definition of the stereoisomerism of some of the components described individually. Selected examples of their extensive study of tobacco composition are presented in Table 2.3.

Periodically between the mid-1970s and the late 1980s, the Swedish Tobacco Company group published excellent reviews of their tobacco component studies and other meaningful related studies in the scientific literature, e.g., Enzell (1149, 1149a), Enzell and Wahlberg (1156), Enzell et al. (1157), Wahlberg and Eklund (4086a), and Wahlberg and Enzell (4089, 4090).

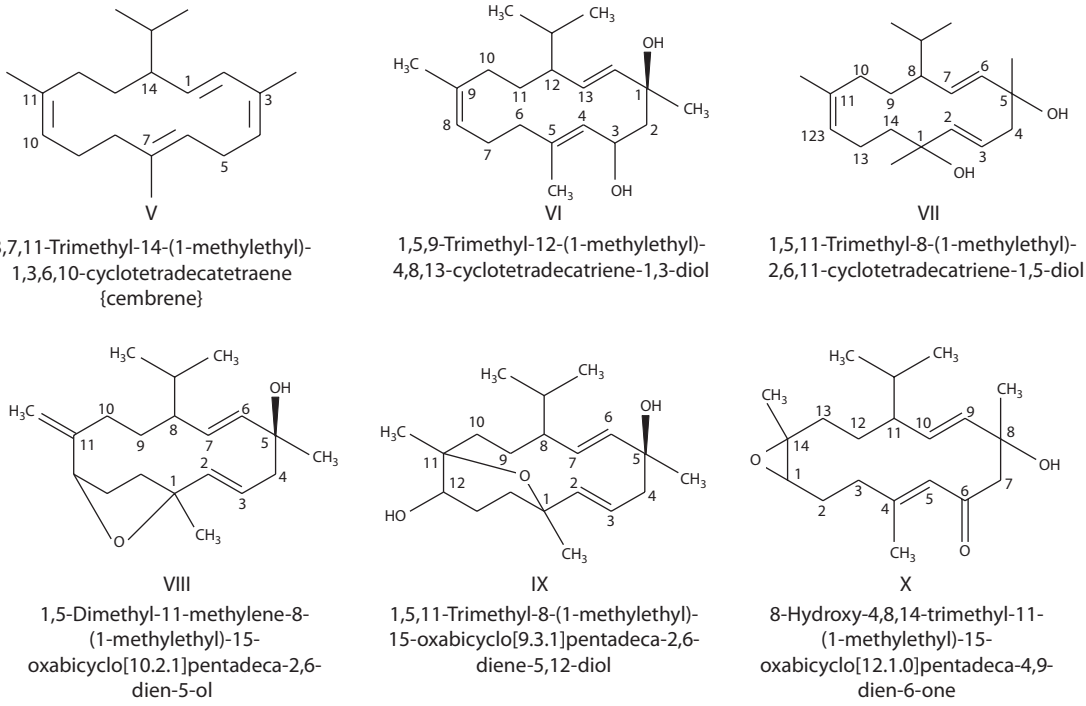
In addition to his isolation of the alcohol solanesol and contribution to its characterization, Rowland was involved in the isolation and characterization of the hydroxylated flue-cured tobacco components solanachromene and α-tocopherol, each of which is a phenol. The solanachromene has not been identified in tobacco smoke, but α-tocopherol, a well-known anticarcinogen, was identified as a cigarette MSS component in 1959 (3271) and many times since in MSS and ETS, e.g., Risner (3170).

In their 1962–1963 study of hydroxylated tobacco components, Rowland and his colleagues next isolated several 1,3- and 1,5-diols from tobacco. Structurally, these diols were shown to be related to the alicyclic diterpenoid hydrocarbon cembrene, previously isolated in 1951 from plant tissue by Haagen-Smit et al. (2A02) and characterized in 1962 as 3,7,11-trimethyl-14-(1-methylethyl)-1,3,6,10-cyclotetradecatetraene (see {V} in Figure 2.2) by Dauben et al. (905a). The 1,3-diol and 1,5-diol isolates were demonstrated to possess the cyclotetradecatriene structures shown as {VI} and {VII}, respectively, in Figure 2.2 [Rowland (3351, 3352), Rowland and Roberts (3360)]. Additional studies indicated the presence in tobacco not only of the diols {VI} and {VII} but also the two oxabicyclo compounds {VIII} and {IX} derived from the 1,5-diol {VII}. A third oxabicyclo type {X} was eventually identified in tobacco (9, 12, 4089–4091). The four compounds {VI}–{IX} were reported by Rowland et al. to be present in cigarette MSS (3361). Cembrene {V} was eventually identified in 1966 in tobacco by Reid (1097a) and in Japanese tobacco in 1980 by Takagi et al. (3853).

The reports of these cyclotetradecatrienediols and their ethers by Rowland, Roberts, and their colleagues led to an intensive study of tobacco by the Swedish Tobacco Company research team. Their study involved the isolation, characterization, and stereochemical definition of nearly 100 compounds containing the 14-carbon ring [Aasen et al. (12), Arndt et al. (94a), Behr et al. (235, 236), Wahlberg et al. (4083–4085, 4091, 4098–4100), Wahlberg and Eklund (4086a, 4088), Wahlberg and Enzell (4091)].

TABLE 2.3
Tobacco Components Identified Post-1975

Year	Investigator (Reference)	Components Identified
1971	Aasen et al. (9a)	5-Methoxy-6,7-dimethylbenzofuran
1971	Enzell et al. (1155)	Norsolanesene
1974	Aasen et al. (6)	(9R)-9-Hydroxy-4-megastigmen-3-one,
1975	Aasen et al. (1)	5,6-Epoxy-3-hydroxy-7-megastigmen-9-one (2 isomers)
1977	Behr et al. (230)	3,3-Dimethyl-7-hydroxy-2-octanone
1977	Behr et al. (231)	2,6-Dimethyl-10-oxo-3,6-undecadien-2-ol, 3-methyl-4-oxo-2-nonen-8-ol
1978	Behr et al. (229)	2,6-Dimethyl-2,7-octadiene-1,6-diol
1979	Behr et al. (234)	5,8-Epoxy-6-megastigmene-3,9-diol, 3,6-epoxy-7-megastigmene-5,9-diol
1982	Wahlberg et al. (4084)	8,11-Epoxy-2,6-cembradiene-4,12-diol
1983	Wahlberg et al. (4087)	7,8-Epoxy-4-basmen-6-one
1983	Wahlberg et al. (4098)	Hydroperoxycembratrienediols [5 in all]
1984	Wahlberg et al. (4083)	Cembratrienols [6 in all]
1986	Wahlberg et al. (4102)	A new sucrose ester



V
3,7,11-Trimethyl-14-(1-methylethyl)-1,3,6,10-cyclotetradecatetraene {cembrene}

VI
1,5,9-Trimethyl-12-(1-methylethyl)-4,8,13-cyclotetradecatriene-1,3-diol

VII
1,5,11-Trimethyl-8-(1-methylethyl)-2,6,11-cyclotetradecatriene-1,5-diol

VIII
1,5-Dimethyl-11-methylene-8-(1-methylethyl)-15-oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol

IX
1,5,11-Trimethyl-8-(1-methylethyl)-15-oxabicyclo[9.3.1]pentadeca-2,6-diene-5,12-diol

X
8-Hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-15-oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one

FIGURE 2.2 Tobacco and/or tobacco smoke alcohols related to cembrene.

Much research was conducted after the mid-1950s to identify alcohol components in the particulate phase of cigarette MSS primarily because some were found to contribute consumer acceptable flavor and aroma properties to the MSS. As noted by Rodgman (3266), many components, including alcohols, used by the tobacco industry in its flavor formulations [see listing by Doull et al. (1053)] are known components of additive-free tobacco and/or its smoke. Thus, such additives are not strangers to the tobacco and/or its smoke, but their addition increases the consumer acceptable flavor. Table 2.4 lists some of the tobacco and/or tobacco smoke alcohol components that have been or are used in flavor formulations.

Table 2.5 is a catalog of the alcohols identified in tobacco and/or tobacco smoke. Of the 1722 alcohols identified to date, 675 have been reported in tobacco smoke, 1360 in tobacco, and 313 in both tobacco and tobacco smoke.

2.2 PHYTOSTEROLS

The alcohol category in tobacco and tobacco smoke includes the phytosterols, the plant-derived sterols. The sterols have been examined in considerable detail over the years, an examination that did not actually originate in the study of tobacco and/or its smoke. In 1928, Kennaway and Sampson demonstrated the tumorigenicity of the pyrolysate from the sterol cholesterol (2080). Their study preceded the first reports of induction of skin cancer in laboratory animals with two individual compounds, the PAHs dibenz[*a,h*]anthracene (DB[*a,h*]A) in 1930 by Kennaway and Hieger (2078) and benzo[*a*]pyrene (B[*a*]P) in 1932 by Cook et al. (796a, 797). Both PAHs subsequently were classified as highly potent tumorigens. Based on the results of their detailed study of the tumorigenicity of several PAHs, Barry et al. (194) reported that a third PAH 3-methylcholanthrene was also a highly potent tumorigen. 3-Methylcholanthrene was subsequently named 1,2-dihydro-3-methylbenz[*j*]aceanthrylene. Because of their structural similarity, 1,2-dihydro-3-methylbenz[*j*]aceanthrylene became the object of the search in the pyrolysate from cholesterol (Figure 2.3).

Cholesterol and several similarly structured phytosterols (campesterol, β-sitosterol, stigmasterol) are components of tobacco, and a portion of each is transferred intact to smoke during the smoking process. The phytosterols in tobacco have been reported by numerous investigators, e.g., Traetta-Mosca (3942b), Kobel and Neuberg (2153a), Shmuk (3656a), Khanolkar et al. (2087), and Venkatarao et al. (4042b). All have been reported in tobacco as glycosides by Bolt and Clarke (390), Dymicky and Stedman (1079), Kallianos et al. (2018, 2019), and Khanolkar et al. (2087) and long-chained saturated and unsaturated acid esters (3296). Theoretically, all could yield 1,2-dihydrobenz[*j*]aceanthrylene and/or 1,2-dihydro-3-methylbenz[*j*]aceanthrylene during the smoking process.

To date, the identification of this PAH in tobacco smoke has been reported by only one investigator, Kröller (2191). Dihydrobenz[*j*]aceanthrylene (cholanthrene) was not among the several PAHs isomeric with 1,2-dihydrobenz[*j*]aceanthrylene reported by Snook et al. (3756–3758). In the late 1940s, there was much interest in 1,2-dihydro-3-methylbenz[*j*]aceanthrylene because of its possible generation from cholesterol during the heating of cholesterol-containing foodstuffs. While 1,2-dihydro-3-methylbenz[*j*]aceanthrylene could actually be synthesized from cholesterol by a series of sophisticated chemical

TABLE 2.4
Tobacco and/or Smoke Alcohols Used in Flavor Formulations

CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Identified in	
			Smoke	Tobacco
60-12-8	Benzeneethanol	Phenethyl alcohol	+	+
100-51-6	Benzenemethanol	Benzyl alcohol	+	+
105-13-5	Benzenemethanol, 4-methoxy-	Anisyl alcohol	–	+
98-85-1	Benzenemethanol, α-methyl-	α-Methylbenzyl alcohol	–	+
122-97-4	Benzenepropanol	3-Phenyl-1-propanol	+	+
507-70-0	Bicyclo[2.2.1]heptane-2ol,endo-1,7,7,-trimethyl-	Borneol	+	+
107-88-0	1,3-Butanediol	1,3-Butanediol	+	+
71-36-3	1-Butanol	Butyl alcohol	+	+
98-55-5	3-Cyclohexene-1-methanol, α,α,4-trimethyl-	α-Terpineol	+	+
562-74-3	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-	4-Carvomenthol	+	+
112-30-1	1-Decanol	Capric alcohol	–	+
7212-44-4	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-	Nerolidol	+	+
64-17-5	Ethanol	Ethyl alcohol	+	+
57-48-7	*D*-Fructose	Sugars	+	+
59-23-4	*D*-Galactose	Sugars	+	+
50-99-7	α-*D*-Glucose	Sugars	+	+
57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose}	Sugars	+	+
50-99-7	α-*D*-Glucose	Sugars	+	+
111-27-3	1-Hexanol	Hexyl alcohol	–	+
104-76-7	1-Hexanol, 2-ethyl-	2-Ethyl-1-hexanol	+	+
544-12-7	3-Hexen-1-ol	3-Hexen-1-ol	–	+
31103-86-3	Mannose	Sugars	+	+
78-70-6	1,6-Octadien-6-ol, 3,7-dimethyl-	Linalool	–	+
106-25-2	2,6-Octadien-1-ol, 3,7-dimethyl-	Nerol	–	+
111-87-5	1-Octanol	1-Octanol	–	+
3391-86-4	1-Octen-3-ol	1-Octen-3-ol	–	+
106-22-9	6-Octen-1-ol, 3,7-dimethyl-	*dl*-Citronellol	+	+
71-41-0	1-Pentanol	Amyl alcohol	–	+
57-55-6	1,2-Propanediol	Propylene glycol	+	+
56-81-5	1,2,3-Propanetriol	Glycerol	+	+
78-83-1	1-Propanol, 2-methyl-	Isobutyl alcohol	+	+
104-54-1	2-Propen-1-ol, 3-phenyl-	Cinnamyl alcohol	+	–
118-71-8	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-	Maltol	+	+
50-70-4	Sorbitol[a]	Glucitol	–	+

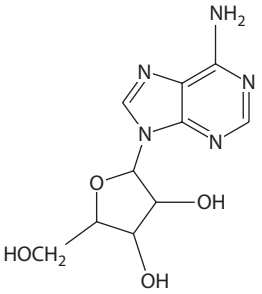
[a] Sorbitol (glucitol) is not included in the Doull et al. list (1053) but is included in flavor formulations used by cigarette manufacturers outside of the United States [see Table 7A in (3266)].

reactions (1184a), attempts to generate it by pyrolysis of cholesterol were unsuccessful.

As shown in Figure 2.4, pyrolysis of cholesterol {Ia} yields chrysene {III}, Diels hydrocarbon {IV}—a methylcyclopentaphenanthrene—and numerous other PAHs. Both PAHs noted have also been identified in pyrolysates of the major tobacco phytosterols [Wynder et al. (4356), Van Duuren (4022)]. More recently in the early 1970s, Hecht et al. (1560) discussed the generation of chrysene and alkylchrysenes by pyrolysis of phytosterols.

Although none of the sterols {Ia–Id} have been shown to generate the potent tumorigen 1,2-dihydro-3-methylbenz[*j*] aceanthrylene (3-methylcholanthrene) on pyrolysis, Falk et al. (1171) reported that cholesterol and cholesterol esters on pyrolysis do generate the mouse-skin tumorigens 4-cholesten-3-one {Va} and 3,5-cholestadiene {VIa}. Veldstra (4042a) reported that the pyrolysis of cholesteryl oleate also yielded 3,5-cholestadiene {VIa}. Cholesteryl oleate was probably a component of the mixture of phytosteryl esters described in flue-cured tobacco by Rowland and Latimer (3358). Its analogs stigmasteryl oleate and β-sitosteryl oleate were among the phytosteryl esters in tobacco smoke characterized by Rodgman et al. (3296). The other identified phytosteryl esters included stigmasterol and β-sitosterol esterified with saturated acids (lauric, palmitic, stearic, and myristic) and unsaturated acids (linolenic and linoleic) (3296).

TABLE 2.5
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	141-46-8	Acetaldehyde, hydroxy- {glycolaldehyde} $HO\text{-}CH_2\text{-}CH{=}O$	568b, 2939, 3553, 3559, 3797, 5811b	568b, 3973, 3974a, 4249, 5811b	3401, 3402, 3405
2.	4293-57-6	Acetamide *N*-(2-hydroxypropyl)- $H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CHOH\text{-}CH_3$	568b, 4249		
3.	79-14-1	Acetic acid, hydroxy- {glycolic acid} $HOCH_2\text{-}COOH$	237, 1099, 1371, 1375a, 1377, 1445, 1674, 1882, 2133, 2493, 2777, 2939, 3059, 3060, 3061, 3255, 3302, 3384, 3394, 3496, 3741, 3743, 5811b	3060, 3194, 3797, 3973, 3974a, 5811b	1375a, 1377, 3393, 3402, 3405
4.	623-50-7	Acetic acid, hydroxy-, ethyl ester $HOCH_2\text{-}COO\text{-}C_2H_5$	3255, 3553		
5.	61892-60-2	Acetic acid, hydroxy-, 2-hydroxypropyl ester $HOCH_2\text{-}COO\text{-}CH_2\text{-}CHOH\text{-}CH_3$	568b, 3553, 4249, 5811b	568b, 2389, 2544, 4249	
6.	96-35-5	Acetic acid, hydroxy-, methyl ester $HOCH_2\text{-}COO\text{-}CH_3$	3553, 3557, 5811b		
7.	1932-50-9	Acetic acid, hydroxy-, potassium salt		5811b	
8.	90357-58-7	Acetic acid, hydroxy-, propyl ester $HOCH_2\text{-}COO\text{-}C_3H_7$	3553	2389, 2544, 3550	
9.		Acetic acid, hydroxymethyl ester $CH_3\text{-}COO\text{-}CH_2OH$	2767		
10.	107-16-4	Acetonitrile, hydroxy- $HOCH_2\text{-}CN$	568b, 1371, 2543, 2773, 3410, 4249, 5770		
11.	58-61-7	Adenosine 		429b, 4249, 4828, 5540	
12.	60-92-4	Adenosine, cyclic 3′,5′-(hydrogen phosphate)		2371a, 4249, 4523	
13.	28542-78-1	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-		683a, 2371a, 4066a	
14.	6025-53-2	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*E*)-		2371a, 4249, 4582	
15.	15896-46-5	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-,(*Z*)-		2371a, 4249	
16.	26190-61-4	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-		2371a, 4249, 4778	
17.	53274-45-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*E*)-		2371a, 4249, 4778	
18.	52049-48-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*Z*)-		960a, 2371a	
19.	22663-55-4	Adenosine, *N*-(4-hydroxy-3-methylbutyl)-		2371a, 4249, 4522	
20.	7724-76-7	Adenosine, *N*-(3-methyl-2-butenyl)-		2371a, 4249, 4523	
21.	75081-82-2	Adenosine, *N*-[3-methyl-4-[(*O*-phosphono-β-*D*-glucopyranosyl)oxy]-2-butenyl]-, (*E*)-		429b, 4249, 4813	
22.	4294-16-0	Adenosine, *N*-(phenylmethyl)-		2371a	
23	56-65-5	Adenosine 5′-(tetrahydrogen triphosphate)		429b	
24.	40922-97-2	Adenosine 5′-(tetrahydrogen triphosphate), *N*-(phenylmethyl)-		2371a	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

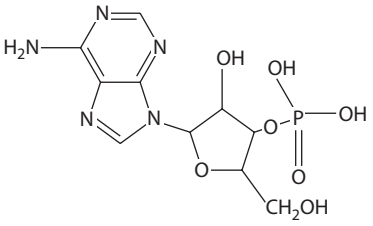
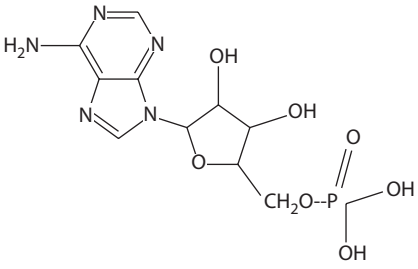
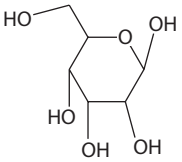
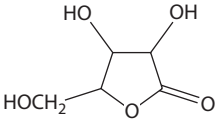
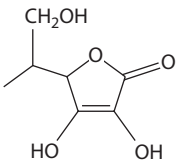
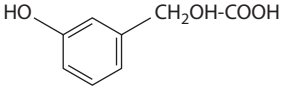
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
25.	58-64-0	Adenosine 5′-(trihydrogen diphosphate)		429b	
26.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P′*→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridine carboxamide		429b, 4249, 4708	—
27.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P′*→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofurano sylpyridinium hydroxide, inner salt		429b	—
28.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	—
29.	55030-93-8	Adenosine 5′-(trihydrogen diphosphate), *N*-(3-methyl-2-butenyl)-		429b	—
30.	22732-83-8	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester		4249, 4617	—
31.	40811-89-0	Adenosine 5′-(trihydrogen diphosphate), *N*-(phenylmethyl)-		2371a	—
32.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P′*→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	—
33.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P′*→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	—
34.	84-21-9	3′-Adenylic acid 		429b, 4249, 4758	
35.	61-19-8	5′-Adenylic acid 		429b, 4249	
36.	20268-93-3	5′-Adenylic acid, *N*-(3-methyl-2-butenyl)-		4249, 4536	
37.	13484-66-7	5′-Adenylic acid, *N*-(phenylmethyl)-		4249	
38.	79-83-4 137-08-8	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- {pantothenic acid} HO-CH_2-$C(CH_3)_2$-CHOH-CO-NH-$(CH_2)_2$-COOH		429b, 1941, 4249, 4758, 5079	
39.	16124-24-6 25127-16-6	*L*-Alanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1063–1066, 1068–1074, 1351, 2337, 3639, 3797, 3923, 4362, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

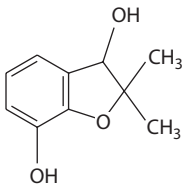
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
40.	2595-97-3	*D*-Allose 		3075	
41.	11078-27-6	Arabinan		373a, 4249	
42.	20261-96-5	Arabinohexonic acid, 3-deoxy-, γ-lactone	4249	4249	
43.	42400-32-8	*D*-Arabinohexonic acid, 2-deoxy-, γ-lactone		4249	
44.	23675-06-1	α-*D*-Arabinohexopyranoside, 2-deoxy-α-*D*-arabino-hexopyranosyl 2-deoxy-		4249, 4599	
45.	154-17-6	*D*-Arabinohexose, 2-deoxy- {also known as *D*-glucose, 2-deoxy-}		429b, 3075, 4249, 4599, 5811b	
46.	16449-30-2	*D*-Arabinohexose, 2-deoxy-4-*O*-β-*D*-glucopyranosyl-		4249, 4599	
47.	13752-83-5	Arabinonic acid $HO\text{-}CH_2\text{-}(CHOH)_3\text{-}COOH$		2362a	
48.	13280-76-7	Arabinonic acid, γ-lactone 	4249		
49.	87-72-9 5328-37-0	*L*-Arabinose $HO\text{-}CH_2\text{-}(CHOH)_3\text{-}CH{=}O$	1351, 2145, 2939, 3302, 4249, 5811	120, 158, 344a, 830a, 1263, 1351, 2070, 2270, 2338, 3059, 3075, 3797, 3973, 3974a, 4249, 5811, 5811b	
50.	147-81-9	*DL*-Arabinose	5580, 5811b	5079, 5785, 5811b	
51.	9040-27-1	Arabinoxylan		429b, 1109, 4249	
52.	7643-75-6	Arabitinol	5580		
53.		Arabitinol, 2,3-di-*O*-methyl- $HO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$		3669	
54.		Arabitinol, 2,5-di-*O*-methyl- $H_3CO\text{-}CH_2\text{-}(CHOH)_2\text{-}(CHOCH_3)\text{-}CH_3$		3669	
55.		Arabitinol, 3,5-di-*O*-methyl- $H_3CO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)\text{-}CHOH\text{-}CH_3$		3669	
56.		Arabitinol, 2,3,4-tri-*O*-methyl- $HO\text{-}CH_2\text{-}(CHOCH_3)_3\text{-}CH_3$		3669	
57.		Arabitinol, 2,3,5-tri-*O*-methyl- $H_3CO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$		3669	
58.	98530-09-7	Arabogalactan		1971, 5777	
59.	50-81-7	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-} 	3257, 3266, 3685, 4249, 4751a	120, 174b, 379, 486, 557, 1053, 1971, 2079, 2270, 2489, 2532, 2939, 3266, 3707, 3922, 4236, 4249, 5079, 5267a, 5811b	
60.	31105-02-9	*L*-Aspartic acid *N*-(1-deoxy-*D*-fructos-1-yl)-		5811	
61.	17119-15-2	Benzeneacetic acid, α,3-dihydroxy- 	3712, 3737, 3741, 3743, 4249, 5811b		

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
62.	1198-84-1	Benzeneacetic acid, α,4-dihydroxy-	3712, 3737, 3741, 3743, 4249, 5811b		
63.		Benzeneacetic acid, α,?-dihydroxy-ethyl-	4249		
64.	90-64-2	Benzeneacetic acid, α-hydroxy- {mandelic acid}		429b	
65.	96937-37-0	Benzeneacetic acid, ar,α-dihydroxy-ar-ethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
66.	51-55-8	Benzeneacetic acid, α-(hydroxymethyl)-(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (atropine}		5811, 5811b	
67.	53392-07-7	Benzenebutanol, 4-methyl-	2767, 2769, 3226, 4249		
68.	497-76-7	1,4-Benzenediol, β-*D*-glucopyranoside {arbutin}		5777	
69.	60-12-8	Benzeneethanol {phenethyl alcohol} C_6H_5-CH_2CH_2-OH	172, 568b, 1215, 1360, 1364, 1371, 1375a, 1586, 1882, 1905, 1907, 1949, 1971, 2270, 2387, 2422, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 3059, 3193, 3224, 3255, 3302, 3410, 3553, 3555, 3557, 3797, 4159, 4249, 4319, 5811b	120, 172a, 174b, 404, 543a, 568b, 937, 1053, 1063–1066, 1068–1074, 1550, 1587a, 1590a, 1949, 1980, 2282, 2283, 2338, 2339a, 2386, 2389, 2422, 2544, 2611, 2861a, 2917a, 2939, 3059, 3188, 3198, 3215, 3219, 3266, 3350, 3370, 3539, 3543, 3547, 3549, 3550, 3555, 3560, 3561, 3797, 3905, 3973, 3974a, 4098a, 4249, 5811b	1360, 1375a, 2387
70.	5040-23-3	Benzeneethanol, α,4-dimethyl-	4249		
71.	7779-78-4	Benzeneethanol, α-(2-methylpropyl)-		1053, 3266	
72.	13398-94-2	Benzeneethanol, 3-hydroxy-	596, 2601a, 3712, 4249	1587a, 2338, 4249	
73.	501-94-0	Benzeneethanol, 4-hydroxy-	596, 1365, 1561, 1884, 3712, 4249	1561, 4249	
74.	2380-78-1	Benzeneethanol, 4-hydroxy-3-methoxy-	596, 3712, 4249, 4897	5811b	
75.	699-02-5	Benzeneethanol, 4-methyl-		937, 4249	
76.	100-51-6	Benzenemethanol {benzyl alcohol} C_6H_5-CH_2OH	155, 172, 568b, 1360, 1371, 1375a, 1426, 1427, 1586, 1882, 1884, 1905, 1907, 2079, 2270, 2387, 2506, 2507, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3059, 3255, 3266, 3302, 3410, 3553, 3555, 3557, 3648, 3794, 3797, 3812, 4159, 4202, 4249, 4319, 4570a, 5079, 5811b	120, 404, 568b, 1053, 1063–1066, 1068–1074, 1550, 1587a, 1590a, 2282, 2283, 2338, 2339a, 2386, 2389, 2544, 2611, 2861a, 2917a, 2939, 3059, 3186, 3188, 3193, 3198, 3215, 3219, 3266, 3350, 3539, 3543, 3547, 3550, 3555, 3560, 3561, 3648, 3797, 3905, 3973, 3974a, 4073b, 4098a, 4202, 4249, 5079, 5811b	1360, 1375a, 2387, 2506, 2507

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
77.	1197-01-9	Benzenemethanol, α,α,4-trimethyl- {*p*,α,α- trimethylbenzyl alcohol} C_6H_5-$C(CH_3)_2OH$	568b, 2570, 4249	568b, 1053, 1156, 2389, 2544, 3266, 4090, 4249, 5811b	
78.	617-94-7	Benzenemethanol, α,α-dimethyl-	2506, 2507	404, 642, 4249	2506, 2507
79.	536-50-5	Benzenemethanol, α,4-dimethyl-		937, 1053, 1156, 2389, 3266, 4090	
80.	4393-06-0	Benzenemethanol, α-ethenyl- C_6H_5-$CH(CH{=}CH_2)OH$	3547, 4249		
81.	93-54-9	Benzenemethanol, α-ethyl- {1-phenyl-1-propanol} C_6H_5-$CH(C_2H_5)OH$		568b, 1053, 3266, 4249	
82.	5349-60-0	Benzenemethanol, α-ethyl-4-methoxy- {1-(4-methoxyphenyl)-1-propanol}		568b, 4249	
83.	98-85-1	Benzenemethanol, α-methyl- C_6H_5-$CH(CH_3)OH$	568b, 2387, 3266, 5811b	568b, 967, 1053, 2283, 2386, 2389, 2544, 3266, 3547, 4249, 5811b	2387
84.	93-03-8	Benzenemethanol, 3,4-dimethoxy-		568b, 4249	
85.	13651-14-4	Benzenemethanol, 2,3-dimethyl-	642, 4249		
86.	89-95-2	Benzenemethanol, 2-methyl-	2768	404, 4249	
87.	620-24-6	Benzenemethanol, 3-hydroxy-	1561, 3712	1561	
88.	623-05-2	Benzenemethanol, 4-hydroxy-	568b, 4249	568b, 4249	
89.	498-00-0	Benzenemethanol, 4-hydroxy-3-methoxy-	568b, 4249, 5811a	5811a	
90.	105-13-5	Benzenemethanol, 4-methoxy- {anisyl alcohol}		172a, 174b, 568b, 1053, 3266, 3370, 3893, 4249	
91.	589-18-4	Benzenemethanol, 4-methyl-	4249, 4504	404	
92.	6282-37-7	Benzenemethanol, 4-methyl-α-propyl-	2767, 4249		
93.	1331-81-3	Benzenemethanol, ar-methoxy-		1217	
94.	27043-34-1	Benzenemethanol, methyl-	642, 4249		
95.	156-05-8	Benzenepropanoic acid, α-hydroxy- {phenyllactic acid} C_6H_5-CH_2-CH_2OH-COOH		120, 2270, 2722, 3532, 3973, 3974a	
96.	7326-19-4	Benzenepropanoic acid, α-hydroxy-, (R)-		3560, 3561	
97.	24696-05-7	Benzenepropanoicacid, 2-(β-*D*-glucopyranosyloxy)-		4249	
98.	122-97-4	Benzenepropanol {3-phenyl-1-propanol} C_6H_5-CH_2-CH_2-CH_2OH	1367, 3266, 4249	172a, 174b, 1053, 3266, 4249	
99.	1992-50-3	Benzenepropanol, α-ethyl- C_6H_5-CH_2-CH_2-$CH(C_2H_5)OH$	2767, 4249		
100.	2845-25-2	Benzenepropanol, γ-ethyl-, (S)- C_6H_5-$CH(C_2H_5)$-CH_2-CH_2OH	2767, 3226, 4249		
101.	10210-17-0	Benzenepropanol, 4-hydroxy-	596, 3712, 4249		
102.	17781-15-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl- 		5811, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

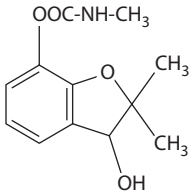
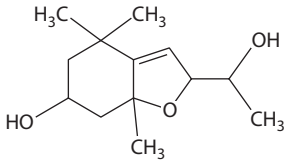
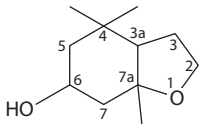
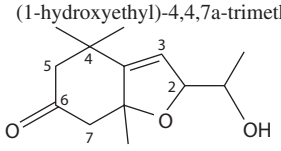
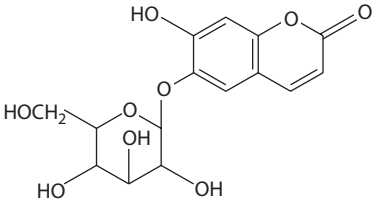
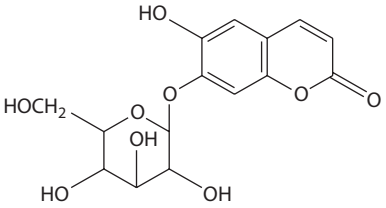
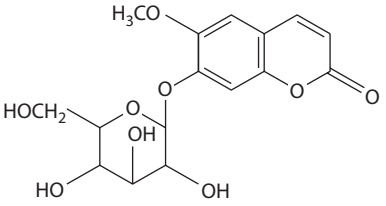
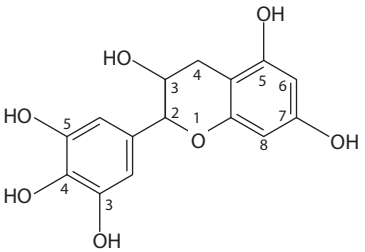
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
103.	16655-82-6	3,7-Benzofurandiol, 2,3-dihydro-2, 2-dimethyl-, 7-(methylcarbamate) {3-Hydroxycarbofuran®} 	1553, 21A19	1280, 1553, 3481, 5811b, 21A19	
104.	73051-72-6	2-Benzofuranmethanol, 2,4,5,6,7,7a-hexahydro-6-hydroxy-α,4,4,7a-tetramethyl-		234, 4249	
105.		2-Benzofuranmethanol, 2,4,5, 7a-tetrahydro-4,4,7a-trimethyl-		3547, 4249	
106.		6-Benzofuranol, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl- 		234, 1156, 3991, 4090	
107.	39815-67-3	6-Benzofuranol, octahydro-4,4,7a-trimethyl- 		943, 1149, 1149a, 1254, 1256, 3205, 3210, 3218, 3219, 3550, 4249, 4780, 5811b	
108.	61892-48-6	2(3*H*)-Benzofuranone,hexahydro-3a-hydroxy-	3553, 4249		
109.	54911-63-6	2 (3*H*)-Benzofuranone, hexahydro-4-hydroxy-	568b, 4249		
110.	82395-89-9	2(4*H*)-Benzofuranone, 6-(β-*D*-glucopyranosyloxy)-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-		234, 4249, 4714	
111.	1133-03-5	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-		5811b	
112.	10481-90-0	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, *Z*-(±)- {loliolide}	1587, 4249	2389, 2544, 2780, 3218, 4249	
113.	5989-02-6	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7, 7a-tetrahydro-4,4,7a-trimethyl-, (6S- *Z*)-		4249, 4573	
114.	117769-21-8	5(4*H*)-Benzofuranone, 2,7a-dihydro-2-(1-hydroxyethyl)-4,4-dimethyl-		4249, 5811b	
115.	70875-03-5	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl- 		234, 1156, 1254, 1256 3206, 3210, 3218, 3549, 3991, 4090, 4249, 5811b	
116.	10366-91-3	Benzoic acid, 2-(β-*D*-glucopyranosyloxy)-		4249, 5811b	
117.	612-20-4	Benzoic acid, 2-(hydroxymethyl)-	4249		
118.	32142-31-7	Benzoicacid, 4-(β-*D*-glucopyranosyloxy)-3-methoxy-		429b, 4249, 4915	
119.	124052-01-3	2*H*-1-Benzopyran-3,4-dione, 2-(3,4-dihydroxyphenyl)-2,5,7-trihydroxy-		4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
120.	74712-71-3	2*H*-1-Benzopyran-2-one, 7-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-6-methoxy-		4249	
121.	60091-00-1	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-		3797, 4249	
122.	531-75-9	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin} 	3257	1309, 2939, 2954, 3103, 3973, 3974a, 4249, 5711, 5811b	
123.	531-58-8	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin} 		1309, 1626, 3797, 4249, 5811b, 5838	
124.	531-44-2	2*H*-1-Benzopyran-2-one,7-(β-*D*-glucopyranosyloxy)-6-methoxy- {scopolin} 		72, 120, 677b, 830a, 831, 834, 835, 840, 890, 966, 1102, 1309, 1626, 1863, 2338, 2395, 2557a, 2911c, 2954, 3194, 3629, 3631, 3646, 3738, 3797, 3973, 3974a, 3974b, 4156, 4249, 4269, 5649, 5650, 5809, 5811b, 5831	
125.	71050-53-8	2*H*-1-Benzopyran-2-one, 6-methoxy-7-(β-*D*-xylofuranosyloxy)- {scopoletin glucoside}		2939, 3797, 4249, 5650, 5808, 5809, 5830, 5842, 5888	
126.	18309-73-4	2*H*-1-Benzopyran-2-one, 6-methoxy-7-[(6-*O*-β-*D*-xylopyranosyl-β-*D*-glucopyranosyl)oxy]-		1863a, 2939, 4249, 5811b	
127.	970-73-0	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*E*)- 		429b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

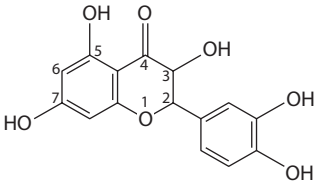
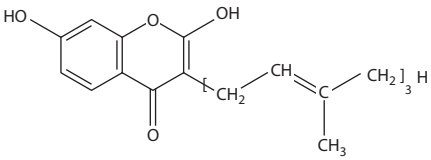
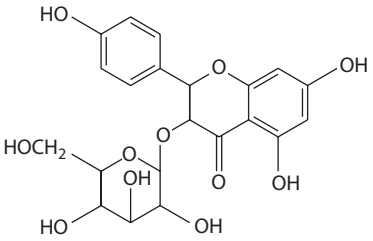
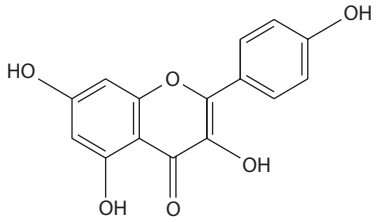
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
128.	970-74-1	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*Z*)-		429b, 4249	
129.	17912-87-7	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricitrin}		5811, 5811b	
130.	124052-00-2	4*H*-1-Benzopyran-4-one,2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,3,5,7-tetrahydroxy-		4249	
131.	21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		120, 1626, 1837a, 1971, 2023, 2270, 2939, 3059, 3194, 3555, 3667, 3794, 3797, 3973, 3974a, 4249, 5079, 5255, 5256, 5724, 5747, 5811b, 5888	
132.	117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin, 3,3a,4a,5,7-pentahydroxyflavone} 	3096, 3555	72, 120, 970, 1077b, 1837a, 2270, 2379, 2704a, 2939, 3059, 3462, 3555, 3685, 3794, 3797, 3974a, 4036, 4403, 4999, 5079, 5255, 5641, 5652, 5750, 5758, 5811b, 5904	
133.	7215-44-3 20188-84-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-O-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy- {quercetin 3,3′-diglucoside}		4249, 5811, 5811b	
134.	491-50-9	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}		3797, 3974a, 4249	
135.	124051-99-6	4*H*-1-Benzopyran-4-one,2-(3,4-dihydroxyphenyl)-7-[[2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,6-dihydroxy-3-oxo-4-benzofuranyl]oxy]- 2, 3-dihydro-3,5-dihydroxy-		4249	
136.	643-57-2	4*H*-1-Benzopyran-4-one, 2,7-dihydroxy-3-(3,7,11-trimethyldodeca-2,6,10-trienyl- {ammoresinol} 		3763, 5079	
137.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3,4-dihydroxyphenyl)- {3a,4a, 5,7-tetrahydroxy-3-methylflavone}		4147, 5776, 5888	
138.		4*H*-1-Benzopyran-4-one,5,7-dihydroxy-3-methyl-2-(3-methyl-4-hydroxyphenyl)- {4a,5,7-trihydroxy-3,3a-dimethylflavone}		4147, 5888	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
139.		4*H*-1-Benzopyran-4-one, 3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)-{3a,4a,5-trihydroxy-3,5-dimethylflavone}		5776	
140.	480-10-4	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glucoside; 3,4a,5,7-tetrahydroxy flavone glucoside} 		120, 641, 830a, 835, 838, 840, 966, 970, 1626, 1971, 2023, 2270, 2939, 3059, 3161, 3555, 3646, 3738, 3797, 3974a, 4072a, 4249, 5079, 5724, 5753, 5758	
141.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(3,4-dihydroxyphenyl)-{3a,4a,5,7-tetrahydroxyflavone, 3-glucoside}		1625, 4147, 5353, 5724, 5834, 5888	
142.	520-18-3	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(4-hydroxyphenyl)-{kaempferol; 3,4a,5,7-tetrahydroxyflavone} 	2767, 3095a, 3555, 4249	1626, 1971, 2939, 3059, 3555, 3794, 4249, 5652, 5758, 5811b	
143.	529-44-2	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricetin}		5811, 5811b	
144.	55136-76-0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
145.	142235-82-3	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2090b	
146.	19895-95-5	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	
147.	522-12-3	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {quercetrin}	970	4036, 4249, 4573	
148.	55696-57-6	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-		4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

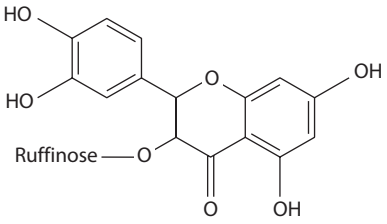
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
149.	55804-74-5	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
150.	153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-{rutin} 		69, 72, 120, 248, 385, 598, 828b, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1063–1066, 1068–1074, 1309, 1329, 1333, 1485, 1626, 1971, 2014, 2079, 2153a, 2270, 2313a, 2338, 2361, 2379, 2395, 2514, 2529, 2531, 2557a, 2704a, 2810–2812, 2939, 3059, 3096, 3161, 3367a, 3400, 3462, 3551, 3555, 3628, 3629, 3631, 3641, 3646, 3700, 3705, 3738, 3767, 3794, 3974a, 3974b, 3984, 3999, 4005–4007, 4036, 4156, 4157, 4249, 4403, 4999, 5079, 5110, 5156, 5157, 5189, 5204, 5217, 5304, 5305, 5310, 5576, 5591, 5596, 5641, 5652, 5661, 5681, 5697, 5698, 5724, 5747, 5750, 5780, 5788, 5808, 5809, 5811b, 5831, 5834, 5888, 5889	
151.	17650-84-9	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		1309, 4249, 5811b	
152.	30311-61-6	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-{rutin-7-glucoside}		2023, 4147, 5777, 5811b, 5888	
153.	34336-18-0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
154.	29859-91-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
155.	27554-19-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxy phenyl)-		1309, 4249	
156.	58934-57-9	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
157.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-glucoside}		4147, 5888	
158.		4*H*-1-Benzopyran-4-one, 7-(β-*D*-rhamnoglucopyranosyloxy)-3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone, 7-rhamnoglucoside}		4147, 5888	
159.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-rhamnoglucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxy-flavone, 3-rhamnoglucoside}		3095a, 4372, 5888	
160.	10236-47-2	4*H*-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}		970, 1305b, 3797, 3974a, 4249	
161.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,5′,7-pentahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2023, 4249	
162.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,7-tetrahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		4249	
163.	528-58-5	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride		4249, 4681	
164.	22688-80-8	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride		4249, 4681, 4710	
165.	528-53-0	1-Benzopyrylium, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-, chloride		2855a	
166.	18719-76-1	1-Benzopyrylium, 3-[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-, chloride		928b, 4249, 4710	
167.	33978-17-5	1-Benzopyrylium, 3-[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride		4249, 4681	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

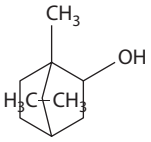
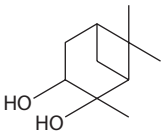
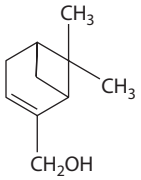
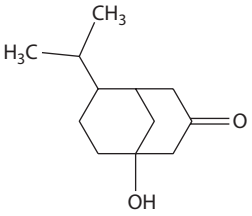
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
168.	27548-56-7	3-Benzoxepin-7-methanol, 5a,6,7,8,9, 9a-hexahydro-α,α,5,9a-tetramethyl-, (5aα,7α,9aα)-(−)-		4249, 5811b	
169.	509-11-5	Bicyclo[2.2.1]heptan-2-ol, 1,7-dimethyl-, (*exo,anti*)-		4249	
170.	124-76-5	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *exo*-		568b, 4249	
171.	464-45-9 507-70-0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *endo*- {borneol} 	568b, 1971, 3266, 3302, 4249, 4319	120, 568b, 909, 1053, 1156, 1971, 2270, 2939, 3266, 3374, 3797, 3971, 3974a, 4090, 4249, 5079, 5811b	
172.	22422-24-0	Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl- {2,3-pinanediol} 		2917a	
173.	515-00-4 36203-31-3	Bicyclo[3.1.1]hept-2-ene-2-methanol,6,6-dimethyl- 		1156, 1248, 2389, 2544, 4090, 4249	
174.	471-16-9	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, [1S-(1α,3β,5α)]- {sabinol}		131, 3555, 4249	
175.	124749-69-5	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy-6-(1-methylethyl)-, *endo*- 	4249		
176.	123695-64-7	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy-6-(1-methylethyl)-, *exo*-	4249		
177.		2,3′-Bipyridine, 6-hydroxy-3,4,5,6-tetrahydro-	568b, 4249		
178.	34764-22-2	Butanal, 3,4-dihydroxy- $HOCH_2$-CHOH-CH_2-CH═O	3553, 4249		
179.	107-89-1	Butanal, 3-hydroxy- {aldol} H_3C-CHOH-CH_2-CH═O	568b, 2170, 2702, 2939, 3302, 3876, 4249, 5079		
180.		Butanal, 3-hydroxy-2-oxo- {methylreductone} H_3C-CHOH-CO-CH═O		3797	
181.	25714-71-0	Butanal, 4-hydroxy- HO-$(CH_2)_3$-CH═O	3553, 4249		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
182.		Butanal, 4-(2-hydroxyethoxy)- $HO\text{-}CH_2CH_2\text{-}O\text{-}(CH_2)_3\text{-}CH{=}O$	3553, 4249		
183.	1758-51-6	Butanal, 2,3,4-trihydroxy-, (R*,R*)- {erythrose} $HOCH_2\text{-}(CHOH)_2\text{-}CH{=}O$		3797, 4249	
184.		Butanedioate, hydroxy- {malate}	2931	3160	
185.	6915-15-7	Butanedioic acid, hydroxy- {malic acid} $HOOC\text{-}CHOH\text{-}CH_2\text{-}COOH$	565, 1371, 2939, 3059, 3061, 3224, 3266, 3302, 3308, 3496, 3555, 3741, 3743, 4249, 5811b	120, 172a, 256, 385, 543a, 555, 634, 677b, 722, 826a, 835, 836, 838–840, 963, 1053, 1063–1066, 1068–1074, 1279, 1289, 1305a, 1330, 1332, 1333, 1548 1923, 1933a, 1982, 2014, 2079, 2154, 2270, 2283, 2356, 2529, 2532, 2543, 2545, 2688, 2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3052, 3107, 3194, 3266, 3353, 3476, 3486, 3555, 3655b, 3656, 3667, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 3974b, 3976, 3984, 4103, 4131, 4249, 4275, 5079, 5109, 5126, 5189, 5244, 5342, 5381, 5384, 5389, 5419, 5430, 5477, 5478, 5745, 5749, 5753, 5811b, 5832, 5896, 17B17	3393
186.		Butanedioic acid, hydroxy-, labeled with ^{14}C {malic acid}-^{14}C	2763	2763	
187.	16426-50-9	Butanedioic acid, hydroxy-, calcium salt		5079, 5189, 5342	
188.	1587-15-1	Butanedioic acid, hydroxy-, dimethyl ester {dimethyl malate; malic acid dimethyl ester} $H_3C\text{-}OOC\text{-}CHOH\text{-}CH_2\text{-}COO\text{-}CH_3$	568b, 2570, 3553, 4249, 5811b		
189.	585-09-1	Butanedioic acid, hydroxy-, dipotassium salt $KOOC\text{-}CHOH\text{-}CH_2\text{-}COOK$		4249, 4560, 5079, 5189, 5342	
190.	676-46-0	Butanedioic acid, hydroxy-, disodium salt $NaOOC\text{-}CHOH\text{-}CH_2\text{-}COONa$		5811b	
191.	869-06-7	Butanedioic acid, hydroxy-, magnesium salt		5079, 5189, 5342	
192.	71608-04-3	Butanedioic acid, (hydroxymethylene)-	1871a, 4249		
193.	3237-44-3	Butanedioic acid, 2-hydroxy-2-(1-methylethyl)-		1259, 2722, 4249	
194.	526-83-0	Butanedioic acid, 2,3-dihydroxy- {tartaric acid} $HOOC\text{-}CHOH\text{-}CHOH\text{-}COOH$	1268, 1270, 3266, 3555, 4249	1268, 1270, 1982, 3266, 3555, 4249, 5529, 5764	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

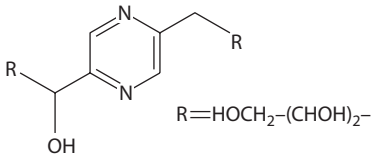
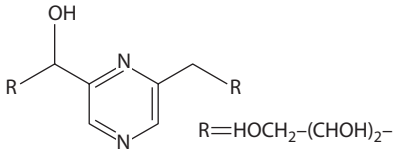
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
195.	147-71-7	Butanedioic acid, 2,3-dihydroxy- {*d*-tartaric acid}		172a, 1053, 3266	
196.	87-69-4	Butanedioic acid, 2,3-dihydroxy- {*l*-tartaric acid}		174c, 1053, 3266, 5811b	
197.	133-37-9	Butanedioic acid, 2,3-dihydroxy- {*dl*-tartaric acid}		1053, 3266	
198.	147-73-9	Butanedioic acid, 2,3-dihydroxy- {*meso*-tartaric acid}		1053, 3266	
199.	921-53-9	Butanedioic acid, 2,3-dihydroxy- [R-(R*,R*)]-, dipotassium salt		2517a, 4249, 4560	
200.	52642-07-6	Butanediol, monoacetate	2767, 3553, 4249, 5811b		
201.	107-88-0	1,3-Butanediol {1,3-butylene glycol} H_3C-CHOH-CH_2-CH_2OH	568b, 627, 2246, 2548, 2549, 2790, 3266, 3302, 3308, 3553, 3689, 4249	568b, 627, 1053, 2188, 2195, 2196, 3264, 3266, 4249, 5811b	
202.	110-63-4	1,4-Butanediol {tetramethylene glycol} $HOCH_2$-$(CH_2)_2$-CH_2OH		2788, 4249	
203.	513-85-9	2,3-Butanediol H_3C-CHOH-CHOH-CH_3	568b, 1365, 1375, 1375b, 1586, 2543, 2767, 2769, 2773, 3553, 3555, 3557, 3559, 4249, 5811b	404, 568b, 2389, 2544, 3549, 3555, 4249, 5811b	
204.	5341-95-7	2,3-Butanediol, (R*,S*)-	2767		
205.	6982-25-8	*DL*-2,3-Butanediol	5811, 5811a, 5811b		
206.	4476-02-2	Butanenitrile, 2-hydroxy- H_3C-CH_2-CHOH-CN	172, 1067, 1364, 1365, 1371, 2545, 2773, 3553		
207.	15344-34-0	Butanenitrile, 2-hydroxy-3-methyl- $(H_3C)_2$=CH-CHOH-CN	172, 1067, 1075		
208.	149-32-6	1,2,3,4-Butanetetrol, (R*,S*)- {erythritol}	2321, 3302, 5580, 5811b	3797, 4249	
209.	68510-02-1	1,2,3,4-Butanetetrol, 1-[5-(2,3,4-trihydroxybutyl) pyrazinyl]- {2,5-deoxyfructosazine} 		480, 1361, 1587a, 2339b, 2420, 2421, 2423, 2424, 4249, 4422, 4747, 5540, 17B57	
210.	68510-03-2	1,2,3,4-Butanetetrol, 1-[6-(2,3, 4-trihydroxybutyl) pyrazinyl]- {2,6-deoxyfructosazine} 		480, 1361, 1587a, 2339b, 2420, 2421, 2423, 2424, 4249, 4422, 4747, 5540, 17B57	
211.	4435-50-1	1,2,3-Butanetriol {1-methylglycerol} H_3C-CHOH-CHOH-CH_2OH	568b, 3553, 4249, 5811b		
212.	3068-00-6	1,2,4-Butanetriol H_2COH-CHOH-CH_2-CH_2OH		4249	
213.	7004-04-8	Butanoic acid, 2-amino-3-hydroxy- H_3C-CHOH-CH(NH_2)-COOH	429b	429b, 4249	
214.	1927-25-9	Butanoic acid, 2-amino-4-hydroxy-		5777, 5905	
215.	565-70-8	Butanoic acid, 2-hydroxy- H_3C-CH_2-CHOH-COOH	568b, 1882, 3553, 4249, 4677, 5811b	568b, 1886, 2336, 2337a, 3553, 4249	3393
216.	3739-30-8	Butanoic acid, 2-hydroxy-2-methyl- H_3C-CH_2 -C(CH_3)(OH)-COOH		1948, 4249	
217.	4026-18-0	Butanoic acid, 2-hydroxy-3-methyl- H_3C-CH(CH_3)-CHOH-COOH	1260	1085, 1260, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
218.	300-85-6	Butanoic acid, 3-hydroxy- H_3C-CHOH-CH_2-COOH	3394, 5811b		3393
219.	625-08-1	Butanoic acid, 3-hydroxy-3-methyl- H_3C-C(CH_3)(OH)-CH_2-COOH	5811b	1948, 4249	
220.	71-36-3	1-Butanol {*n*-butyl alcohol} H_3C-(CH_2)$_2$-CH_2OH	172, 568b, 1140, 1218, 1373, 1375a, 1377, 1378, 1416, 2559, 2559a, 3255, 3257, 3265, 3266, 3302, 3559, 3797, 4249, 5811b	568b, 1053, 1550, 2339a, 3186, 3188, 3266, 3328, 3905, 3973, 4249	1375a, 1377, 1378
221.	20281-85-0	1-Butanol, 2,3-dimethyl-		2339a	
222.		1-Butanol, 2-ethoxy-		2339a	
223.	97-95-0	1-Butanol, 2-ethyl-	568b, 4249	568b, 4249	
224.	91599-03-0	1-Butanol, 4-[(7-β-*D*-glucopyranosyl-7*H*-purin-6-yl)amino]-2-methyl-		4249	
225.	137-32-6	1-Butanol, 2-methyl-	568b, 1589, 2543, 2761, 2765, 2777, 4249	568b, 937, 2339a, 3547, 4249, 5811b	
226.	23599-75-9	1-Butanol, 2-methyl-4-(1*H*-purin-6-ylamino)- {dihydrozeatin}	2777	4249, 5811, 5811b	
227.	123-51-3	1-Butanol, 3-methyl- {isoamyl alcohol}	568b, 1589, 2761, 2765, 3559, 4249, 5811b	404, 568b, 1587a, 1590a, 2282, 2339a, 2917a, 3186, 3188, 3905, 4249, 5811b	
228.	78-92-2 15892-23-6	2-Butanol {*sec*-butyl alcohol} H_3C-CH_2-CHOH-CH_3	568b, 1140, 1416, 2559, 2559a, 3302, 3797, 4249, 5811b	568b, 984, 4249	
229.	6291-17-4	2-Butanol, 3-amino-2-methyl-	1375, 1375b, 3557		
230.	155728-85-1	2-Butanol, 1-(4-bromophenoxy)-3-[(phenylmethyl)amino]-, (R*,R*)-		4249	
231.	75-85-4	2-Butanol, 2-methyl-	568b, 3559, 4249		
232.	598-75-4	2-Butanol, 3-methyl-	568b, 4249		
233.	3293-47-8	2-Butanol,4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-		2917a	
234.	35734-62-4	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-	1364	2032, 4249, 5811b	
235.	51769-21-2	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (±)-		4249, 4495	
236.	59578-62-0	1-Butanone, 4-hydroxy-1-(3-pyridinyl)-	5087, 5508	4249, 5508	
237.		1-Butanone, 4-(methylamino)-1-(2,6-dihydroxy-3-pyridinyl)-		1101, 4249	
238.		1-Butanone,4-(methylamino)-1-(6-hydroxy-pyridinyl)-		1101, 4249	
239.	5077-67-8	2-Butanone, 1-hydroxy- H_3C-CH_2-CO-CH_2OH	568b, 1063–1066, 1068–1074, 1215, 2777, 4249, 5811b	568b, 2386, 3555, 4249, 5811b	3401, 3402, 3404, 3405
240.	38895-88-4	2-Butanone, 3,3-dimethyl-4-hydroxy-	568b, 4249		
241.	57011-15-1	2-Butanone, 3,4-dihydroxy- H_3C-CO-CHOH-CH_2OH	3553, 4249, 5811b		
242.	513-86-0	2-Butanone, 3-hydroxy- {acetoin} H_3C-CO-CHOH-CH_3	568b, 1063–1066, 1068–1074, 1426, 1427, 1882, 2337, 2761, 2762, 2765, 2766, 2777, 3266, 3410, 3555, 3559, 4249, 5811b	174b, 404, 568b, 1053, 2339a, 2339b, 2386, 2917a, 3266, 3549, 4249, 5811b	2244, 3401, 3402, 3404
243.	590-90-9	2-Butanone, 4-hydroxy- H_3C-CO-CH_2-CH_2OH	568b, 3553, 3555, 4249, 5811b	404, 568b, 4249, 5811b	
244.	1823-90-1	2-Butanone, 4-hydroxy-3,3-dimethyl- H_3C-CO-C(CH_3)$_2$-CH_2OH	3553, 4249, 5811b		

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

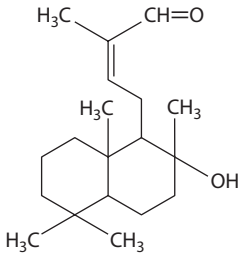
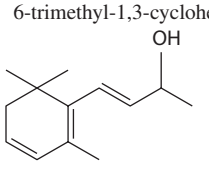
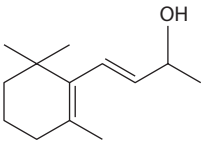
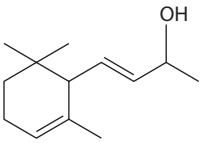
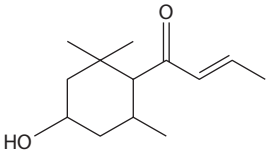
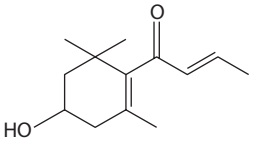
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
245.	158815-72-6	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-,(*E*)-		4249, 5811b	
246.	158815-73-7	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-,(*Z*)-		4249, 5811b	
247.	160115-51-5	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-,(*E*)-(+)-		4249	
248.	160115-52-6	2-Butanone, 4-[3,6-dihydro-6- hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-,(*Z*)-(−)-		4249	
249.	83841-47-8	2-Butenal, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-2-methyl-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		4249, 4950, 5811b	
250.	6923-22-4	2-Butenamide, 3-hydroxy-*N*-methyl-, dimethylphosphate, (*Z*)-{Monocrotophos®}		5811, 5811b	
251.	497-06-3	3-Butene-1,2-diol $HOCH_2$-CHOH-CH═CH_2	568b, 3553, 3559, 4249, 5811b		
252.	43000-45-9	1-Buten-1-ol, 3-methyl-	1387, 2775, 4249	1157	
253.	4675-87-0	2-Buten-1-ol, 2-methyl-		3547, 4249	
254.	556-82-1	2-Buten-1-ol, 3-methyl-		404, 1157, 2339a, 3547, 4249	
255.	1637-39-4	2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylamino)-, (*E*)-		2241a, 4249, 4514, 5811b	
256.		2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylaminoribosyl)-		4249, 4514	
257.	29736-33-2	2-Buten-1-ol, 2-methyl-4-[[2-(methylthio)-1*H*-purin-6-yl]amino]-, (*E*)-		4249, 4703	
258.	72074-11-4	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2-yl)-, [2S- [2α(*E*),3aα,5aβ,9aα,9bβ]]-		4249	
259.	87584-34-7	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetra methylnaphtho[2,1-*b*]furan-2-yl)-, [2R-[2α(*E*),3aβ,5aα,9aβ,9bα]]-		4249, 5811b	
260.	627-27-0	3-Buten-1-ol H_2C═CH-CH_2-CH_2OH	568b, 1360, 1375a, 4249		1360, 1375a
261.	115-18-4	3-Buten-2-ol, 2-methyl- H_2C═CH-CHOH═$(CH_3)_2$	2559, 2559a	2339a	
262.	1504-55-8	3-Buten-2-ol, 4-phenyl- C_6H_5-CH═CH-CHOH-CH_3		1053, 3266	
263.	13215-89-9	3-Buten-2-ol, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- 		1252, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
264.	33759-63-6	3-Buten-2-ol, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {3-hydroxy-β-ionol}	1364	1156, 1251, 4090	
265.	27185-80-4	3-Buten-2-ol, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-ionol}		1254, 1256, 2338, 3549	
266.	27008-60-2 22029-76-1	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- {β-ionol} 		568b, 1156, 2336, 2339b, 2389, 2544, 2917a, 3218, 3760a, 4090, 4249, 5811b	
267.	472-80-0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3*E*)- {β-ionol, (*E*)}		5811, 5811b	
268.	472-78-6 25312-34-9	3-Buten-2-ol, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-ionol} 		4249	
269.	79925-80-7	3-Buten-2-ol, 4-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)-		2138, 3547, 4249, 4780	
270.	102488-09-5	2-Buten-1-one, 1-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {3-hydroxy-β-damascone}	568b, 2601a, 4249	568b, 2338, 2917a, 4098a, 4249, 4495, 5811b	
271.	53398-17-7	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethycyclohexanyl)- {4-hydroxydihydro-β-damascone} 		233, 2032, 5811, 5811b	
272.	56915-02-7	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-damascone} 	568b, 1063–1066, 1068–1074, 1360, 1361, 1365, 1371, 1375, 1375a, 1375b, 2543, 2545, 2761, 2762, 2767, 3410, 3553, 3557, 4249, 5811b	404, 568b, 1063–1066, 1068–1074, 1156, 1254, 1256, 1587a, 1590a, 2032, 2338, 2339a, 2339b, 2386, 2389, 2544, 3218, 3543, 3546, 3549, 3550, 3560, 3561, 4090, 4159, 4249, 5811b	1360, 1375a
273.	35734-61-3	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-	2765, 2766, 2773, 2775	404, 5811b	
274.	160550-79-8	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, [R-(*E*)]-		4249	
275.	62512-25-8	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-		4249, 4715	
276.	160550-77-6	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		4249, 4715	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

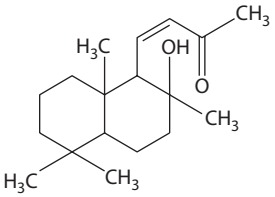
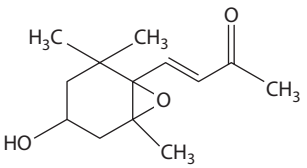
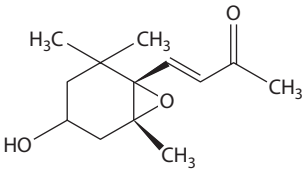
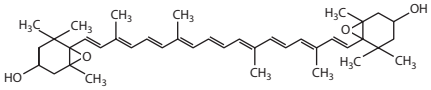
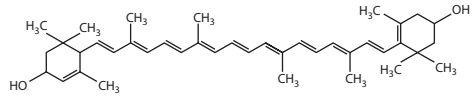
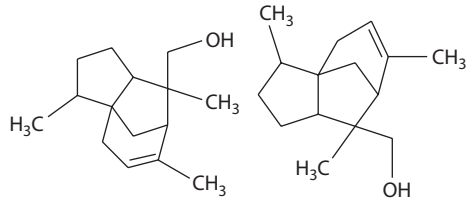
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
277.	52811-61-7	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-	5811, 5811a, 5811b		
278.	42569-64-2	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		5, 1151, 1156, 1248, 3561, 4090, 4249, 4780, 5811b	
279.	54656-80-3	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1α(*E*),2α,4aβ,8aα]-(±)-		1151, 1156, 3561, 4090, 4249	
280.	36340-49-5	3-Buten-2-one, 4-(1,2-epoxy-2,6,6-trimethyl-cyclohexyl)-, (*E*)-		5811, 5811b	
281.	15356-75-9	3-Buten-2-one, 4(1-hydroxy-2,2-dimethyl-6-methylenecyclohexyl)-		568b, 4249, 5811, 5811b	
282.	15356-76-0	3-Buten-2-one, 4-(1-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)-		5811, 5811b	
283.	15401-34-0	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-		5811, 5811b	
284.	14398-34-6	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-		909, 1249, 1256, 4249	
285.	61892-82-8	3-Buten-2-one,4-(4-hydroxy-1-cyclohexen-1-yl)-	568b, 2767, 3553, 4249, 5811b		
286.	31253-95-9	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)		5811, 5811b	
287.	50281-42-0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1S-[1α(*E*),4α,6α]]- 		1, 1156, 3547, 4090, 4249, 4780, 5811b	
288.	61116-99-2	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1R-[1α(*E*),4β,6α]]- 		1, 1156, 2338, 4090	
289.	72491-46-4	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-ionone}		1156, 1249, 1254, 1256, 2386, 4090, 5811b	
290.	38963-41-6	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)- {4-hydroxy-α-ionone}	2767, 2769, 4249		
291.	9064-51-1 54724-00-4	Callose {1,3-β-*D*-glucan}		1102, 3075, 4249, 4907, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
292.	14660-91-4	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R, 5′R,6R,6′S,9′-*cis*)- {neoxanthin}		943, 2338, 2339a, 3973, 5811b	
293.	30743-41-0	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S)-		943, 2338, 2339a, 2939, 3973, 4249	
294.	29472-68-2	β,β-Carotene-3,3′-diol {zeaxanthin}	3971, 3972	585, 830a, 971, 972, 1156, 2939, 3059, 3194, 3218, 3797, 3971, 3973, 3974a, 4090, 4249	
295.	144-68-3	β,β-Carotene-3,3′-diol, (3R,3′R)- {zeaxanthin}		830a, 1156, 3194, 3218, 3973, 4090	
296.	126-29-4	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R, 5′R,6S,6′S)- {violaxanthin} 		543a, 585, 830a, 832, 835, 838, 943, 971, 972, 1156, 2338, 2339b, 2939, 3194, 3218, 3797, 3973, 3974a, 4090, 5811b	
297.	26927-07-01	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S,9-*cis*)-		429c	
298.	68831-78-7	β,β-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,9-*cis*)-		429c, 5811b	
299.	472-70-8	β,β-Caroten-3-ol, (3R)- {cryptoxanthin}		971, 972, 1156, 3194, 3218, 3797, 3973, 3974a, 4090	
300.	17539-43-4	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-		429c	
301.	28368-08-3	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,6′R)-		429c	
302.	512-29-8	β,ε-Carotene-3,3′-diol, 5,8-epoxy-5,8-dihydro-, (3S,3′R,5R,6′R,8R)- {flavoxanthin}		2939, 3797, 3974a	
303.	127-40-2	β,ε-Carotene-3,3′-diol, (3R,3′R,6′R)- {xanthophyll; lutein} 		120, 367, 543a, 585, 830a, 832, 835, 838, 840, 922b, 943, 971, 972, 1156, 1254, 1256, 2079, 2270, 2283, 2338, 2339b, 2356, 2543, 2545, 2765, 2766, 2914, 3059, 3194, 3218, 3971, 3973, 3974a, 4090, 4159, 4222, 4249, 4286, 5079, 5189, 5300, 5811b	
304.	28231-03-0	Cedrenol 		2917a	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

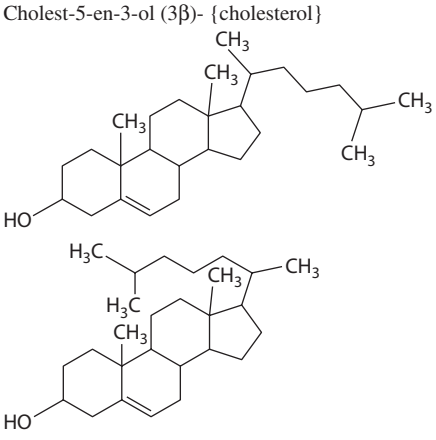
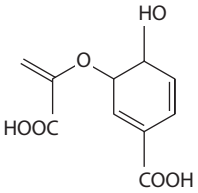
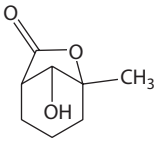
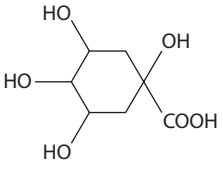
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
305.	9004-34-6	Cellulose	5811b	120, 172, 248, 277, 337, 385, 385a, 420, 451, 535, 539, 601, 602, 629, 665, 722, 1053, 1063–1066, 1068–1074, 1077, 1228, 1289, 1329, 1330, 1333, 1352, 1878a, 1885, 1887, 1933a, 2014, 2042, 2044, 2046, 2070, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2454, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2913, 2919, 2939, 3029, 3059, 3087, 3192, 3264, 3266, 3305, 3371, 3372, 3393, 3395, 3401, 3402, 3404, 3405, 3409, 3430, 3449, 3450, 3462, 3468, 3551, 3665a, 3702, 3797, 3871, 3973, 3974a, 3975, 3976, 4104, 4151, 4249, 4261, 4262, 4418, 4999, 5079, 5189, 5344, 5811b, 5841	
306.		Cellulose, labeled with ^{14}C {cellulose-^{14}C}		2764, 4249	
307.	9000-11-7	Cellulose, carboxymethyl ether		172b, 2086a	
308.	9004-57-3	Cellulose, ethyl ether		429b	
309.	9004-67-5	Cellulose, methyl ether		429b	
310.	80-97-7	Cholestan-3-ol (3β) {dihydrocholesterol}		5811, 5811b	
311.	96443-01-5	Cholest-4-en-3-ol, 4-methyl- (3α)	2601a		
312.	57-88-5	Cholest-5-en-3-ol (3β)- {cholesterol} 	126a, 126b, 172, 237, 1099, 1100, 1171, 1352, 1360, 1373, 1375a, 1434, 1445, 1586, 1651, 1674, 1842, 1933, 2080, 2570, 2601a, 2767, 2939, 3255, 3257, 3265, 3484, 3557, 3608, 3741, 4249, 5079, 5108, 5109, 5189, 5300, 5413, 5811b	832, 840, 907a, 1076a, 1171, 1329, 1352, 1651, 1933a, 2080, 2338, 2400, 2939, 3072, 3263, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3608, 3755, 3797, 3867, 3920, 3973, 3974a, 4249, 5079, 5242, 5811b, 4A03, 4A04, 4A05, 25A54, 25A58	1360, 1375a

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
313.	474-77-1	Cholest-5-en-3-ol, (3α)-) {epicholesterol}		429c	
314.	1253-88-9	Cholest-5-en-3-ol, 4,4-dimethyl-, (3β)-		429c, 4249	
315.	6036-58-4	Cholest-7-en-3-ol, (3β)-		429c, 4249, 4820	
316.	481-25-4	Cholest-7-en-3-ol, 4-methyl-, (3β,4α,5α)-		429c	
317.	6062-47-1	Cholest-8-en-3-ol, 14-methyl-, (3β,5α)-		429c	
318.	5241-24-7	Cholest-8-en-3-ol, 4,4-dimethyl-, (3β,5α)-		429c	
319.	5241-22-5	Cholest-8-en-3-ol, 4-methyl-, (3β,4α,5α)-		429c	
320.	100017-41-2	Cholest-9(11)-en-3-ol, 14-methyl-, (3β,5α)-		429c	
321.	60485-38-3	9,19-Cyclocholest-24-en-3-ol, 4, 14-dimethyl-, (3β,4α,5α)-		429c	
322.	34443-88-4	9,19-Cycloergost-24(28)-en-3-ol, 14-methyl-,(3β,5α)-		429c	
323.	469-39-6	9,19-Cycloergost-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c, 3098, 4249, 4429, 5811b	
324.	34347-58-5	9,19-Cycloergostan-3-ol,14-methyl-, (3β,5α,9β)-		429c	
325.	59780-40-4	9,19-Cycloergostan-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-		429c	
326.	617-12-9	1,5-Cyclohexadiene-1-carboxylic acid, 3-[(1-carboxyethenyl)oxy]-4-hydroxy-, (3R-*E*)- {chorismic acid} 		429b, 4249, 4476	
327.	2474-72-8	2,5-Cyclohexadiene-1,4-dione, 2-hydroxy-	1586, 2767, 4249		
328.	3361-10-2	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11, 15-tetramethylhexadecyl)-6-methyl-		1394, 4249, 4462	
329.	7559-04-8	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15-tetramethylhexadecyl)-3,5,6-trimethyl-, [3R-(3R*,7R*,11R*)]-		4249, 4462	
330.		2,5-Cyclohexadien-1-one, 2,6-bis (1,1-dimethylethyl)-4-hydoxy-4-methyl-		2917a	
331.	110053-64-0	1,3-Cyclohexanecarbolactone,2-hydroxy-3-methyl- 	5811, 5811a, 5811b		
332.	34214-77-2	Cyclohexanecarboxylic acid, [[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]trihydroxy-, (1α,3α,4α,5β)-	3302, 3792, 4249	1309, 3797, 4249, 5811b	
333.	77-95-2 562-73-2	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy- {quinic acid} 	1083, 2675, 3302	120, 1086, 2079, 2270, 2531, 2892c, 2939, 3059, 3655b, 3797, 3973, 3974a, 4249, 4999, 5079, 5189, 5383, 5389, 5698, 5713, 5722, 5779, 5784, 5786, 5811b, 5831	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

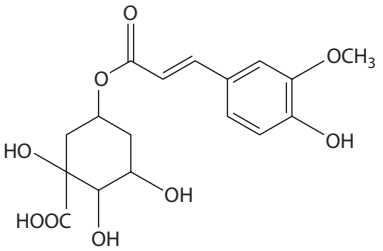
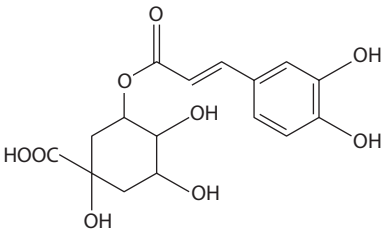
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
334.	36413-60-2	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, (1α,3α,4α,5β)-		2892c, 2939, 3797, 4249	
335.	1899-29-2	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)-{3-*O*-feruloylquinic acid} 		3797, 3973, 3974a, 4249, 4402, 4913, 5811b	
	27044-07-1	Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-			
336.	1899-30-5	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]-, [1S-(1α,3α,4α,5β)]-{*p*-coumaroylquinic acid}		3973, 3974a, 4402	
337.	2450-53-5	Cyclohexanecarboxylic acid, 3,5-bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4-dihydroxy-, [1R-(1α,3α,4α,5β)]-{isochlorogenic acid}		1309, 4249, 5705	
338.	15016-60-1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*Z*),4α,5α]]-	3302, 3792, 4249	3797, 4249	
339.	15076-00-3	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*E*),4α,5α]]-		4249	
340.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-{chlorogenic acid; 3-*O*-caffeoylquinic acid} 	172, 602, 1884, 3257, 3302, 3792, 3797, 4249	69, 72, 120, 254, 385, 486, 598, 602, 657, 665, 677b, 718, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1040, 1063–1066, 1068–1074, 1077b, 1309, 1329, 1333, 1352, 1485, 1625, 1626, 1923, 2014, 2056a, 2079, 2154, 2250a, 2270, 2283, 2313a, 2338, 2361, 2395, 2514, 2531, 2529, 2557a, 2810–2812, 2911c, 2911d, 2914, 2939,	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid; 3-*O*-caffeoylquinic acid} (cont.)		2954, 3029, 3059, 3096, 3161, 3302,3366a, 3367a, 3400, 3459–3462, 3551, 3616, 3628, 3631, 3641, 3646, 3655b, 3700, 3705, 3738, 3748, 3749, 3751, 3754, 3792, 3794, 3797, 3806, 3973, 3974a, 3974b, 3984, 3999, 4005–4007, 4156, 4221, 4249, 4275, 4279, 4372, 4402, 4403, 4421, 4999, 5079, 5189, 5200, 5246, 5353, 5389, 5576, 5592–5594, 5596, 5604, 5652, 5665, 5672, 5673, 5681, 5697. 5698, 5700, 5705, 5713, 5722, 5737, 5761, 5782, 5784, 5788, 5808–5810, 5811b, 5812, 5827, 5831, 5834, 5839, 5850, 5856, 5889, 5890, 5896, 5900, 5908	
341.	906-33-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-(1α,3α,4α,5β)]- {neochlorogenic acid; 5-*O*-caffeoylquinic acid} Also listed as cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxxy-	3302, 3792, 5811b	120, 602, 830a, 831, 834, 835, 838, 840, 890, 970, 1206a, 1626, 2557a, 2939, 3646, 3738, 3792, 3797, 3973, 3974a, 4249, 4402, 5705, 5811b, 5831	
342.	24321-18-4	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dioxo-1,5-cyclohexadien-1-yl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-		3633, 3973, 4271a, 5811b	
343.	534-61-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl] oxy]-1,4,5-trihydroxy- [1S-(1α,3β,4β,5 α)]- {isochlorogenic acid}	5811, 5811b	5811b	
344.	70898-22-5	Cyclohexanecarboxylic acid, 3-[[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-		4249, 4785, 4984	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

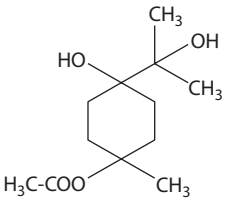
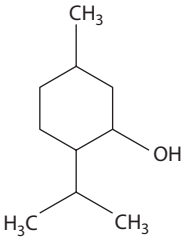
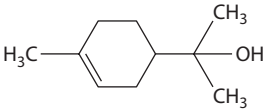
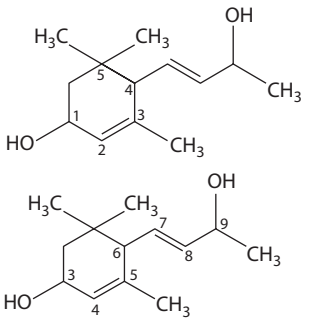
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
345.	17608-52-5	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-{4-*O*-caffeoylquinic acid}		831, 834, 835, 838, 840, 890, 1206a, 3646, 3738, 3973, 3974a, 4249, 5705, 5889	
346.		Cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-5-phenyl		5705, 5749	
347.	905-99-7	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-,(1α,3α,4α,5β)-		4249	
348.	931-17-9	1,2-Cyclohexanediol, (*E*)-		568b, 4249	
349.	82612-14-4	1,2-Cyclohexanediol, 4-[1-(acetyloxy)-1-methylethyl]-1-methyl-, (1α,2β,4α)-(±)-		4249, 4664	
350.	6296-84-0	1,2-Cyclohexanediol, 1-methyl-		568b, 4249	
351.		1,2-Cyclohexanediol, 1-methyl- {isomer}		568b, 4249	
352.	56859-02-0	1,2-Cyclohexanediol, 2-(3-hydroxy-1-butenyl)-1,3,3-trimethyl-		5811, 5811b	
353.	112019-00-8	1,2-Cyclohexanediol, 2-(3-hydroxy-1-butenyl)-1,3,3-trimethyl-, [1R-[1α,2α,2(1*E*,3S*)]]-		4249	
354.	38713-11-0	1,2-Cyclohexanediol, 1,3,3-trimethyl-		937, 3218, 4249	
355.	23832-27-1	1,2-Cyclohexanediol, 4-methyl-		568b, 4249	
356.	556-48-9	1,4-Cyclohexanediol		568b, 4249	
357.	88663-71-2	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*E*)- 		4249, 4734	
358.	88663-72-3	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*Z*)-		4249, 4734	
359.	59632-88-1	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*Z*)-		4249, 4734	
360.	59632-87-0	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*E*)-		4249, 4734	
361.	54993-31-6	1,4-Cyclohexanediol, 2,2,6-trimethyl-		568b, 4249	
362.	639-99-6	Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)-,[1R-(1α,3α,4β)]-		131, 4249	
363.	80-53-5	Cyclohexanemethanol, 4-hydroxy-α,α,4-trimethyl- {*p*-menthane-1,8-diol}	5811, 5811a, 5811b		
364.	2451-01-6	Cyclohexanemethanol, 4-hydroxy-α,α,4-trimethyl-, monohydrate, (*Z*)- {terpin hydrate}	1587, 4249		
365.	104153-60-8	1,2,3-Cyclohexanetriol,1-methyl-4-(1-methylethyl)-		2917a	
366.	108-93-0	Cyclohexanol	2761, 2762, 4249	5811b	
367.	60759-94-6	Cyclohexanol, 1-(3-hydroxy-1-butenyl)-2,2-dimethyl-6-methylene-		4249, 4780	
368.	586-81-2	Cyclohexanol,1-methyl-4-(1-methylethylidene)-		4249, 4734	
369.	619-01-2	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-		568b, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
370.	22567-22-2	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, [1R-(1α,2α,5β)]-		4249, 4663	
371.	51773-45-6	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, [1R-(1α,2α,5α)]-		4249, 4663	
372.	89-79-2	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, [1R-(1α,2β,5α)]-		4249, 4573	
373.	491-01-0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {*D*-neomenthol}		5811, 5811b	
374.	1490-04-6	Cyclohexanol, 5-methyl-2-(1-methylethyl)-	5811b	3561, 5811b	
375.	89-78-1	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {menthol} 	172, 174e, 309, 315, 355, 391, 409, 449, 568b, 873, 874, 1104, 1106–1108, 1269, 1360, 1361, 1375a, 1377, 1426, 1427, 1448, 1482, 1627, 1637, 1874, 1933, 1936, 1949, 2020, 2062, 2143, 2242, 2299, 2410, 2415, 2522, 2562, 2628, 2761, 2762, 2765, 2766, 2770–2773, 2775–2777, 2800, 2923, 2939, 3072b, 3132, 3153, 3154, 3187, 3193, 3228, 3266, 3302, 3308, 3553, 3603, 3662, 4103, 4249, 4259, 4268, 4319, 5055, 5058, 5079, 5506, 5530, 5544, 5545, 5549, 5556, 5575	172a, 174b, 309, 315, 355, 449, 568b, 722, 873, 1053, 1104, 1106–1108, 1156, 1482, 1627, 1874, 1933a, 1936, 1949, 2020, 2242, 2284, 2339a, 2356, 2386, 2389, 2402, 2415, 2544, 2562, 2761, 2762, 2770–2772, 2776, 2800, 2923, 2939, 3153, 3154, 3266, 3354, 3370, 3476, 3497, 3547, 3549, 3560, 3561, 3603, 3905, 3974a, 3988, 4090, 4103, 4249, 4259, 5058, 5079, 5506, 5549, 5811b	1360, 1375a, 1377
376.		Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-^{14}C(U) {^{14}C-menthol (U)}	1936, 2770–2772, 2776	1936, 2770–2772, 2776	
377.	23283-97-8 490-99-3	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5β)- {isomenthol}		568b,4249	
378.	2216-51-5	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, [1R-(1α,2β,5α)]-		172a, 174b	
379.	7500-42-7	Cyclohexanone, 2-hydroxy-2,6,6-trimethyl-		404, 2389, 2544, 3547, 3550, 4249, 4780, 5811b	
380.	20548-02-1	Cyclohexanone, 4-hydroxy-2,2,6-trimethyl-	568b, 937, 4249, 5811b	568b, 937, 943, 1254, 1256, 3206, 3218, 3219, 3543, 3550, 3561, 4249, 5811b	
381.	20548-03-2	Cyclohexanone, 4-hydroxy-3,3,5-trimethyl-	937, 4249	943, 1254, 1256, 3550, 4249, 5811b	
382.	138-59-0	1-Cyclohexene-1-carboxylic acid, 3,4,5-trihydroxy-, [3R-(3α,4α,5β)]- {shikimic acid}		3059, 3797, 3973, 3974a, 4249, 5778, 5783, 5786	
383.	6082-44-6	1-Cyclohexene-1-carboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-4,5-dihydroxy-, (3α,4α,5β)-		4249	

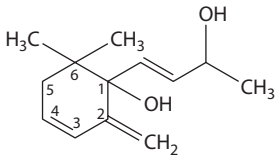
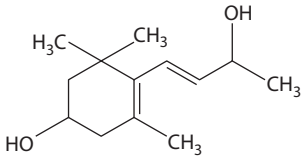
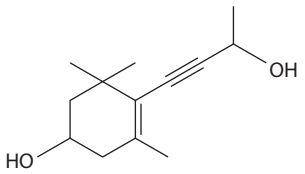
(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
384.	19894-91-8	1-Cyclohexene-1,4-dimethanol, α4,α4-dimethyl-, (S)-		4249	
385.	35692-98-9	2-Cyclohexene-1,4-dione,2-hydroxy-3,5,5-trimethyl-		404, 943, 2092, 3219, 5811b	
386.	472-65-1	1-Cyclohexene-1-ethanol, 2,6,6-trimethyl- {β-cyclohomogeraniol}		5811, 5811b	
387.	13835-30-8	3-Cyclohexene-1-ethanol, β,4-dimethyl- {8-menthen-2-ol}		568b, 4249	
388.	88663-73-4	1-Cyclohexene-1-methanol, 4-(acetyloxy)-α,α,4-trimethyl-		4249, 4734	
389.	472-20-8	1-Cyclohexene-1- methanol, 2,6,6-trimethyl- {β-cyclogeraniol}		5811, 5811b	
390.	42370-41-2	3-Cyclohexene-1-methanol, 5-hydroxy-α,α,4-trimethyl-, *trans*-		4249, 4664	
391.	8000-41-7	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {terpineol}	5811, 5811a, 5811b	5811, 5811a, 5811b	
392.	98-55-5	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {α-terpineol} 	568b, 1054, 2543, 2773, 3266, 3555, 4249	172a, 174b, 568b, 1053, 1254, 1256, 2389, 2544, 2917a, 3215, 3266, 3370, 3547, 3550, 3555, 4249, 5811b	
393.	498-71-5	3-Cyclohexene-1-methanol, 5-hydroxy-α, α,4-trimethyl-		429b	
394.	10482-56-1	3-Cyclohexene-1-methanol,α,α,4-trimethyl-,(S)-	568b, 3266, 4249	172a, 174b, 568b, 1053, 3266, 4249, 5811b	
395.	822-67-3	2-Cyclohexen-1-ol	3559	404	
396.	536-30-1	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethyl)-, (1S-*Z*)-		4249	
397.	27185-80-4	2-Cyclohexen-1-ol, 3-(3-hydroxy-1-butenyl)-2,4,4-trimethyl-		4249, 5811b	
398.	470-99-5	2-Cyclohexen-1-ol, 3,5,5-trimethyl- {isophorol}		2917a	
399.		2-Cyclohexen-1-ol,3,5,5-trimethyl-4-methylene-		1149, 1149a	
400.	13215-90-2	2-Cyclohexen-1-ol, 4-(2-butenylidene)-3,5,5-trimethyl- {megastigmatrienol}		1854, 3547, 4249	
401.	62660-03-1	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- 		233, 1156, 4090, 4249, 4575, 5811b	

Nomenclature by Enzell et al.

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
402.	68831-80-1	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [1S-[1α,4α(1*E*,3S*)]]-		233, 1156, 4090, 4249, 5811b	
403.	68831-81-2	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [1S-[1α,4α(1*E*,3R*)]]-		233, 1156, 4090, 4249, 5811b	
404.	78830-91-8	3-Cyclohexen-1-ol, 1-(3-hydroxy-1-butenyl)-6,6-dimethyl-2-methylene- 		232, 1156, 4090	
405.	33759-63-6	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- 		1156, 3852, 4090, 5811b	
406.	121269-03-2	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, (*E*)-		1156, 3852, 4090, 5811b	
407.	31162-45-5 58023-72-6	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butynyl)-3,5,5-trimethyl- 	568b, 1063–1066, 1068–1074, 4249	568b, 1149a, 1254, 1256, 1587a, 3550, 4249, 4780, 5811b	
408.	562-74-3	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- {4-carvomenthenol}	3266, 3555, 4249	131, 172a, 174b, 1053, 2339a, 3266, 3370, 3555, 4249	
409.	23811-18-9	3-Cyclohexen-1-ol, 3,5,5-trimethyl-, (±)-		3547, 4249	
410.	133304-85-5	2-Cyclohexen-1-one, 3,4-dimethyl-2-hydroxy-	91c, 5811b		
411.	2748-09-6	2-Cyclohexen-1-one, 3,5-dimethyl-2-hydroxy-	91c, 5811b		
412.	2748-08-5	2-Cyclohexen-1-one, 3,6-dimethyl-2-hydroxy-	91c, 5811b		
413.	41577-83-7	2-Cyclohexen-1-one, 3-ethyl-2-hydroxy-	91c, 5811b		
414.	74051-80-2	2-Cyclohexen-1-one, 2-[1-(ethoximino) butyl]-5-[2-(ethylthio)-propyl]-3-hydroxy- {Sethoxydim®}		3633	
415.	10316-66-2	2-Cyclohexen-1-one, 2-hydroxy-	91c, 5811b		
416.	490-03-9 3400-78-0	2-Cyclohexen-1-one, 2-hydroxy-3-methyl- {diosphenol}	91c, 5811, 5811a, 5811b	2917a	
417.	55310-49-1	2-Cyclohexen-1-one, 2-hydroxy-3-propyl-	91c, 5811, 5811a, 5811b		
418.		2-Cyclohexen-1-one, 2-hydroxy-3,5,5-trimethyl-	91c		
419.	77761-55-8	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)-3,5,5-trimethyl-		3973, 4249, 4909	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

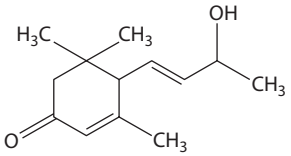
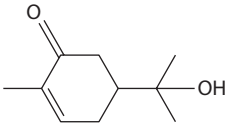
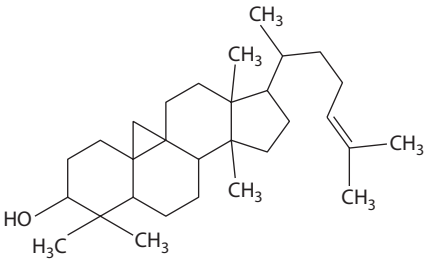
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
420.	77842-24-1	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)-3,5,5-trimethyl-		4249, 4909	
421.	62512-22-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-		4249, 4715, 5811b	
422.	77699-19-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-		4249, 4715	
423.	159813-37-3	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [4R-[4R*(1*E*,3S*)]]-		4249, 4715	
424.	54835-70-0	2-Cyclohexen-1-one,4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-4-hydroxy-3,5,5-trimethyl-, [R-[R*,S*-(*E*)]]-		321c, 1361, 4249, 4713	
425.	62512-23-6	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butyl]-3,5,5-trimethyl-		4249, 4715, 5811b	
426.	91048-13-4	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butylidene]-3,5,5-trimethyl-		4249, 4715	
427.	34318-21-3	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {4-keto-α-ionol} 	568b, 1361, 1371, 1375, 1375b, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3255, 3553, 3557, 4249, 4570a, 5811b	404, 568b, 908, 1063–1066, 1068–1074, 1149, 1149a, 1156, 1254, 1256, 1587a, 1590a, 2338, 2339b, 2386, 2389, 2544, 3547, 3549, 3550, 4090, 4249, 5811b	2387
428.	52210-15-8	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-	1371, 2601a, 3410	1149, 1149a, 1156, 1587a, 4090	
429.	68759-08-0	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [S-[R*,S*-(*E*)]]-	1371	1149, 1149a, 1156, 1587a, 4090	
430.		2-Cyclohexen-1-one, 4-hydroxy 4-(3-methyl-1,3-dibutenyl)-3,5,5-trimethyl-	568b, 4249		
431.	60047-19-0	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl- {4-ketodihydro-α-ionol}	1375, 1375b, 3553, 3557, 4249, 5811b	52, 404, 937, 943, 1149a, 1254, 1256, 1590a, 2386, 2389, 2544, 3218, 3547, 3549, 4249, 5811b	
432.	36151-02-7	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl-, [R-(R*,R*)]-	568b, 2601a, 4249	568b, 1063–1066, 1068–1074, 2917a, 4249, 5811b	
433.	60026-24-6	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-	2570	1254, 1256, 2338, 2389, 2544, 4249, 4790, 5811b	
434.	102488-07-3	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-, (*E*)	5811, 5811b	5811, 5811b	
435.	19620-37-2	2-Cyclohexen-1-one, 4-hydroxy-2,6,6-trimethyl-		943, 2389, 2544, 3218, 4249, 5811b	
436.	14203-59-9	2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-		568b, 937, 4249	
437.	23526-45-6	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- (+) {blumenol A}		5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
438.	24427-77-8	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {vomifoliol}	568b, 1365, 1587, 4249, 5811b	568b, 1587, 1587a, 2338, 3549, 4249	
439.	7070-24-8	2-Cyclohexen-1-one, 4-hydroxy-4-(3-oxo-1-butenyl)-3,5,5-trimethyl-		5811, 5811b	
440.	23069-00-3	2-Cyclohexen-1-one, 4-hydroxymethyl-3,5,5-trimethyl-	568b, 4249	568b, 4249	
441.	7712-46-1	2-Cyclohexen-1-one, 5-(1-hydroxy-1-methylethyl)-2-methyl- 		937, 1156, 4090, 4249	
442.	4657-58-3	9,19-Cyclolanostan-3-ol, (3β)-		4249, 4686	
443.	26955-76-0	9,19-Cyclolanostan-3-ol, 24,25-epoxy-, (3β)-		4249, 4686	
444.	1449-09-8	9,19-Cyclolanostan-3-ol, 24-methylene-, (3β)-		3098, 4249, 5811b	
445.	469-38-5	9,19-Cyclolanost-24-en-3-ol, (3β)- {cycloartenol} 	663, 1651, 3608	1117, 1651, 3098, 3608, 3616, 4249, 5811b	
446.	25692-13-1	9,19-Cyclolanost-24-en-3-ol, 24-methyl-, (3β)-		4484, 4249	
447.	51088-90-5	9,19-Cyclolanost-25-en-3-ol,24-methyl-,(3β,24S)-	4249	4249	
448.	511-61-5	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3β,24S)-		4249	
449.	124713-05-9	9,19-Cyclolanost-5-en-3-ol,24-methylene-,(3β)-		1651	
450.	142750-40-1	4,10(1*H*,5*H*)-Cyclopentacycloundecenedione, 2,3,3a,6,7,11,12,12a-octahydro-1,3,12-trihydroxy-3,8,12-trimethyl-5-(1-methylethyl)-, (1R*,3S*,3aR*,5S*,8Z,12R*,12aR*)-(−)-		4249, 5811b	
451.		2,4-Cyclopentadien-1-one, 2,3-dimethyl-4-hydroxy-	1586, 2767		
452.	20497-93-2	Cyclopentanecarboxaldehyde, 2-hydroxy-1-methyl-		568b, 3547, 4249	
453.		1,2-Cyclopentanedione, hydroxy-	1367, 4249		
454.		1,4-Cyclopentanedione, 2-hydroxy-3,5,5-trimethyl-	568b, 4249		
455.	473-84-7	Cyclopentanone, 2-hydroxy-	5811b		3404, 3405, 4249
456.		Cyclopentene, 2-acetyl-4-hydroxy-4-(1-methylethyl)-		3543	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

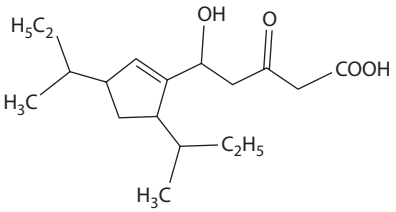
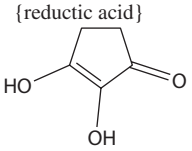
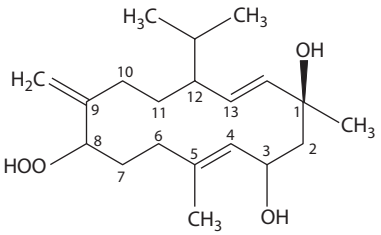
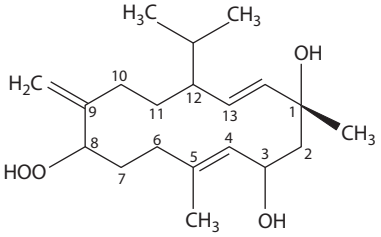
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
457.	53109-18-5	1-Cyclopentene-1-pentanoic acid, δ-hydroxy-3, 5-bis(1-methylpropyl)-β-oxo- 		4249	
458.	61205-39-8	2-Cyclopenten-1-one, ethyl-2-hydroxy-	92, 93		
459.	17190-74-8	2-Cyclopenten-1-one, 2-(2-butenyl)-4-hydroxy-3-methyl-		404	
460.	80-72-8	2-Cyclopenten-1-one, 2,3-dihydroxy- {reductic acid} 	92, 93, 1352, 1375a, 1377, 1882, 2939, 3127, 3302, 3797, 4079, 4249, 5811b		1375a, 1377, 3402
461.	10493-98-8	2-Cyclopenten-1-one, 2-hydroxy-	93, 5811, 5811a, 811b		
462.	29798-72-9	2-Cyclopenten-1-one, 2-hydroxy-3-(1-butyl)-	93, 5811, 5811b		
463.	80-71-7	2-Cyclopenten-1-one, 2-hydroxy-3-methyl- {methylcyclopentenolone}	92, 93, 596, 597, 1099, 1133, 1375, 1375b, 1586, 1958, 1960, 2327c, 2337, 2387, 2493, 2601a, 3255, 3266, 3553, 3555, 3557, 4249, 5034, 5811b	174b, 1053, 2337, 2389, 2544, 3266, 3370, 3430, 3555, 4249, 5811b	2387, 3402, 3404
464.	109682-92-0	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylbutyl)-	93, 5811b		
465.	109682-91-9	2-Cyclopenten-1-one, 2-hydroxy-3-(3-methylbutyl)-	93, 5811b		
466.	109682-81-7	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-(1-methylethyl)-	93, 5811b		
467.	55277-47-9	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylethyl)-	93, 5811, 5811a, 5811b		
468.	29798-73-0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylpropyl)-	93, 5811, 5811b		
469.	25684-05-3	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylpropyl)-	93, 5811, 5811a, 5811b		
470.	109682-89-5	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-propyl-	93, 5811b		
471.	109682-85-1	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-5-propyl-	92, 93, 1586, 5811b		
472.	15899-72-6	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-	93, 5811, 5811a, 5811b		
473.	109682-88-4	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-3-propyl-	93, 5811b		
474.	55007-08-4	2-Cyclopenten-1-one, 2-hydroxy-3-pentyl-	93		
475.	25684-04-2	2-Cyclopenten-1-one, 2-hydroxy-3-propyl-	92, 93, 1352, 1586, 1587, 4249, 5811b		
476.	82147-26-0	2-Cyclopenten-1-one, 2-hydroxy-4-propyl-	92, 93, 568b, 1587, 4249		
477.	61205-40-1	2-Cyclopenten-1-one, 2-hydroxypropyl-	4249	4249	
478.	109682-87-3	2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl-	93, 5811b		
479.	61364-95-2	2-Cyclopenten-1-one, 3,4-diethyl-2-hydroxy-	93, 5811, 5811a, 5811b		
480.	21835-00-7	2-Cyclopenten-1-one, 3,4-dimethyl-2-hydroxy-	92, 93, 1586, 5811, 5811a, 5811b		
481.	52808-97-6	2-Cyclopenten-1-one, 3,5-diethyl-2-hydroxy-	92, 93, 1586, 5811, 5811a, 5811b		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

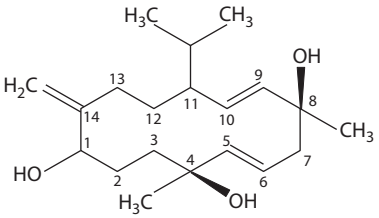
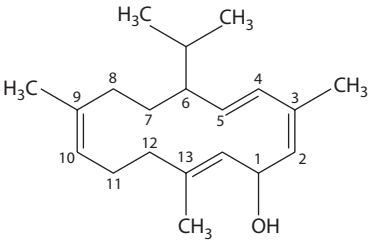
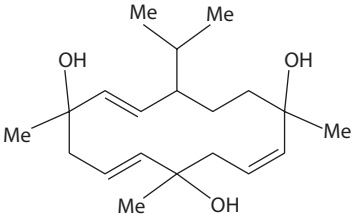
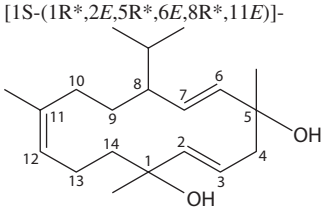
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
482.	109682-90-8	2-Cyclopenten-1-one, 3,5-dimethyl-4-ethyl-2-hydroxy-	93, 5811b		
483.	21834-98-0	2-Cyclopenten-1-one, 3,5-dimethyl-2-hydroxy-	93, 1364, 1586, 5811, 5811a, 5811b		
484.	21835-01-8	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- {ethylcyclopentenolone}	92, 93, 1063–1066, 1068–1074, 1133, 1364, 2857, 3266, 4249, 5811b	172a, 174b, 1053, 2917a, 3266, 4249, 5811b	3402
485.	42348-12-9	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-4-methyl-	93, 5811, 5811a, 5811b		
486.	58228-72-1	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-5-methyl-	93, 5811, 5811a, 5811b		
487.	78210-63-6	2-Cyclopenten-1-one, 3-ethyl-4-hydroxy-	568b, 1587, 4249, 5811b		
488.	5870-63-3	2-Cyclopenten-1-one, 3-hydroxy-2-methyl-		3072a, 3430, 5811b	
489.	28017-62-1	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-	93, 5811, 5811a, 5811b		
490.	71387-71-8	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-3-methyl-	93, 5811b		
491.	10288-24-1	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-	568b, 1586, 2767, 3553, 3557, 4249		
492.	53263-58-4	2-Cyclopenten-1-one, 5-ethyl-2-hydroxy-3-methyl-	92, 93, 1586, 5811, 5811a, 5811b		
493.	70919-26-5	2-Cyclopenten-1-one, 5-hydroxy-		4249	3401, 3402, 3405, 4249
494.	70919-27-6	2-Cyclopenten-1-one, 5-hydroxy-3-methyl-	1371, 1586, 2767, 2774, 3553, 4249		
495.	2516-33-8	Cyclopropanemethanol		568b, 4249	
496.	18383-59-0	Cyclopropanemethanol, 2,2-dimethyl-3-(2-methylpropenyl)- {chrysanthemyl alcohol} 		2917a	
497.	50906-50-8	9,19-Cyclostigmast-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24Z)-		429c	
498.	89288-59-5	4,13-Cyclotetradecadiene-1,3-diol, 8-hydroperoxy-1,5-dimethyl-9-methylene-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,8R*,12R*,13*E*)]- 		4089, 4098, 4249, 5811b	
499.	89362-05-0	4,13-Cyclotetradecadiene-1,3-diol, 8-hydroperoxy-1,5-dimethyl-9-methylene-12-(1-methylethyl)-,[1R-(1R*,3R*,4*E*,8S*,12S*,13*E*)]- 		4089, 4098, 4249, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
500.	102734-57-6	5,10-Cyclotetradecadiene-1,2,7,9-tetrol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*, 2R*,5*E*,7S*,9R*,10*E*,12R*)]-		4249	
501.	89362-08-3	4,13-Cyclotetradecadiene-1,3,8-triol, 1, 5-dimethyl-9-methylene-12-(1-methylethyl-		5811, 5811b	
502.	89362-09-4	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,8S*,12S*,13*E*)]-		4083, 4089, 4100, 4249, 5811b	
503.	91200-13-4	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8S*,12R*,13*E*)]-		4083, 4089, 4100, 4249	
504.	80802-00-2	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-		4083, 4089, 4100	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
505.	91163-46-1	5,9-Cyclotetradecadiene-1,4,8-triol, 4,8-dimethyl-14-methylene-11-(1-methylethyl)-,[1S-(1R*,4R*,5*E*,8S*,9*E*,11R*)]- 		3778, 4089	
506.	90660-18-7	4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-(1-methylethyl)-		4249, 4811, 5811b	
507.	119613-98-8	5,10-Cyclotetradecadien-1-one, 7,9-dihydroxy-7,11-dimethyl-4-(1-methylethyl)-, [4S-(4R*,5*E*,7R*,9S*,10*E*)]-		4249, 5811b	
508.	39815-66-2	2,4,9,13-Cyclotetradecatetraen-1-ol, 3, 9,13-trimethyl-6-(1-methylethyl)- 		9, 453, 3219, 4089, 5811b	
509.	95334-70-6	2,6,10-Cyclotetradecatriene -1,5, 9-triol, 1,5,9-trimethyl-12-(1-methylethyl)- 		5811, 5811b	
510.	57688-99-0 59284-87-6	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5, 11-trimethyl-8-(1-methylethyl)-	1365, 2726, 4249	5811b	
511.	59284-88-7	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, (1S, 2*E*, 5R, 6*E*, 8S, 11*E*) {β-3,8,13-duvatriene-1,5-diol}	5811, 5811a, 5811b	5811, 5811a, 5811b	
512.	84367-90-8	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1S-(1R*,2*E*,5R*,6*E*,8R*,11*E*)]- 	1063–1066, 1068–1074, 1373, 2543, 2545, 2726, 2761, 2762, 2765, 2766, 2773, 2781, 3255, 3257, 4249	9, 227, 671, 943, 1149, 1149a, 1591, 2529, 3198, 3215, 3219, 3220, 3329, 3352, 3360, 3493, 3703, 3704, 3706, 3971, 3974a, 3999, 4089, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

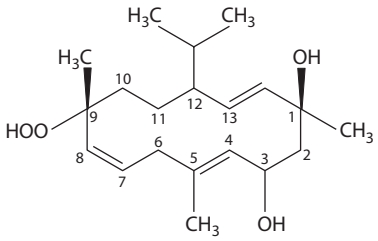
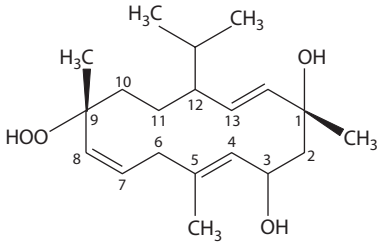
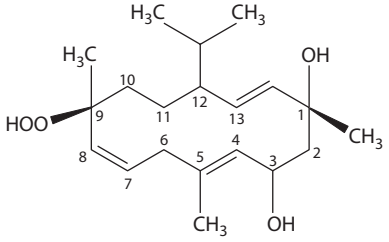
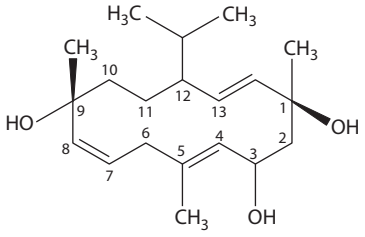
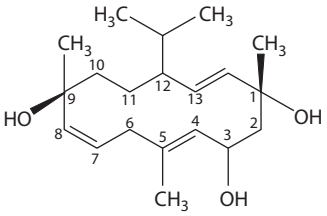
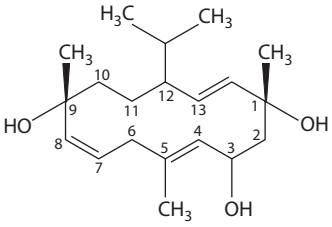
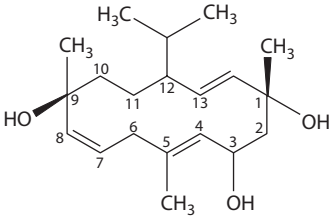
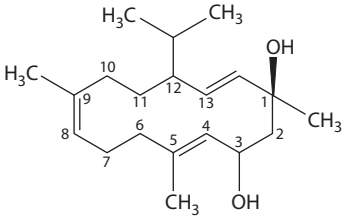
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
513.	84367-92-0	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8S*,11*E*)]-		9, 671, 1591, 3352, 3360, 3703, 3704, 3706, 3974a, 5811b	
514.	89288-60-8	4,7,13-Cyclotetradecatriene-1,3-diol, 9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,7*E*,9R*,12R*,13*E*)]- 		4089, 4098, 5811b	
515.	89362-06-1	4,7,13-Cyclotetradecatriene-1,3-diol, 9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,7*E*,9S*,12R*,13*E*)]- 		4089, 4098, 5811b	
516.	89362-07-2	4,7,13-Cyclotetradecatriene-1,3-diol, 9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-,[1R-(1R*,3R*,4*E*,7*E*,9S*,12S*,13*E*)]- 		4089, 4098, 5811b	
517.	82003-46-1	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5, 9-trimethyl-12-(1-methylethyl)-, [1S-(1R*, 3S*,4*E*,7*E*,9R*,12R*,13*E*)]- 		4083, 4089, 4100, 5811b	
518.	89362-10-7	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5, 9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*, 4*E*,7*E*,9R*,12R*,13*E*)]-		4083, 4089, 4100, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
					
519.	89362-11-8	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5, 9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*, 4*E*,7*E*,9R*,12R*,13*E*)]-		4083, 4089, 4100, 5811b	
					
520.	91200-14-5	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5, 9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*, 4*E*,7*E*,9R*,12R*,13*E*)]-		4083, 4089, 4100, 5811b	
					
521.	116348-80-2	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5, 9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-		4249	
522.	121916-90-3	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3R*, 4*E*,8*E*,12S*,13*E*)]-		4249, 5811b	
523.	122620-36-4	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5, 9-trimethyl-12-(1-methylethyl)-, (1R*,3R*, 4*E*,8*E*,12S*,13*E*)-(±)-	5811b	4249	
524.	57605-80-8	4,8,13-Cyclotetradecatriene-1, 3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-	1063–1066, 1068–1075, 1373, 2543, 2570, 2601a, 2726, 2761, 2762, 2765, 2766, 3255, 3257, 3265, 3971, 4249	9, 227, 297, 404, 675, 676, 909, 943, 1149, 1149a, 1591, 2054, 2338, 2341a, 2786, 2914, 2939, 3195, 3197, 3215, 3219, 3221, 3329, 3389, 3613a, 3621, 3703, 3704, 3706, 3797, 3971, 3973, 3974a, 4089, 4249, 5811b	
					

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

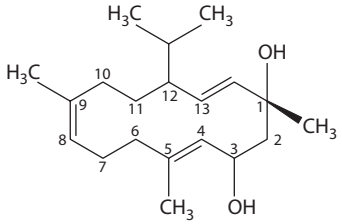
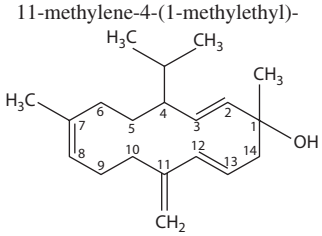
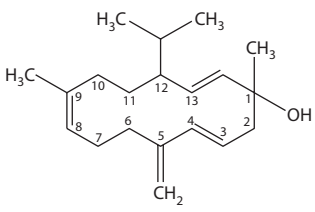
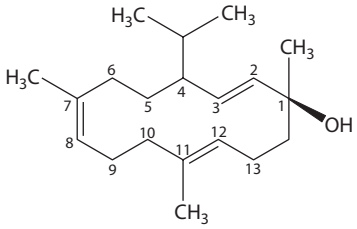
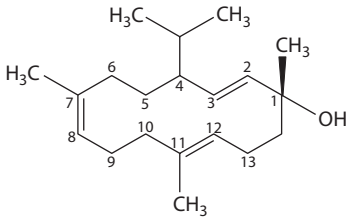
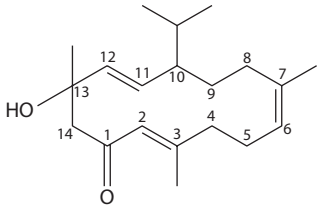
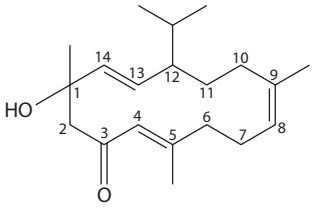
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
525.	57605-81-9	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-1R*,3R*,4*E*,8*E*,12S*,13*E*)]- 	1373, 2726, 3255, 3257, 3265, 4249	9, 227, 675, 676, 909, 943, 1149, 1149a, 1591, 2054, 2338, 2341a, 2786, 2914, 2939, 3195, 3197, 3215, 3219, 3221, 3389, 3607, 3613a, 3621, 3703, 3704, 3706, 3778, 3797, 3971, 3973, 3974a, 4089, 4249, 5811b	
526.	87554-04-9	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*Z*)]-		4249	
527.	7220-78-2	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5, 9-trimethyl-12-(1-methylethyl)-	1360, 1375a, 2601a	2917a	1360, 1375a
528.	2043-08-1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, 3-acetate, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-		4249	
529.	146564-67-2	4,8,13-Cyclotetradecatriene-1,3-diol, 9-(hydroxymethyl)-1,5-dimethyl-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,8*Z*,12R*,13*E*)]-		4249, 5811b	
530.	149403-67-8	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7S*,8*E*,12R*)]-		4249	
531.	149403-68-9	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7R*,8*E*,12R*)]-		4249	
532.	149403-69-0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7R*,8*E*,12S*)]-		4249	
533.	149403-70-3	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7S*,8*E*,12S*)]-		4249	
534.	149403-71-4	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7S*,8*Z*,12S*)]-		4249	
535.	146564-66-1	4,9,13-Cyclotetradecatriene-1,3,8-triol, 3,9,13-trimethyl-6-(1-methylethyl)-, [1R-(1R*, 3R*,4*E*,6S*,8R*,9*E*,13*E*)]-		4249, 5811b	
536.	146609-95-2	4,9,13-Cyclotetradecatriene-1,3,8-triol, 3,9, 13-trimethyl-6-(1-methylethyl)-, [1R-(1R*, 3S*,4*E*,6S*,8R*,9*E*,13*E*)]-		4249	
537.	60026-11-1	2,7,12-Cyclotetradecatrien-1-ol, 1,7-dimethyl-11-methylene-4-(1-methylethyl)-  *Chem, abstracts numbering*  *Alternate numbering*		1149, 1149a, 2389, 2544, 4089	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

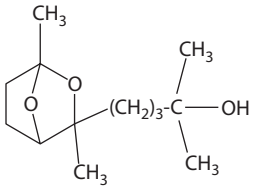
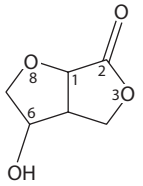
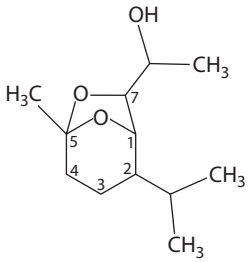
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
538.	87387-80-2	2,6,12-Cyclotetradecatrien-1-ol, 3,7,13-trimethyl-10-(1-methylethenyl)-		4249	
539.	119864-28-7	2,7,10-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1R- (1R*,2*E*,4S*,7*E*,10*E*)]-		1591, 5811b	
540.	119944-62-6	2,7,10-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-,[1S-(1R*,2*E*,4R*,7*E*,10*E*)]-		1591, 5811b	
541.	25269-17-4	2,7,11-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1R-(1R*,2*E*,4S*,7*E*,11*E*)]- 	2601a	453, 3219, 4089, 3613a	
542.	80126-41-6	2,7,11-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1S-(1R*,2*E*,4R*,7*E*,11*E*)]- 		453, 3219, 4089, 3613a, 5811b	
543.	149312-90-3	2,6,11-Cyclotetradecatrien-1-one, 5,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-,[5S-(2*E*,5R*,6*E*,10R*,11*E*,13R*)]-		4249	
544.	98064-74-5	2,5,11-Cyclotetradecatrien-1-one, 7,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-,[7S-(2*E*,5*E*,7R*,10R*,11*E*,13R*)]-		4098, 4249	
545.	149312-89-0	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-,[6S-(2*E*,6R*,7*E*,9R*,11S*,12*E*)]-		4249	
546.	149403-72-5	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-,[6S-(2*E*,6R*,7*E*,9S*,11S*,12*E*)]-		4249	
547.	41429-54-3	2,6,11-Cyclotetradecatrien-1-one, 13-hydroxy-3,7,13-trimethyl-10-(1-methylethyl)- = 4,8,13-Cyclotetradecatrien-1-ol-3-one,-1, 5,9-trimethyl-12-(1-methylethyl)-, 	1364 	671, 1149, 1149a, 1591, 4089, 4249, 4401, 4780, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
548.		13-Cyclotetradecene-1,3,4,8-tetrol-1-methyl-5, 9-dimethylene-12-(1-methylethyl)-		94a, 4089, 4401	
549.		1-Cyclotetradecen-1-one, 3,6,13-triol-3,13-dimethyl-7-methylene-10-(1-methylethyl)-		94a	
550.	65-46-3	Cytidine {2(1*H*)-pyrimidinone, 4-amino-1-β-*D*-ribofuranosyl-}		429b, 4249, 4477	
551.	65-47-4	Cytidine 5′-(tetrahydrogen triphosphate)		429b, 4249, 4505	
552.	63-37-6	5′-Cytidylic acid		429b, 4249, 4774	
553.	158815-70-4	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-		736, 4249, 5811b	
554.	160115-53-7	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-, methyl ester		4249	
555.		Decanoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-	2092, 4249	2092, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
556.	112-30-1	1-Decanol {capric alcohol} $H_3C\text{-}(CH_2)_8\text{-}CH_2OH$	172, 568b, 1333, 1365, 3255, 3559, 5811b	568b, 1053, 1157, 1333, 2650a, 2650b, 3266, 3370, 3633, 3811a, 3973, 3977, 4098a, 4249, 5811b	
557.	60924-66-5	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-		737, 4249	
558.	129777-23-7	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-, [R-[R*,S*-(*E*)]]-		737, 4249, 5811b	
559.	77288-98-3	6-Decen-2-one, 8,10-dihydroxy-8-methyl-5-(1-methylethyl)-		4249, 4948	
560.	9004-53-9	Dextrin		120, 174b, 2079, 2283, 2939, 2947b, 2947c, 3266, 3449, 4249, 5079, 5189, 5344, 5449, 5811b	
561.	5894-59-7	Digalacturonic acid		5811, 5811b	
562.	117210-54-5	2,7-Dioxabicyclo[2.2.1]heptane-3-butanol, α,α,1,3-tetramethyl- 		5811, 5811b	
563.	121927-15-9	13,14-Dioxabicyclo[10.2.2]hexadec-6-ene-2,3,5-triol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2S*,3R*,5S*,		4249	
564.	52886-15-4	2,9-Dioxabicyclo[3.3.1]nonan-4-ol, 1,3,3-trimethyl-6-(1-methylethyl)- {2 isomers reported}		3547, 5811b	
565.	110053-63-9	3,8-Dioxabicyclo[3.3.0]octan-2-one,6-hydroxy- 	5811, 5811a, 5811b		
566.	58001-00-6	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,5-dimethyl-[1α,2β,5α,7α(R*)] 		1149, 1149a	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

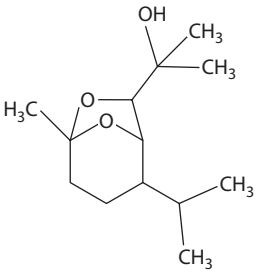
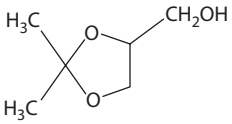
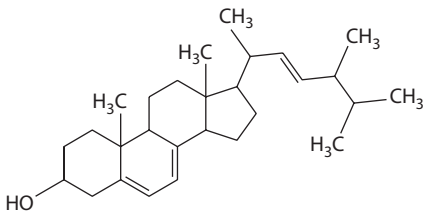
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
567.	58001-10-8	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-, (2-endo,7-exo)-(±)- 		4249	
568.	52992-36-6	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-		4249, 5811b	
569.	5464-28-8	1,3-Dioxalane-4-methanol	568b, 4249		
570.	100-79-8	1,3-Dioxalane-4-methanol, 2,2-dimethyl- 	568b, 1375, 3553, 3557, 4249, 5811b		
571.	931-40-8	1,3-Dioxalan-2-one, 4-(hydroxymethyl)- {glycerol carbonate}	568b, 1371, 1375, 3255, 3553, 3557, 4249, 5811b		
572.	86687-05-0	1,3-Dioxane, 5-hydroxy-	568b, 4249		
573.	30303-65-2	Docosanol		5811, 5811b	
574.	661-19-8	1-Docosanol {behenyl alcohol} H_3C-$(CH_2)_{20}$-CH_2OH	172, 568b, 614, 812, 1651, 3059, 3251, 3299, 3302, 3608, 3797, 4249	568b, 812, 1591, 1651, 1893b, 2389, 2544, 3198, 3219, 3299, 3329, 3350, 3604, 3605, 3608, 3613a, 3755, 3973, 3974a, 4073b, 4249	
575.		1-Docosanol, 20-methyl-		3613a, 4249, 4964	
576.		1-Docosanol, 21-methyl-		3613a	
577.	65596-29-4	3,6-Dodecadienedioic acid, 10-hydroxy-4, 9-dimethyl- $HOOC$-CH_2-$CHOH$-$CH(CH_3)$-CH_2-CH═CH-CH_2-$C(CH_3)$═CH-CH_2-$COOH$		739, 1156, 4090, 4249	
578.	7226-86-0	2,6-Dodecadien-1-ol, 3,7,11-trimethyl-	4249		
579.	117232-64-1	5,10-Dodecadien-2-one,9-hydroxy-6,11-dimethyl-		3285, 4249, 5811b	
580.	27342-88-7	Dodecanol	5811, 5811a, 5811b		
581.	112-53-8	1-Dodecanol {lauryl alcohol} H_3C-$(CH_2)_{10}$-CH_2OH	172, 568b, 2601a, 3559, 4249	568b, 2356, 3633, 4098a, 4249	
582.	6750-34-1	1-Dodecanol, 3,7,11-trimethyl- {hexahydrofarnesol}		2917a	
583.		2,6,9,11-Dodecatetraen-1-ol, 2,6,10-trimethyl-, (2*E*,6*E*,9*E*)- {α-sinensol}	4570a		
584.		2,6,10,?-Dodecatetraenol {dehydrofarnesol}	3251, 3285, 4249		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
585.	7212-44-4	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- {nerolidol}	3224, 3266, 4249	172a, 174b, 1053, 2389, 2544, 2611, 3266, 4098a, 4249, 5811b	
586.	142-50-7	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-,[S-(*Z*)]-		568b, 2917a, 4249, 5811b	
587.	4602-84-0 3790-71-4	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- {farnesol}	1586, 2601a, 2767, 3224, 3251, 3266, 3284, 3285, 3302, 3557, 4249, 4570a, 5811b	172a, 174b, 404, 909, 1053, 2386, 2917a, 3266, 4249	
588.	106-28-5	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- {farnesol isomer}	568b, 2601a, 4249		
589.	28679-05-2	Eicosanol		5811, 5811b	
590.	629-96-9	1-Eicosanol {arachic alcohol} $H_3C\text{-}(CH_2)_{18}\text{-}CH_2OH$	172, 568b, 812, 1651, 3059, 3251, 3276, 3302, 3299, 4249, 5811b	568b, 812, 1651, 2389, 2544, 3299, 3613a, 3755, 3797, 3974a, 4249	
591.		1-Eicosanol, 18-methyl-		3613a, 4249, 4964	
592.		1-Eicosanol, 19-methyl-		3613a	
593.	4340-76-5	2-Eicosanol	2601a		
594.	22104-85-4	2-Eicosen-1-ol $H_3C\text{-}(CH_2)_{16}\text{-}CH{=}CH\text{-}CH_2OH$		4249, 4964	
595.	474-60-2	Ergostan-3-ol,(3β,5α,24R)- {campestanol}		5811, 5811b	
596.	20304-54-5	Ergost-4-en-3-ol, (24R)- {campest-7-en-3-β-ol}		5811, 5811b	
597.	474-62-4	Ergost-5-en-3-ol, (3β,24*R*)- {campesterol}	172, 1099, 1100, 1352, 1360, 1375a, 1586, 1651, 1842, 2018, 2019, 2570, 2601a, 2767, 3059, 3255, 3308, 3484, 3557, 3608, 5512, 5811, 5811b	832, 838, 907a, 082, 1329, 1352, 1651, 2018, 2019, 2338, 2400, 2939, 3059, 3072, 3435, 3476, 3484, 3493, 3511, 3608, 3755, 3797, 3867, 3920, 3973, 3974a, 5811, 5811b	1360, 1375a
598.	26047-31-4	Ergost-7-en-3-ol, (3β)-		429c	
599.	17105-75-8	Ergost-7-en-3-ol, (3β,24ξ)-	273, 429c		
600.	33860-48-9	Ergost-8-en-3-ol, 14-methyl-, (3β,5α)-		429c	
601.	16910-33-1	Ergost-8-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c, 4479	
602.	70116-48-2	Ergost-8-en-3-ol, 4,14-dimethyl-,(3β,4α,5α,24ξ)-		429c	
603.	474-67-9	Ergosta-5,22-dien-3-ol, (3β,22*E*)-		429c, 2400, 5811b	
604.	474-63-5	Ergosta-5,24(28)-dien-3-ol, (3β)-		429c, 1971, 5777, 5811, 5811b	
605.	52936-69-3	Ergosta-5,25-dien-3-ol, (3β)-		429c	
606.	57-87-4	Ergosta-5,7,22-trien-3-ol, (3β,22*E*)- {ergosterol}	3059	334, 1080, 3867, 3973, 3974a, 5811b	



(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
607.	21490-25-5	Ergosta-7,24(28)-dien-3β-ol, 4β-methyl-		429c, 3098, 4249	
608.	474-68-0	Ergosta-7,24(28)-dien-3-ol, (3β,5α)-		429c, 4249, 4431	
609.	1176-52-9	Ergosta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α)-		429c, 4249, 4851, 5811b	
610.	74635-33-9	Ergosta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-		429c, 1971, 4249	
611.	23839-47-6	Ergosta-8,14-dien-3-ol, (3β,5α)-		429c	
612.	33886-74-7	Ergosta-8,24(28)-dien-3-ol,14-methyl-, (3β,5α)-		429c	
613.	16910-32-0	Ergosta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c, 5811b	
614.	80736-41-0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R,23R,24S)-		429c	
615.	121468-15-3	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3β,5α,22R,23R,24S)-		429c	
616.	92751-21-8	Ergostan-6-one, 3,22,23-trihydroxy-, (3β,5α,22R,23R,24S)-		429c	
617.	87734-68-7	Ergostan-6-one, 3,22,23-trihydroxy-, (3α,5α,22R,23R,24S)-		429c	
618.	97190-07-3	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monooctadecadienoate monooctadecatrienoate, (all-*Z*)-		4249	
619.	97190-09-5	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecatrienoate, (*Z,Z,Z*)-		4249	
620.	97190-10-8	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecadienoate, (*Z,Z*)-		4249	
621.	97190-12-0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*- trimethyl-, hydroxide, inner salt, monooctadecadienoate		4249	
622.	62-49-7 123-41-1	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl- {choline} $HO\text{-}(CH_2)_2\text{-}N^+\equiv(CH_3)_3$		120, 1351, 2079, 2270, 2337, 2808a, 2939, 3491, 3555, 3797, 3973, 3974a, 4249, 5079, 5189, 5435, 5436	
623.	107-21-1	1,2-Ethanediol {ethylene glycol} $HOCH_2\text{-}CH_2OH$	568b, 1209, 1350, 1354, 1360, 1371, 1375, 1375a, 1375b, 1445, 1437, 1586, 2079, 2170, 2171, 2387, 2493, 2570, 2761, 2762, 2765–2767, 2775, 2939, 3100, 3254, 3255, 3302, 3100, 3308, 3410, 3553, 3557, 3559, 3797, 3999, 4249, 5079, 5811b	568b, 865, 1024, 1241, 1294, 1296, 1383, 2170, 2188, 2195, 2246, 2789, 3264, 4249, 5079, 5467, 5811b	1354, 1360, 1375a, 2387, 3402, 3405
624.	534-82-7	1,2-Ethanediol,1-(4-hydroxy-3-methoxyphenyl)-		4249	
625.	542-59-6	1,2-Ethanediol, monoacetate {acetic acid, 2-hydroxyethyl ester} $HO\text{-}(CH_2)_2\text{-}OOC\text{-}CH_3$	568b, 1371, 1375, 1375b, 1586, 2767, 3553, 3557, 4249, 5811b		
626.	40460-44-4	1,1,2-Ethanetriol		4249	3402

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
627.	64-17-5	Ethanol {ethyl alcohol} $H_3C\text{-}CH_2OH$	37, 38, 172, 222–224, 314, 568b, 605, 916, 1140, 1375a, 1377, 1378, 1412–1414, 1416, 1419, 1422, 1449, 1481, 1905, 1907, 2088, 2270, 2634, 2858, 2939, 3224, 3255, 3257, 3265, 3302, 3308, 3530, 3692, 3797, 3882, 3901, 4005–4007, 4052, 4056, 4162, 4249, 4319, 4570a, 5811b	120, 172a, 174b, 568b, 1053, 1481, 1550, 2702a, 2339a, 2861a, 2939, 3266, 3328, 3370, 3797, 3973, 3974a, 4249, 5079, 5811b	1375a, 1377, 1378, 4052, 4056
628.		1-^{14}C-Ethanol {ethyl alcohol-^{14}C}	1481	1481	
629.	107-07-3	Ethanol, 2-chloro- {chlorohydrin}	5811, 5811a	5811, 5811a	
630.	108-01-0	Ethanol, 2-(dimethylamino)-	1371, 3410, 3559, 4249		
631.	109-83-1	Ethanol, 2-(methylamino)-		4249, 4829	
632.	1116-54-7	Ethanol, 2,2′-(nitrosoimino)bis- {NDELA} $(HO\text{-}CH_2CH_2)_2{=}N\text{-}NO$	126, 126a, 126b, 172, 237, 239, 458, 471, 477–479, 481, 482, 485, 486, 510, 603, 1058, 1148, 1159, 1217, 1445, 1674, 1704, 1705, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1867, 1870–1872, 2516, 2825, 2655, 3190, 3255–3257, 3265, 3300, 3370, 3480, 3714, 3973, 3992, 4010, 4011, 5512, 5869a	458, 468, 471, 477–479, 481, 482, 485, 486, 490, 498, 1704, 1705, 1727, 1867, 1870–1872, 2990, 3265, 3300, 3480, 3481, 3491, 3947, 3948, 3973, 4010, 4011, 4249, 5001, 5811b	
633.	112-27-6	Ethanol, 2,2′-(1,2-ethanediylbis(oxy)) bis- {triethylene glycol} $HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$	174e, 331, 627, 974, 1371, 1603, 2761, 2762, 2939, 3302, 3797, 3835, 4249, 4319	627, 1241, 1296, 2188, 2192, 2193, 2195, 2788, 2939, 3264, 3797, 3974a, 4249, 5811b, 5903	
634.	112-60-7	Ethanol, 2,2′-[oxybis(2,1-ethanediyloxy)] bis- {tetraethylene glycol} $HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$		3264	
635.	30934-97-5	Ethanol, 2,2-dimethoxy- $(H_3C\text{-}O)_2{=}CH\text{-}CH_2\text{-}OH$	3406, 4249, 5811b		
636.	111-42-2	Ethanol, 2,2′-iminobis- {diethanolamine} $(HO\text{-}CH_2CH_2)_2{=}NH$	479, 490	479, 490, 3973	
637.	111-46-6	Ethanol, 2,2′-oxybis- {diethylene glycol} $(HO\text{-}CH_2CH_2)_2{=}O$	43, 568b, 627, 1603, 2170, 2171, 2543, 2549, 2761, 2767, 2773, 2777, 2939, 3302, 3308, 3553, 4319, 5079, 5189, 5286, 5811b	568b, 627, 1241, 1296, 2170, 2188, 2195, 2246, 2788, 3264, 3605, 3689, 3797, 3974a, 5079, 5206, 5228, 5254, 5286, 5307, 5811b	
638.	141-43-5	Ethanol, 2-amino- {ethanolamine} $HO\text{-}CH_2CH_2\text{-}NH_2$		568b, 622, 749, 752–754, 3705	
639.	110-80-5	Ethanol, 2-ethoxy- $HO\text{-}CH_2CH_2\text{-}O\text{-}CH_2CH_3$	2761, 2762, 2765, 2766, 2777, 4249, 4570a	2917a	
640.	109-86-4	Ethanol, 2-methoxy- $HO\text{-}CH_2CH_2\text{-}O\text{-}CH_3$	3559	2385a, 3905, 4249	
641.	122-99-6 1321-27-3	Ethanol, 2-phenoxy- $C_6H_5O\text{-}CH_2CH_2\text{-}OH$		1256, 2339a, 4249	
		Ethanol, phenyl-: See 60-12-8 Benzeneethanol	2400a	5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

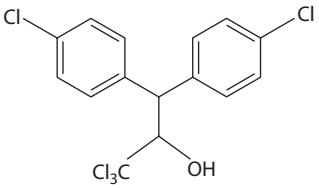
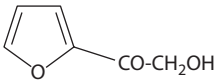
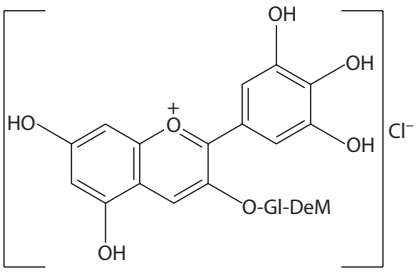
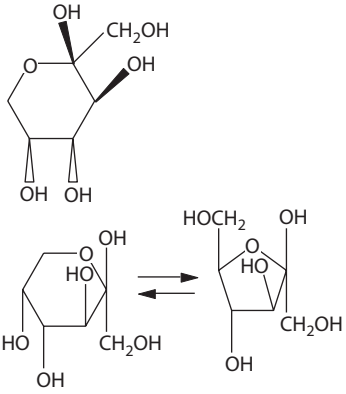
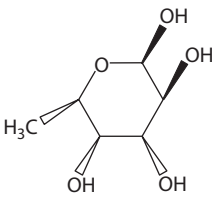
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
642.	115-32-2	Ethanol, 2,2,2-trichloro-1,1-bis(4-chlorophenyl)-{Dicofol®} 		3633	
643.	17678-19-2	Ethanone, 1-(2-furanyl)-2-hydroxy- 	568b, 3553, 3557, 4249, 5811b	568b, 3797, 4249	3402, 3404, 3405, 4249
644.	3420-59-5	Ethanone, 1-(3-hydroxy-2-furanyl)-{isomaltol}		2917a	
645.	120056-06-6	Ethanone, 1-[3-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl) oxiranyl]-, [1S-[1α(2S*,3R*),2β,4a		4249, 5811b	
646.		Ethanone, 1-(5-methyl-2-furanyl)-2-hydroxy- = Furan, 2-(1-oxo-2-hydroxyethyl)-5-methy-	568b, 4249		
647.	55087-82-6	Ethanone, 1-[5-(hydroxymethyl)-2-furanyl]-	568b, 1586, 2767, 3553, 3557, 4249, 5811b		
648.	123695-66-9	Ethanone, 1-[6-hydroxy-6-methyl-3-(1-methylethyl)-2-cyclohexen-1-yl]-	4249		
649.	119-53-9	Ethanone, 1,2-diphenyl-2-hydroxy- C_6H_5-CHOH-CO-C_6H_5		1053, 3266	
650.	582-24-1	Ethanone, 2-hydroxy-1-phenyl- C_6H_5-CO-CH_2OH	5811, 5811b		
651.	29732-48-7	Flavylium, 3-[[O-(6-deoxymannosyl)glucosyl] oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride 		4249, 4527, 4710	
652.		Flavylium, 3-[[O-(6-deoxymannosyl)glucosyl] oxy]-3′,4′,5,7-tetrahydroxy-, chloride		4249, 4527, 4644	
653.	9037-90-5	*D*-Fructan		429b, 4249, 4806	
654.	10247-46-8	*D*-Fructofuranose		429b, 3333a	4923
655.	71385-82-5	β-*D*-Fructofuranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2155, 4249	
656.	79082-92-1	β-*D*-Fructofuranose, 2,6-bis(dihydrogen phosphate)		429b	
657.	79886-47-8	β-*D*-Fructopyranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		3667, 3668, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
658.	57-48-7	*D*-Fructose {levulose} 	1089a, 1352, 1360, 1361, 1375a, 1587, 1887a, 1944, 2079, 2145, 2321, 2524a, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	71, 120, 321b, 480, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1141, 1142, 1289, 1352, 1361, 1435a, 1916, 1971, 2070, 2270, 2283, 2313a, 2337, 2338, 2381, 2532, 2818, 2911c, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3462, 3551, 3555, 3580, 3667, 3797, 3871, 3913, 3973, 3974a, 3974b, 4159, 4249, 4275, 4411, 5079, 5105, 5108, 5109, 5114, 5189, 5344, 5387, 5449, 5562, 5652, 5748, 5768, 5811b, 5819	1360, 1375a
659.	51767-72-7	*D*-Fructose, labeled with ^{13}C, labeled with ^{13}C {*D*-fructose-^{13}C}		976a	
660.		*D*-Fructose, labeled with ^{14}C, labeled with ^{14}C {*D*-fructose-^{14}C}		5644	
661.	29118-61-4	*D*-Fructose, 1-(2-carboxy-1-pyrrolidinyl)-1-deoxy-, (S)-		434, 1063–1066, 1068–1074, 1351, 2337, 2339b, 3555, 3639, 3923, 3973, 3974a, 4159, 4249, 5811b	
662.	488-69-7	*D*-Fructose, 1,6-bis(dihydrogen phosphate)		429b	
663.	70954-04-0	*D*-Fructose, 1-[(1-carboxy-2-hydroxypropyl) amino]-1-deoxy-, [R-(R*,S*)]-		434, 1351, 3555, 3973, 3974a	
664.	34393-27-6	*D*-Fructose, 1-[(3-amino-1-carboxy-3-oxopropyl)amino]-1-deoxy-, (S)-		1351, 2337, 4362	
665.	10003-63-1	*D*-Fructose,1-[(3-carboxypropyl)amino]-1-deoxy-		1351, 2337, 3639, 3923, 3973, 3974a, 5811b	
666.	70906-15-9	*D*-Fructose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		4159	
667.	643-13-0	*D*-Fructose, 6-(dihydrogen phosphate)		429b, 4249, 4670	
668.	36119-15-0	*D*-Fructose, mono(dihydrogen phosphate)		429b, 4249, 4960	
669.	2438-80-4	Fucose 		3075, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

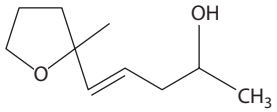
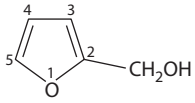
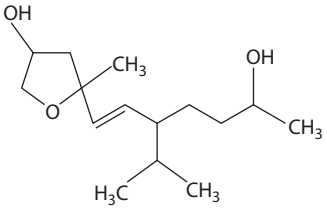
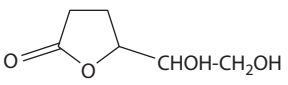
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
670.		Furan,tetrahydro-2-methyl-2-(4-hydroxy-1-pentenyl)- 		1156, 2389, 2544, 4090	
671.		2-Furancarboxaldehyde, hydroxy-	1375a, 1377		1375a, 1377
672.	25376-49-2	2-Furancarboxaldehyde, (hydroxymethyl)-		2939	
673.	67-47-0	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	341, 568b, 722, 723, 924, 1063–1066, 1068–1074, 1350, 1354, 1360, 1364, 1365, 1371, 1375a, 1377, 1882, 1958, 1960, 2337, 2387, 2493, 2543, 2545, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 2939, 3302, 3308, 3397, 3410, 3462, 3530, 3553, 3557, 3559, 4159, 4163, 4249, 4378, 4379, 4407, 5034, 5811b	120, 568b, 965, 984, 2337, 2389, 2544, 2722, 2860a, 2930, 2917a, 2939, 3194, 3430, 3547, 3549, 3973, 3974a, 4249, 5811b	1354, 1375a, 1360, 1375a, 1377, 2387, 3393, 3401, 3402, 3404, 3405
674.	71278-16-5	2-Furancarboxylic acid, 3-hydroxy-	1375a, 1377	1883, 4249	1375a, 1377
675.	6338-41-6	2-Furancarboxylic acid, 5-(hydroxymethyl)-	1089a, 1886m, 1887a, 2524a, 3741, 3743, 4249, 5811b		3393
676.	61892-94-2	3,4-Furandiol, tetrahydro-3-methyl-	3553, 5811b		
677.	40795-25-3	Furanmethanol	1205a, 5034	5811b	
678.	98-00-0	2-Furanmethanol {furfuryl alcohol} 	172, 568b, 1099, 1140, 1215, 1338, 1339, 1350, 1352, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1378, 1427, 1461, 1586, 1882, 1963, 2088, 2270, 2337, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2607, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 2939, 3059, 3255, 3302, 3308, 3397, 3410, 3553, 3555, 3557, 3559, 3648, 3795, 3797, 4104, 4159, 4249, 4319, 4407, 5811b	120, 404, 524, 543a, 568b, 937, 953, 984, 1063–1066, 1068–1074, 1590a, 1848, 2079, 2337, 2339a, 2386, 2389, 2544, 2607, 2649, 2861a, 2917a, 2939, 3059, 3547, 3549, 3550, 3555, 3648, 3797, 3905, 3973, 3974a, 4052, 4249, 5079, 5811b	1360, 1375a, 1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404, 3405
679.		2-Furanmethanol, 2,3-dihydro-5-methoxy-	2775		
680.	60047-17-8	2-Furanmethanol, 5-ethenyltetrahydro-α,α, 5-trimethyl-		404, 937, 2389,2544, 3555, 4249	
681.	5989-33-3 60047-17-8	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*Z*)- {*cis*-linalool oxide}		172a, 174b, 404, 568b, 1053, 2336, 2338, 2339a, 2386, 2389, 2544, 2917a, 3266, 3555, 4249	
682.	23007-29-6	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*E*)- {*trans*-linalool oxide}		172a, 174b, 568b, 1053, 2339a, 2917a, 3266	
683.	55664-77-2	2-Furanmethanol, methyl-		4012, 4249	
684.	3857-25-8	2-Furanmethanol, 5-methyl-	1586, 1882, 2543, 2767, 2775, 3410, 3557, 5811b	404, 1590a, 2917a, 3547, 3549	
685.	54774-28-6	2-Furanmethanol, 5-methyltetrahydro-		2917a	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
686.	61481-02-5	2-Furanmethanol, 5-(1-pyrrolidinylmethyl)-	4249		
687.	97-99-4	2-Furanmethanol, tetrahydro-	222–224, 568b, 2543, 2773, 4249	568b, 2389, 2544, 4249, 5811b	
688.	4412-91-3	3-Furanmethanol	4249	5811b	
689.	29848-46-2	3-Furanol, tetrahydro-5,5-dimethyl-	3553, 4249		
690.	66607-70-3	3-Furanol, tetrahydro-5-[6-hydroxy-3-(1-methylethyl)-1-heptenyl]-5-methyl- 		1156, 3851, 4090	
691.	61892-43-1	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-4-hydroxy-	568b, 1351, 1352, 1375, 1375b, 1586, 3553, 3557, 5811b		
692.		2(3*H*)-Furanone, 4-(acetyloxy)dihydro-5-hydroxy-	568b, 4249		
693.	61892-44-2	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-4-hydroxy-	1351, 1352, 3553, 5811b		
694.	13092-55-2	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-	1351, 1352, 1882, 2777, 3553, 4249		
695.	17675-99-9	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-, (*Z*)-	2777, 5811b		
696.	25596-90-1	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-(3R,4S)	5811, 5811a, 5811b		
697.		2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-	568b, 2321, 4249		
698.	61892-57-7	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-4-methyl-	1351, 1352, 3553, 3557, 4249, 5811b		
699.	18465-71-9	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-, (3R-*Z*)-	1351, 1352, 1360, 1375a, 1586, 2767, 3553, 3557		1360, 1375a
700.	63700-30-1	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-	568b, 4249, 5811b		
701.		2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-methyl-	568b, 4249		
702.		2(3*H*)-Furanone, dihydro-3,4-dihydroxy-4-methyl-	1375, 1375b, 1586, 2761, 2762, 2765–2767, 2777, 3553, 3557, 4249		
703.		2(3*H*)-Furanone, dihydro-4,4-dimethyl-5-hydroxymethyl-	568b, 4249		
704.	72902-81-9	2(3*H*)-Furanone, dihydro-3,3-dimethyl-4-hydroxy-	568b, 4249		
705.	61989-58-0	2(3*H*)-Furanone, dihydro-5-(1,2-dihydroxyethyl)- 	5811, 5811a, 5811b		
706.	158815-74-8	2(3*H*)-Furanone, dihydro-5-(3-ethyl-4-methyl-1-pentenyl)-3-hydroxy-5-methyl-		4249, 5811b	
707.	61892-46-4	2(3*H*)-Furanone, dihydro-4-ethynyl-5-hydroxy-3-methyl-	1351, 1352, 3553, 4249, 5811b		
708.		2(3*H*)-Furanone, dihydro(hydroxy)-	2570		
709.		2(3*H*)-Furanone, dihydro(hydroxymethyl)-	1360, 1375a, 1586, 2570, 2767, 4249		1360, 1375a
710.	18132-98-4	2(3*H*)-Furanone, dihydro-3-(hydroxymethyl)-	568b, 1350, 1375, 1375b, 2543, 3553, 3557, 4249, 5811b		3402, 3404,

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

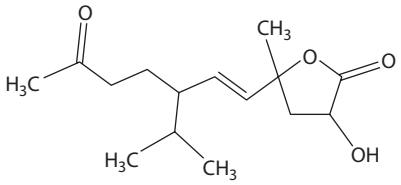
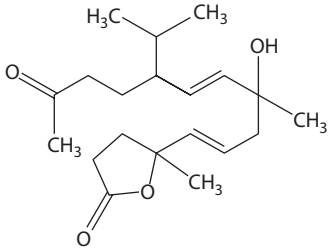
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
711.	19444-84-9	2(3*H*)-Furanone, dihydro-3-hydroxy-	568b, 1350–1352, 1354, 1360, 1371, 1375, 1375a, 1375b, 2493, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3553, 3557, 5811b		1354, 1360, 1375a, 3401, 3402, 3404, 3405
712.	19444-86-1	2(3*H*)-Furanone, dihydro-3-hydroxy-3-(hydroxymethyl)-	1351, 1352, 3553, 5811b		
713.	1192-42-3	2(3*H*)-Furanone, dihydro-3-hydroxy-3-methyl-	4249		
714.	6969-43-3	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4,5-trimethyl-		2544, 4249	
715.	52126-90-6	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-	568b, 1235, 1351, 1352, 1375, 1375b, 2387, 2570, 2761, 2762, 3302, 3410, 3553, 3557, 4249, 5811b	404, 568b, 1256, 2386, 2389, 2544, 2917a, 3188, 4249	2387
716.	599-04-2	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (R)-	1360, 1375a, 1586, 2543, 2767, 2775, 2777, 3553, 3557	404, 1256, 2389, 2544, 3549, 3550	1360, 1375a
717.		2(3*H*)-Furanone, dihydro-3-hydroxy-5-(1-hydroxyethyl)-	568b, 1351, 1352, 2570, 2765–2767, 2777, 3553, 4249		
718.		2(3*H*)-Furanone, dihydro-3-hydroxy-5-(1-hydroxyethyl)- {isomer}	568b, 4249		
719.	61892-52-2	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-	568b, 1351, 1352, 2570, 2761, 2762, 2767, 3553, 4249, 5811b		
720.	61892-50-0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-5-methyl-	568b, 1351, 1352, 1375, 1375b, 1586, 2767, 3553, 3557, 4249, 5811b		
721.	53561-62-9	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-	568b, 1351, 1352, 3553, 4249		
722.		2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl- {isomer}	568b, 4249		
723.	158815-71-5	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1*E*,3S*)]]- 		4249, 5811b	
724.		2(3*H*)-Furanone, dihydro-3-hydroxy-3,4,4-trimethyl-	568b, 4249		
725.	5469-16-9	2(3*H*)-Furanone, dihydro-4-hydroxy-	568b, 1351, 1352, 1371, 1586, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3553, 3557, 4249, 5811b	568b, 3550, 4249	3402, 3405
726.	3285-47-0	2(3*H*)-Furanone, dihydro-4-hydroxy-3,3-dimethyl-	2775		
727.	61892-45-3	2(3*H*)-Furanone, dihydro-4-hydroxy-3-(hydroxymethyl)-	568b, 1351, 1352, 3553, 4249, 5811b		
728.	36679-81-9	2(3*H*)-Furanone, dihydro-4-(hydroxymethyl)-	1352, 1360, 1371, 1375, 1375a, 1375b, 1586, 2387, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3553, 3557, 4249, 5811b	2389, 2544	1360, 1375a, 2387
729.	34945-05-6	2(3*H*)-Furanone, dihydro-4-hydroxy-4-methyl-	568b, 1351, 1352, 3553, 4249, 5811b		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
730.	50768-69-9	2(3*H*)-Furanone, dihydro-5-hydroxy-	1586, 2761, 2762, 2765–2767, 2773, 2775, 4249		
731.	27610-27-1	2(3*H*)-Furanone, dihydro-5-(1-hydroxyethyl)-	1351, 1352, 1586, 3553, 5811b	2389, 2544, 3219	
732.	61892-47-5	2(3*H*)-Furanone, dihydro-5-hydroxy-4-methyl-	1351, 1352, 3553, 4249, 5811b		
733.	10374-51-3	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-	568b, 1351, 1352, 2387, 2543, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3410, 3553, 3557, 4249, 5811b	568b, 3550, 4249	2387, 3405
734.	61892-55-5	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-4-methyl-	1351, 1352, 3553, 4249, 5811b		
735.	102734-52-1	2(3*H*)-Furanone,dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-,[5S-[5R*(1*E*,4R*,5*E*,7R*)]]- 		453, 4089, 4249, 5811b	
736.	102734-53-2	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5S-[5R*(1*E*,4S*,5*E*,7R*)]]-		4089, 5811b	
737.	102734-54-3	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5R-[5R*(1*E*,4S*,5*E*,7S*)]]-		4089, 5811b	
738.	102734-55-4	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5R-[5R*(1*E*,4R*,5*E*,7S*)]]-		4089	
739.	80744-25-8	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1, 5-undecadienyl]-5-methyl-		4249, 4947	
740.		2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl- {stereoisomer}		4249, 4947	
741.	61892-58-8	2(3*H*)-Furanone, 3-(hydroxymethyl)-5-methyl-	568b, 1352, 1371, 2543, 2570, 2773, 2775, 3553, 4248, 5811b		
742.	28664-35-9	2(5*H*)-Furanone, 3-hydroxy-4,5-dimethyl-		172a, 174b, 1053, 3255, 4249, 4771, 5811b	
743.		2(5*H*)-Furanone,3-hydroxy-5-(1-hydroxyethyl)-	3553, 4249		
744.	54621-96-4	2(5*H*)-Furanone,5-(1-hydroxyethyl)-,[R-(R*,S*)]-	1371, 4249		
745.		2(5*H*)-Furanone, 3-(hydroxymethyl)-	2388, 4249		
746.	80904-75-2	2(5*H*)-Furanone, 4-(hydroxymethyl)-	1351, 3397		
747.	27538-09-6	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl-		174b, 3266	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

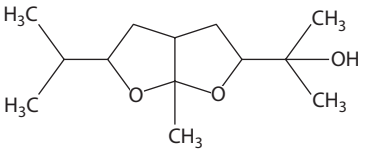
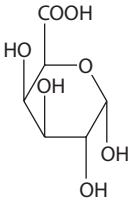
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
748.	17678-20-5	3(2*H*)-Furanone, 4-hydroxy-2-(hydroxymethyl)-5-methyl-	1375, 1375b, 4249		
749.	3658-77-3	3(2*H*)-Furanone, 4-hydroxy-2,5-dimethyl- {furaneol}	568b, 1063–1066, 1068–1074, 1364, 1371, 1882, 2493, 2570, 2601a, 2767, 3266, 3397, 4249, 4407, 5811b	172a, 174b, 568b, 1053, 2917a, 3266, 3370, 4249, 5811b	
750.		Furo[3,2-*b*]furan-2(3*H*)-methanol, tetrahydro-α,α, 3a-trimethyl-5-(1-methylethyl)- 		3543, 3545	
751.	72686-97-6	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, (2α,3aα,5aβ,8β,9aS*)-		4249, 4594	
752.	72747-21-8	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, [2R- (2α,3aβ,5aα,8α,9aR*)]-		4249, 4594	
753.	56857-64-8	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, [3aR-(3αα,5aβ,8β,9aR*)]- {phytuberol}		4101, 4249, 4594, 4910, 5071, 5811b	
754.	9037-55-2	*D*-Galactan		2939, 3797, 3974a, 4249	
755.	9051-94-9	β-(1→4)-*D*-Galactan		5811, 5811b	
756.	526-99-8	Galactaric acid $HOOC-(CHOH)_4-COOH$		1263, 1971, 4249, 5079	
757.		Galactitol, 2,3-di-*O*-methyl- $HOH_2C-[CH(OCH_3]_2-(CHOH)_2-CH_2OH$		3669	
758.		Galactitol, 2,4-di-*O*-methyl- $HOH_2C-CH(OCH_3)-CHOH-CH(OCH_3)-CHOH-CH_2OH$		3669	
759.		Galactitol, 2,6-di-*O*-methyl- $HOH_2C-CH(OCH_3)-(CHOH)_3-CH_2OCH_3$		3669	
760.		Galactitol, 2-*O*-methyl-		3669	
761.		Galactitol, 3-*O*-methyl-		3669	
762.		Galactitol, 2,3,4,6-tetra-*O*-methyl-		3669	
763.		Galactitol, 2,3,4-tri-*O*-methyl-		3669	
764.		Galactitol, 2,3,6-tri-*O*-methyl-		3669	
765.		Galactitol, 2,4,6-tri-*O*-methyl-		3669	
766.	9036-66-2	*D*-Galacto-*L*-arabinan	4249, 4751a	429b, 2939, 3797, 4249	
767.	33818-21-2	α-*D*-Galactofuranose, 1,6-anhydro-	2321, 4249, 5811b		
768.	107389-81-1	Galactoglucomannan		5811b	
769.	9040-29-3	*D*-Galacto-*D*-gluco-*D*-mannan		429b, 4249, 4583	
770.	644-76-8	β-*D*-Galactopyranose, 1,6-anhydro-	2321, 4249, 5811b		
771.	26656-33-7	*D*-Galactopyranuronic acid, homopolymer		4249	
772.	6118-79-2	2-*O*-α-*D*-Galactopyranuronosyl-*L*-mannose,6-deoxy-		5811, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
773.	1948-54-5	Galactose, 2-amino-2-deoxy-		3797, 3974a, 4249	
774.	35381-83-0	Galactose, diether with 1,2,3-propanetriol (1:2)		908, 4249, 4640, 8A09	
775.	59-23-4	*D*-Galactose	3266, 4249, 5580	120, 158, 344a, 933, 1053, 1263, 2070, 2270, 2338, 2939, 3075, 3266, 3555, 3797, 3973, 3974a, 4249, 4411, 5079, 5114, 5768, 5785, 5811b	
776.	7535-00-4	*D*-Galactose, 2-amino-, 2-deoxy- {galactosamine}		3973, 4224, 4226, 4422, 5811b	
777.	1949-89-9	*D*-Galactose, 2-deoxy-		3075	
778.	9001-34-7	Galactosidase		1837b	
779.	97234-09-8	*D*-Galactoside, [(1-oxohexadecatrienyl) oxy][(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249	
780.	97234-10-1	*D*-Galactoside, [(1-oxohexadecyl)oxy] [(1-oxooctadecatrienyl)oxy]propyl, (*Z,Z,Z*)-		4249	
781.	97276-55-6	*D*-Galactoside, [(1-oxooctadecadienyl) oxy][(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249	
782.	97232-94-5	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl) oxy]propyl *O*-*D*-galactosyl-, (all-*Z*)-		4249, 4570	
783.	97170-15-5	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl) oxy]propyl, (all-*Z*)-		4249, 4570	
784.	97233-43-7	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl) oxy]propyl *O*-*D*-galactosyl-, (all-*Z*)-		4249, 4570	
785.	97170-14-4	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl) oxy]propyl, (all-*Z*)-		4249, 4570	
786.	97275-71-3	*D*-Galactoside, 2,3-dihydroxypropyl, 2′(or 3′)-hexadecanoate 3′(or 2′)-octadecadienoate, (*Z,Z*)-		4249	
787.	100092-00-0	Galactoxyloglucan {amyloid}		5811, 5811b	
788.	14982-50-4	Galacturonic acid 	2321, 4249	120, 344a, 722, 1263, 2079, 2939, 3107, 3555, 3797, 3973, 3974a, 4249, 5079, 5114, 5189, 5306	
789.	25990-10-7	Galacturonic acid, homopolymer		1051a, 1971, 4249, 5079, 5114	
790.	685-73-4	*D*-Galacturonic acid	2321, 4249	344a, 722, 2070, 2270, 2939, 3797, 4249, 5811b	
791.	34150-36-2	*D*-Galacturonic acid, anhydro-		4249, 4933	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

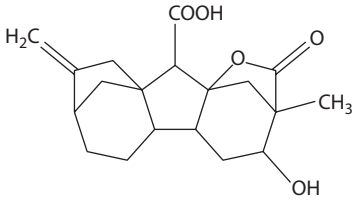
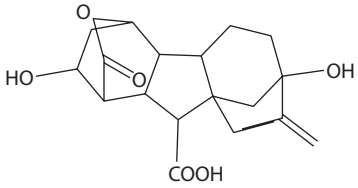
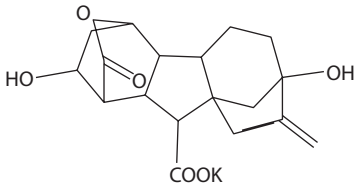
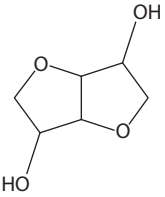
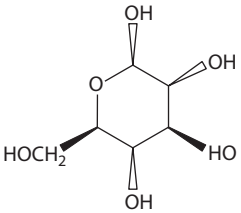
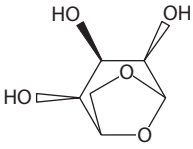
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
792.	25249-06-3	*D*-Galacturonic acid, homopolymer		1051a, 1334e, 1971, 4249	
793.	554-91-6	Gentiobiose		120, 2079, 2270, 3075, 3667, 5079, 5288	
794.	19147-78-5	Gibbane-1,10-dicarboxylic acid, 2,3-epoxy-4a,7-dihydroxy-1-methyl-8-methylene-, 1, 4a-lactone, (1α,2β,3β,4aα,4bβ,10β)-		4249, 4635	
795.	545-97-1	Gibbane-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		429b, 4249, 4831	
796.	468-44-0	Gibbane-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1, 4a-lactone, (1α,2β,4aα,4bβ,10β)- 		2260a, 4249, 4635	
797.	561-56-8	Gibb-2-ene-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,4aα,4bβ,10β)-		429b, 4635	
798.	77-06-5	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)- {gibberellic acid} 		527a, 683a, 5804, 5811b	
799.	125-67-7	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, potassium salt {gibberellic acid, potassium salt} 		3633, 4249	
800.	510-75-8	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		429b, 683a	
801.	9037-91-6	Glucan		842, 1102	
802.	9051-97-2	β-*D*-Glucan, (1→3)-		842, 1102, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
803.	9012-72-0	β-(1,3)-*D*-Glucan {glucan}		5811	
804.	9044-93-3	β-1,3-Glucanase		1111, 1430a	
805.	652-67-5	*D*-Glucitol, 1,4:3,6-dianhydro- 	5811, 5811a, 5811b		
806.	4451-30-3	β-*D*-Glucofuranose, 1,5:3,6-dianhydro-	5811, 5811a, 5811b	5811, 5811a, 5811b	
807.	7425-74-3	β-*D*-Glucofuranose, 1,6-anhydro-	1883, 2939, 4249, 5811b	429b, 5811b	2466, 3402, 3405, 4249
808.	66537-22-2	Glucometasaccharinic acid, γ-lactone	2493, 5811b	4249	
809.	492-62-6	α-*D*-Glucopyranose 		2079, 3667, 4249	
810.	492-61-5	β-*D*-Glucopyranose	5811b	2079, 3667, 4249	
811.	60517-74-0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)		5811b	
812.	25545-13-5	*D*-Glucopyranose, 4-(4-hydroxybenzoate)		4249, 4915	
813.	23445-11-6	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)		4249, 4915	
814.	41682-52-4	β-*D*-Glucopyranose, 1-(3-phenyl-2-propenoate)		429b, 4249, 4915	
815.	59-56-3	α-*D*-Glucopyranose, 1-(dihydrogen phosphate)		120	
816.	498-07-7	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan} 	277, 568b, 1089a, 1351, 1354, 1364, 1371, 1375a, 1377, 1378, 1586, 1887a, 1971, 2170, 2270, 2493, 2524a, 2601a, 2607, 2761, 2762, 2765–2767, 2777, 2850, 2939, 3302, 3308, 3462, 3553, 3557, 3653, 3797, 3963, 4199, 4200, 4202, 4249, 5079, 5811b	568b, 2607, 3430, 3973, 4249, 5079, 5811b	1354, 1375a, 1377, 1378, 3402, 3405, 4249
817.	61891-55-2	β-*D*-Glucopyranose, 1,6-anhydro-, monoacetate	568b, 3553, 4249, 5811b		
818.	10139-18-1	α-*D*-Glucopyranose, 1,6-bis(dihydrogen phosphate)		429b	
819.	21056-52-0	β-*D*-Glucopyranose, 1-benzoate		4249, 4915	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

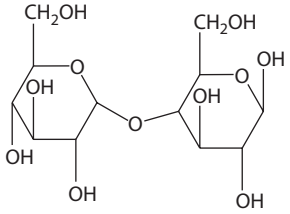
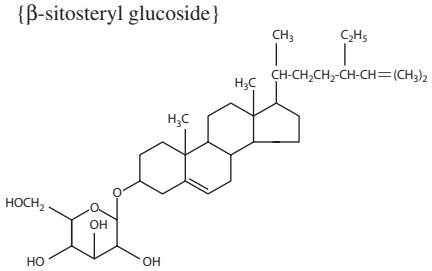
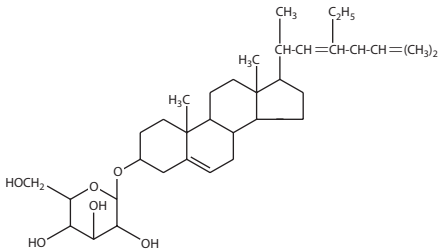
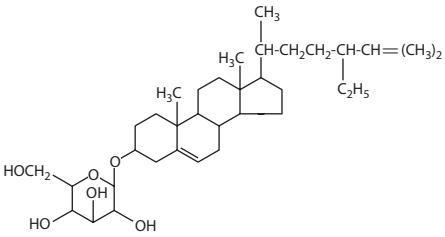
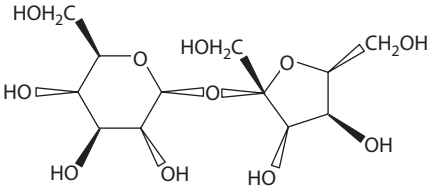
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
820.	69-79-4 4482-75-1 9005-84-9	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin; α-maltose} 		120, 429b, 1063–1066, 1068–1074, 1835b, 2079, 2270, 2283, 3018, 3075, 3555, 3667, 3974a, 4249, 4411, 4841a, 5079, 5189, 5344, 5449, 5768, 5819	
821.		α-*D*-Glucopyranose, 1,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
822.		α-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
823.	133-99-3	β-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {β-maltose}		429b, 2079, 3555, 3667, 3974a, 4249	
824.	64461-84-3	β-*D*-Glucopyranose, 6-(3-phenyl-2-propenoate)		3367a, 4249, 4915	
825.		β-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
826.	7724-09-6	β-*D*-Glucopyranoside, (2-hydroxyphenyl) methyl		4249, 4790	
827.	7073-61-2	β-*D*-Glucopyranoside, (3β)-cholest-5-en-3-yl {cholesteryl glucoside}	648, 1434, 4249, 4534	390, 4249	
828.	32214-82-7	β-*D*-Glucopyranoside, (3β)-ergost-5-en-3-yl {campesteryl glucoside}	648, 2018, 2019, 2079, 3308, 3667, 4249	2018, 2019, 4249, 5777	
829.		β-*D*-Glucopyranoside, 3-hexen-1-yl {3-hexen-1-yl glucoside; leaf acid glucoside}		740	
830.	474-58-8 20431-48-5	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl {β-sitosteryl glucoside} 	648, 2018, 2019, 2939, 3296, 3302, 3308, 4249	1079, 2018, 2019, 2270, 2939, 3296, 3302, 3346, 3349, 4249	
831.	19716-26-8	β-*D*-Glucopyranoside, (3β,22*E*)-stigmasta-5, 22-dien-3-yl {stigmasteryl glucoside} 	648, 908, 2018, 2019, 2939, 3296, 3302, 3308, 4249, 4534	908, 2018, 2019, 3302, 3346, 3349, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

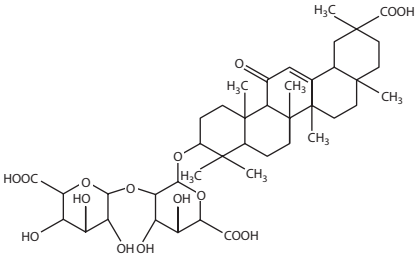
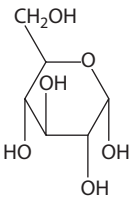
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
832.	51064-38-1	β-*D*-Glucopyranoside, (3β,24S)-stigmast-5-en-3-yl {γ-sitosteryl glucoside} 	2018	120, 2087, 3346, 4249	
833.	57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose} 	1264, 1265, 1361, 4249, 5811b	71, 120, 172c, 248, 321b, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1264, 1265, 1289, 1361, 1933a, 1958, 1960, 1971, 2070, 2079, 2270, 2283, 2313a, 2337, 2532, 2818, 2911c, 2939, 2947c, 3059, 3075, 3266, 3370, 3398, 3409, 3449, 3461, 3462, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3973, 3974a, 3974b, 4249, 4411, 4990, 5079, 5108, 5109, 5126, 5189, 5449, 5562, 5679, 5692, 5748, 5768, 5811b, 5819, 5836, 5896	
834.	126-14-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate		1053, 3266	
835.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-		4990	
836.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-3′-acetyl-		4990	
837.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-4′-acetyl-		4990	
838.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-		4990	
839.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′-*O*-acetyl-		4990	
840.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-4′-*O*-acetyl-		4990	
841.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′,4′-*O*-diacetyl-		4990	
842.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-1′,3′,4′-*O*-triacetyl-		4990	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
843.	470-55-3	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)-O-α-*D*-galactopyranosyl-(1→6)-{stachyose}		429b, 1971, 3797, 4249, 5811b	
844.	512-69-6	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)- {raffinose}		3075, 1971, 3797, 4249, 5768, 5811b	
845.	13101-54-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→4)- {erlose}		429b, 3667, 4249	
846.	25954-44-3	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-β-*D*-glucopyranosyl-(1→6)-		429b, 4249, 4460	
847.	98913-58-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 3-methylpentanoate		4249, 5811b	
848.	154063-13-5	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(2-methylbutanoate)		3606	
849.	97614-61-4	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(3-methylpentanoate)		3606, 5811b	
850.	106033-38-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(3-methylpentanoate), [2(S),3(S),4(S)]-		4249, 5811b	
851.	41055-68-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, labeled with ^{13}C		4249, 4720,	
852.	21291-36-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→6)-		429b, 3667, 4249	
853.	88848-61-7	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7- (1-methylethenyl)-2-naphthalenyl 2-*O*-β-*D*-glucopyranosyl-,[1S-(1α,2β,3α,7β)]-		4249, 4716, 4717, 5811b	
854.	99499-89-5	β-*D*-Glucopyranoside,1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl*O*-6-deoxy-α-*L*-mannopyranosyl-(1→4)-*O*-β-*D*-glucopyranosyl-(1→4)-, [1S-(1α,2β,3α,7β)]-		4249, 5811b	
855.	138-52-3	β-*D*-Glucopyranoside, 2-(hydroxymethyl) phenyl		4249, 4790	
856.	136448-99-2	β-*D*-Glucopyranoside, 2-[5-(acetyloxy)-1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl]-2-hydroxypropyl, 2,3,4,6-tetraacetate, [2R-[2α(S*),5α,8β,8aα]]-		4249, 5811b	
857.	75039-16-6	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl, mono(dihydrogen phosphate) (ester), (*E*)-		4249, 4813	
858.	62512-96-3	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)butyl		4249	
859.	78081-83-1	β-*D*-Glucopyranoside, 3-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0] hept-1-yl)-1-methyl-2-propenyl		4249, 4713	
860.	63648-83-9	α-*D*-Glucopyranoside, 3-*O*-acetyl-β-*D*-fructofuranosyl		4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
861.	470-57-5	α-*D*-Glucopyranoside, *O*-α-*D*-galactopyranosyl-(1→6)-β-*D*-fructofuranosyl {theanderose}		3667, 4249	
862.	1464-44-4	β-*D*-Glucopyranoside, phenyl		689a, 2527, 4249	
863.	1405-86-3	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid {3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid; glycyrrhizin} 		174e, 242, 743, 1356, 1361, 1671, 2313a, 3390, 3555, 4623, 5019, 5811b	
864.	53596-04-0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated 3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated; glycyrrhizin ammoniated}		172a, 174b, 1053, 3266	
865.	50-99-7 26655-34-5	α-*D*-Glucose 	1264, 1265, 1352, 1360, 1361, 1371, 1375a, 1883, 1944, 2145, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	72, 120, 172c, 174b, 248, 321b, 480, 727, 840, 924, 933, 1053, 1063–1066, 1068–1074, 1077b, 1128a, 1141, 1142, 1264, 1265, 1289, 1352, 1361, 1835b, 1835d, 1863, 1916, 1933a, 1971, 2070, 2079, 2270, 2283, 2313a, 2338, 2339b, 2381, 2394a, 2532, 2704a, 2850, 2911c, 2913, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3913, 3973, 3974a, 4103, 4159, 4249, 4275, 4411, 4999, 5079, 5108, 5109, 5126, 5189, 5255, 5344, 5449, 5562, 5655, 5656, 5698, 5748, 5768, 5774, 5811b, 5819, 5831	1360, 1375a

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

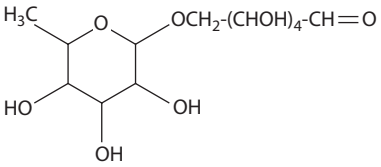
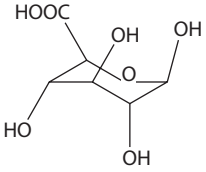
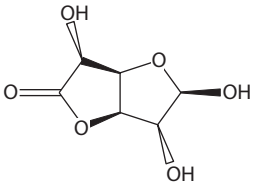
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
866.	110187-42-3	Glucose, labeled with ^{13}C		4249, 4720	
867.	9050-36-6	α-*D*-Glucose, labeled with ^{14}C		1264, 1265, 5785, 25A30, 25A74	
868.	3416-24-8	*D*-Glucose, 2-deoxy-, 2-amino- {glucosamine}		1032, 1063–1066, 1068–1074, 2445a, 3705, 3797, 3973, 3974a, 4224, 4226, 4249, 4422, 5540, 5811b	
869.	90-74-4	*D*-Glucose, *6-O*-(6-deoxy-α-*L*-mannopyranosyl)- {rutinose} 		1971. 5777, 5811	
870.	1398-61-4	*D*-Glucose, β-(1,4)-2-acetamido-2-deoxy-		1102	
871.	28905-12-6	β-*D*-Glucose	1354, 1360, 1375a, 2761, 2762, 2765, 2766, 2777	3667, 4275	1354, 1360, 1375a
872.	37294-28-3	Glucoxylan		429b, 4248	
873.	66369-21-9	Glucuronoarabinoxylan		5811	
874.	576-37-4	Glucuronic acid 	312, 4249	120, 2070, 2939, 3973, 4249, 4360a, 5079, 5478, 5785	
875.	6556-12-3	*D*-Glucuronic acid		5811	
876.	14984-34-0	*D*-Glucuronic acid, monosodium salt		5811b	
877.	28905-07-9	α-*D*-Glucuronic acid, methyl ester		4249	
878.	32449-92-6	*D*-Glucurono-3,6-lactone 	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249		1360, 1375a
879.	62930-75-0	Glucuronomannan		2042a, 2618a	
880.	77272-02-7	Glucuronomannoarabinan		4249, 4428	
881.	37317-38-7	Glucuronoxylan		5811	
882.	4429-05-4	Glycine, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
883.	9034-32-6	Hemicellulose		120, 385, 385a, 842, 1838, 1887, 2056, 2154, 2283, 2850, 2939, 3059, 3372, 3665a, 3702, 3973, 4249, 5079, 5189, 5344, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
884.	63100-39-0	Hemicellulose A		120, 3973, 4249	
885.	63100-40-3	Hemicellulose B		120, 3973, 4249	
886.	65058-12-0	Hemicellulose C		3973, 4249, 4805	
887.	15594-90-8	1-Heneicosanol $H_3C\text{-}(CH_2)_{19}\text{-}CH_2OH$	172, 812, 3059, 3251, 3276, 3302, 3299, 5811b	812, 1893b, 3299, 3613a, 3797, 3973, 3974a	
888.	2004-39-9	1-Heptacosanol $H_3C\text{-}(CH_2)_{25}\text{-}CH_2OH$		3613a, 3755, 4249, 4678	
889.	63785-26-2	1-Heptacosanol, 26-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{24}\text{-}CH_2OH$		4249, 4964	
890.	150462-99-0	Heptadecanoic acid, 16-methyl-, 2-(acetyloxy)-1-(hydroxymethyl)ethyl ester		4249	
891.	150462-98-9	Heptadecanoic acid, 16-methyl-, 3-(acetyloxy)-2-hydroxypropyl ester		4249	
892.	1454-85-9	1-Heptadecanol $H_3C\text{-}(CH_2)_{15}\text{-}CH_2OH$	172, 812, 3251, 3276, 3299, 3302, 5811b	812, 3299, 3797, 3973, 3974a	
893.	41744-75-6	1-Heptadecanol, 16-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{14}\text{-}CH_2OH$	1586, 2570	4249, 4964	
894.	51945-98-3	1,5-Heptadiene-3,4-diol $H_3C\text{-}CH{=}CH\text{-}CHOH\text{-}CHOH\text{-}CH{=}CH_2$		4249	
895.		1,6-Heptadien-4-ol	5770		
896.	77411-76-8	3,5-Heptadien-2-ol, 2,6-dimethyl-		2917a	
897.	57935-33-8	4,6-Heptadien-1-ol, 6-methyl-3-(1-methylethyl)-, (*E*)-		404, 940, 1156, 3547, 3550, 4090, 4249	
898.	535-24-0	Heptanedioic acid, 2,6-diamino-3-hydroxy- $HOOC\text{-}CH(NH_2)\text{-}(CH_2)_2\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$		4249, 4602	
899.	53535-33-4	Heptanol		5811, 5811b	
900.	111-70-6	1-Heptanol $H_3C\text{-}(CH_2)_5\text{-}CH_2OH$	172, 568b, 3255, 4249	568b, 2389, 2544, 4249	
901.	1653-40-3	1-Heptanol, 6-methyl-		4249, 5811b	
902.	543-49-7	2-Heptanol		404, 2339a	
903.	4730-22-7	2-Heptanol, 6-methyl-		568b, 4249	
904.	52812-43-8	2-Heptanone, 5-[3-(1-hydroxy-1-methylethyl) oxiranyl]-6-methyl-	2545	940, 942, 4249	
905.	72693-12-0	2-Heptanone, 6-hydroxy-	3553, 4249		
906.		4-Heptanone, 5-hydroxy-	568b, 4249		
907.	34098-52-7	*D*-xylo-Hept-2-enaricacid,2,6-anhydro-3-deoxy-{2*H*-pyran-2,4-dicarboxylic acid, 3,4-dihydro-3,4-dihydroxy-}		4249	
908.	77288-93-8	2-Heptene-1,6-diol, 3-(1-methylethyl)-, (*E*)- $H_3C\text{-}CHOH\text{-}(CH_2)_2\text{-}C[CH(CH_3)_2]{=}CH\text{-}CH_2OH$		1156, 4090, 4249, 4948	
909.	105728-84-5	4-Heptenoic acid, 6-hydroxy-		2917a	
910.	1335-09-7	Heptenol, methyl-		174b, 3266	
911.	33467-78-4	2-Hepten-1-ol (*E*) $H_3C\text{-}(CH_2)_3\text{-}CH{=}CH\text{-}CH_2OH$		3550	
912.	55454-22-3	2-Hepten-1-ol (*Z*)		4249	
913.	70898-26-9	3-Hepten-2-ol, 5-ethyl-2,6-dimethyl-		1660, 4249	
914.		3-Hepten-2-ol, 5-(1-methylethy)-2-methyl-		1660	
915.	58927-84-7	4-Hepten-2-ol, 6-methyl-, (*E*)-		3547, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

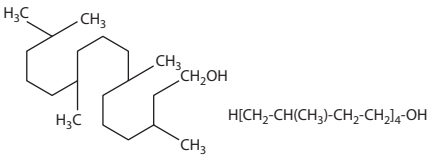
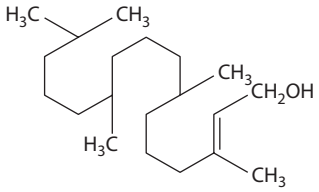
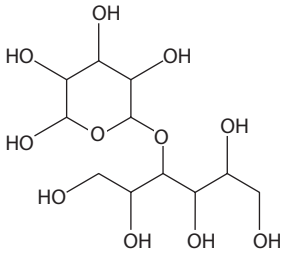
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
916.	1569-60-4	5-Hepten-2-ol, 6-methyl-		404, 1156, 2338, 2339a, 2389, 2544, 2917a, 3205, 3215, 3219, 4090, 4249, 5811b	
917.	42201-30-9	6-Hepten-2-ol, 4-methylene-		404, 937	
918.	57782-61-3	6-Hepten-2-ol, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)-		943, 944, 1156, 4090, 4249, 5811b	
919.	133561-46-3	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-		5811, 5811b	
920.	129742-47-8	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-, [R-(*E*)]-		4249, 5811b	
921.	104669-35-4	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-4-hydroxy-2-methyl-2-furanyl)-		232, 943, 944, 1156, 3852, 4090, 4249, 4780, 5811b	
922.	160115-55-9	6-Hepten-2-one, 7-[4-(acetyloxy)tetrahydro-5-hydroxy-2-methyl-2-furanyl]-5-(1-methylethyl)-		4249	
923.		Heptose		5777	
924.	506-52-5	1-Hexacosanol	5811b	3613a, 3755, 4249, 4573	
925.	63785-25-1	1-Hexacosanol, 24-methyl-		3613a, 4249, 4964	
926.		1-Hexacosanol, 25-methyl-		3613a	
927.	23470-00-0	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester H_3C-$(CH_2)_{14}$–COO-CH═$(CH_2OH)_2$ {glyceryl 2-hexadecanoate}	2601a		
928.	3233-90-7	Hexadecanoic acid, 10,16-dihydroxy-		3973, 3974a, 4249, 4822	
929.	506-13-8	Hexadecanoic acid, 16-hydroxy- $HOCH_2$-$(CH_2)_{14}$-COOH		2326a, 4249, 4774	
930.	124-29-8	1-Hexadecanol H_3C-$(CH_2)_{14}$-CH_2OH	172, 568b, 3299, 4249, 5811b	404, 568b, 2339a, 3299, 4098a, 4249, 4964	
931.	2490-43-9	1-Hexadecanol, 14-methyl-		4249, 4964	
932.	645-72-7	1-Hexadecanol, 3,7,11,15-tetramethyl- {dihydrophytol}  	2871, 3251, 3282–3285, 3302, 4249	4098a	
933.	60054-55-9	1-Hexadecanol, 7,11,15-trimethyl-3-methylene-		2389, 2544, 4249	
934.	76540-54-0	1,6,10,14-Hexadecatetraene-3,9-diol, 3,7,11,15-tetramethyl-		4112, 4249	
935.	76540-55-1	2,6,10,15-Hexadecatetraene-1,14-diol, 2,6,10,14-tetramethyl-, [S-(*Z,E,E*)]-		4112, 4249	
936.	63871-00-1	Hexadecatrien-1-ol, 3,7,11,15-tetramethyl-	5811a		
937.	505-32-8 60046-87-9	1-Hexadecen-3-ol, 3,7,11,15-tetramethyl- {isophytol}	1663, 3251, 3284, 3285, 4249, 5811, 5811b	404, 2386, 2389, 2544, 2611, 2917a, 3547, 4249, 5811, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

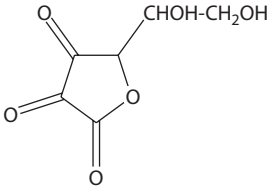
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
938.	22104-83-2	2-Hexadecen-1-ol		4249, 4964	
939.	102608-53-7	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-		2917a	
940.	150-86-7	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(*E*)]]- {phytol} 	172, 568b, 1360, 1375a, 1651, 2601a, 2761, 2762, 2777, 3251, 3282–3285, 3302, 3308, 3608, 4249, 4336, 5067, 5811b	537, 543a, 568b, 722, 1590a, 1651, 1854, 2260, 2270, 2338, 2386, 2389, 2544, 2611, 2917a, 3086, 3547, 3549, 3550, 3608, 3611, 3755, 4098a, 4249, 4336, 5067, 5539, 5811b	1360, 1375a
941.	94806-37-8	1,5-Hexadien-3-ol, 5-methyl-	5770		
942.	50-70-4	Hexane, hexahydroxy- {sorbitol; glucitol} $HOCH_2$-$(CHOH)_4$-CH_2OH	627, 1360, 1375a, 1586, 2761, 2762, 2765–2767, 2777, 2850, 5580	120, 174b, 627, 773, 933, 1221, 1971, 2079, 2195, 2705, 2939, 3075, 3163, 3264, 3266, 3667, 3797, 3973, 3974a, 5079, 5180, 5216, 5811b	1360, 1375a
943.	585-88-6	Hexane, hexahydroxy-, 4-*O*-β-*D*-glucopyranosyl- {maltitol; 4-*O*-β-*D*-glucopyranosyl-*D*-glucitol} 		3163	
944.		Hexane, hexahydroxy-, 2,6-di-*O*-methyl-		3669	
945.		Hexane, hexahydroxy-, 2,3,6-tri-*O*-methyl-		3669	
946.		Hexane, hexahydroxy-, 2,3,4,6-tetra-*O*-methyl-		3669	
947.	1462-11-9	1,5-Hexanediol, 5-methyl-	568b, 4249		
948.	102488-05-1	1,5-Hexanediol, 2-(1-methylethyl)-		5811, 5811b	
949.	77289-00-0	1,5-Hexanediol,2-(1-methylethyl)-,[S-(R*,R*)]-		738, 1156, 4090, 4249, 4948	
950.	2935-44-6	2,5-Hexanediol	568b, 3553, 4249, 5811b	568b, 2389, 2544, 4249	
951.	29044-06-2	2,5-Hexanediol, 2-methyl-		2389, 2544, 4249, 5811b	
952.	61892-85-1	2,5-Hexanedione, 3-hydroxy-	568b, 2767, 3553, 3557, 4249, 5811b		
953.	64350-07-8	Hexanenitrile, 2-hydroxy-	4249	4249	
954.	106-69-4	1,2,6-Hexanetriol	5811		
955.	18990-98-2	1,3,6-Hexanetriol	1586, 2767, 4249		
956.		Hexanoic acid, hydroxy-	3741, 3743		
957.	6064-63-7	Hexanoic acid, 2-hydroxy-		4101, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
958.	6946-90-3	Hexanoic acid, 2-hydroxy-, ethyl ester		5811	
959.	2305-25-1	Hexanoic acid, 3-hydroxy-, ethyl ester		5811	
960.	40309-49-7	Hexanoic acid, 3-hydroxy-5-methyl-		4101, 4249	
961.	1191-25-9	Hexanoic acid, 6-hydroxy-	4249, 4897, 5811b		
962.	25917-35-5	Hexanol	4249	701a, 3973	
963.	111-27-3	1-Hexanol {caproyl alcohol} $H_3C\text{-}(CH_2)_4\text{-}CH_2OH$	172, 568b, 1419, 3555, 4249, 5811b	172a, 174b, 568b, 937, 1053, 2339a, 2917a, 3266, 3547, 3555, 4249, 5811b	
964.	104-76-7	1-Hexanol, 2-ethyl-	1445, 2570, 2767, 2769, 3266, 3557, 4249, 5811b	1053, 1550, 2917a, 3266, 3547, 4249, 5811b	
965.	61949-26-6	1-Hexanol, methyl-	3553, 4249, 5811b		
966.	818-49-5	1-Hexanol, 4-methyl-		404, 5811b	
967.	627-98-5	1-Hexanol, 5-methyl-		674, 4249	
968.	3452-97-9	1-Hexanol, 3,5,5-trimethyl-		172a, 174b, 1053, 3266	
969.	626-93-7	2-Hexanol	568b, 3559, 4249	568b, 2339a, 4249	
970.		2-Hexanol, 2-cyclohexanyl-		2917a	
971.	625-23-0	2-Hexanol, 2-methyl-	568b, 4249	568b, 4249	
972.	627-59-8	2-Hexanol, 5-methyl-	568b, 4249	568b, 4249	
973.	623-37-0	3-Hexanol	568b,1365, 1371, 2775, 3410, 4249	568b, 2337a, 4098a, 4249	
974.	2180-43-0	3-Hexanol, 1-phenyl-	2767, 2769, 4249		
975.		4-Hexanol, 1-phenyl-	2767, 2769		
976.	72693-13-1	2-Hexanone, 5,6-dihydroxy-	3553, 4249	4249	
977.	56745-61-0	2-Hexanone, 5-hydroxy-	2767, 4249		
978.	68208-73-1	2-Hexanone, 6-hydroxy-5-methyl-	2570, 4249		
979.	60924-87-0	2,6,10,14,18,22,26,30,35-Hexatriacontanonaene-1,34-diol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)-		1156, 4090, 4249, 4382	
980.	60924-86-9	2,6,10,14,18,22,26,30,33-Hexatriacontanonaene-1,35-diol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)-		1156, 4090, 4382	
981.	101330-76-1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, labeled with ^{14}C, (*Z,Z,Z*)- {solanesol-^{14}C}		3616	
982.	13190-97-1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)- {solanesol} $H\text{-}[CH_2\text{-}C(CH_3)\text{=}CH\text{-}CH_2]_9\text{-}OH$	85a, 86, 172, 173a, 614, 663, 744, 966, 1099, 1100, 1139, 1231, 1286, 1352, 1375, 1375b, 1431, 1432, 1445, 1651, 1744, 1842, 1944, 2079, 2529, 2590, 2691–2695, 2829, 2832, 2834, 2838, 2939, 3059, 3097, 3133, 3137, 3230, 3251, 3255, 3257, 3270, 3295, 3302, 3308, 3557, 3608, 3797, 3868, 4103, 4249, 4271, 4326, 4336, 4797, 4797a, 4797b, 5512, 5563, 5811b	116, 120, 433, 552, 568a, 614, 657, 669, 840, 908, 965, 1062, 1110, 1149, 1149a, 1352, 1651, 1888, 1893a, 1893b, 1943, 2079, 2338, 2394a, 2529, 2590, 2682, 2914, 2939, 3059, 3097, 3215, 3219, 3269, 3291, 3295, 3329, 3347–3349, 3357, 3359, 3435,	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)- {solanesol} (cont.)		3459–3461, 3470, 3472, 3476, 3493, 3560, 3561, 3604, 3605, 3608, 3611, 3613, 3616, 3630, 3707, 3755, 3797, 3811, 3924, 3971, 3973, 3974a, 3974b, 4103, 4150, 4249, 4276, 4336, 4382, 5009, 5050, 5658, 5682, 5811b, 5867, 5896, 2A01, 2A02, 2A03	
983.	28261-03-2	Hexenol		5811, 5811b	
984.	928-95-0	2-Hexen-1-ol		172a, 174b, 1053, 2917a, 3266	
985.	2305-21-7	2-Hexen-1-ol, (*E*)-	5811b	174b, 3266	
986.	544-12-7	3-Hexen-1-ol		1053, 3266, 3370, 5811b	
987.	928-97-2	3-Hexen-1-ol, (*E*)-		404, 1053, 1157, 2389, 2544, 3266, 3547, 4249	
988.	928-96-1	3-Hexen-1-ol, (*Z*)- {leaf alcohol}	297, 316, 568b,3186, 4249	297, 316, 404, 568b,740, 1053, 1590a, 2339a, 2339b, 2386, 2389, 2544, 2914, 3186, 3188, 3219, 3266, 3354, 4098a, 4249, 5811b	
989.		3-Hexen-1-ol, (*Z*)-, labeled with ^{14}C {leaf alcohol-^{14}C}	316, 3186,4249	316	
990.	58461-27-1	4-Hexen-1-ol, 5-methyl-2-(1-methylethyl)-	568b, 4249		
991.	821-41-0	5-Hexen-1-ol	568b, 4249		
992.	121197-12-4	5-Hexen-3-one, 4,5-dihydroxy-	4249	5811b	
993.	33124-69-5	threo-2,3-Hexodiulosonic acid, γ-lactone {2,3-diketogulonic acid, γ-lactone} 		4249	
994.	490-83-5	*L*-threo-2,3-Hexodiulosonic acid, γ-lactone {*L*-2,3-diketogulonic acid, γ-lactone}		429b	
995.	45009-62-9	Hexoses		429b, 3430	
996.	8064-26-4	Holocellulose		3702, 3973, 4249, 4261, 4262, 4573	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

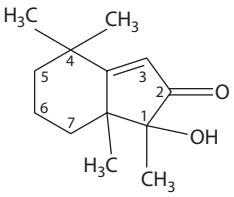
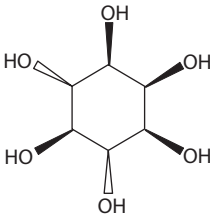
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
997.	498-19-1	Homoserine {2-amino-4-hydroxybutanoic acid}	3557	1351, 2337, 2939, 3491, 3797, 3974a	
	672-15-1	HO-$(CH_2)_2$-CH(NH_2)-COOH			
998.	1415-93-6	Humic acids		2665a	
999.	39815-71-9	2*H*-Inden-2-one, 1,4,5,6,7,7a-hexahydro-1-hydroxy-1,4,4,7a-tetramethyl- 		937, 3219, 4249, 5811b	
1000.	526-55-6	1*H*-Indole-3-ethanol		4249	
1001.	6917-35-7	Inositol	966, 1354, 1360, 1375a, 2761, 2762, 2765, 2766, 2777, 2939, 3302, 3876, 4249, 5580	120, 840, 2079, 2270, 2283, 2704, 2939, 2947b, 3075, 3656, 3797, 3876, 4249, 5079, 5189, 5383, 5384, 5595, 5768, 5852	1354, 1360, 1375a
1002.	87-89-8	myo-Inositol 	1572, 5811b	1572, 3667, 3974a, 4249, 4427, 5811b	
1003.	3615-82-5	myo-Inositol, hexakis(dihydrogen phosphate), calcium magnesium salt {phytin}		429b, 4249, 5079, 5384	
1004.	71608-14-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl- (1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]octadecyl hydrogen phosphate], disodium salt		429b	
1005.	71608-17-8	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl- (1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-1-[(2-hydroxy-1-oxopentacosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838	
1006.	71608-15-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1007.	71608-16-7	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4- dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838	
1008.	71608-19-0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl) amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838	
1009.	71608-20-3	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl) amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838	
1010.	71608-21-4	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838	
1011.	71608-22-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-,1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxopentacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838	
1012.	71608-23-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxohexacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838	
1013.	89194-80-9	myo-Inositol, *O*-*D*-glucopyranosyl-		3667	
1014.	49741-70-0	*D*-myo-Inositol, *O*-*D*-glucopyranosyl-		429b	
1015.		myo-Inositol, phosphatidyl-		3973	
1016.	8013-90-9	Ionone, 4-hydroxy- {see 3-buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- and 3-buten-2-one, 4-(4-hydroxy-2, 6,6-trimethyl-2-cyclohexen-1-yl)-}	2767		
1017.	52655-10-4	Isoeicosanol		4249	
1018.	63-42-3	Lactose		933, 1361, 1835b, 3075, 5079, 5811b	
1019.	79-62-9	Lanost-8-en-3-ol, (3β)-		4249, 4686	
1020.	6890-88-6	Lanost-8-en-3-ol, 24-methylene-, (3β)-		4249, 4431	
1021.	26409-08-5	Lanost-9(11)-en-3-ol, 24,25-epoxy-, (3β)-		429c	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

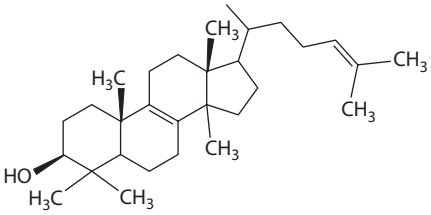
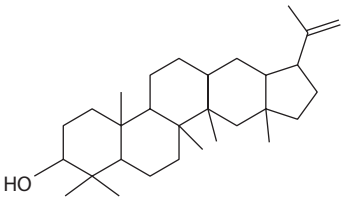
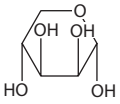
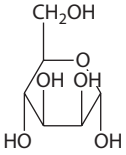
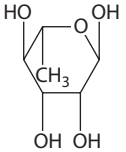
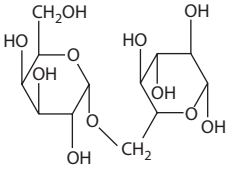
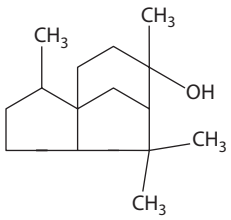
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1022.	79-63-0	Lanosta-8,24-dien-3-ol, (3β)- {lanosterol} 		1117, 4249, 4480	
1023.	67493-77-0	Lanostane-3,7,11-triol, 3,7-diacetate, (3β,7β,11β)-		4249, 4497	
1024.	70898-27-0	Lanostane-3,7-diol, (3β,7β)-		4249, 4497	
1025.	545-47-1	Lup-20(29)-en-3-ol, (3β)- 		1157a, 3098, 4249	
1026.	1190-94-9 28902-93-4	Lysine, hydroxy-		726, 749, 752–754, 4249	
1027.	1114-34-7	Lyxose 	5580	3075	
1028.	69-65-8	*D*-Mannitol {cordycepic acid} $HOCH_2$-$(CHOH)_4$-CH_2OH	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249, 5580	312, 1360, 2761, 2777, 3075, 3555, 3973, 4249, 5811b	1360, 1375a
1029.	31103-86-3	Mannose 	1587, 2761, 2762, 2765, 2766, 2777, 3266, 3555, 4249	1053, 2070, 3266, 3555, 3797, 3973, 3974a, 4249, 5768	
1030.	3458-28-4	*D*-Mannose {seminose}	1360, 1375a, 2765, 2766, 4249	3797, 4249, 5811b	1360, 1375a
1031.	14307-02-9	*D*-Mannose, 2-amino-2-deoxy- {mannosamine}		1063–1066, 1068–1074, 1370, 4249, 4422, 5811b	
1032.	3615-41-6	*L*-Mannose, 6-deoxy- {α-rhamnose} 	3555, 5580	71, 120, 158, 344a, 2070, 2079, 2270, 2338, 2704a, 2939, 3075, 3555, 3655b, 3797, 3973, 3974a, 4249, 5079, 5698, 5768, 5811b, 5831	
1033.	585-99-9	Melibiose 		3075	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1034.	77-53-2	1*H*-3a,7-Methanoazulen-6-ol, octahydro-3,6,8, 8-tetramethyl-, [3R-(3α,3aβ,6α,7β,8aα)]- 		2611	
1035.	4586-22-5	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, stereoisomer		4249	
1036.	105300-09-2	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 1a-[(β-*D*-glucopyranosyloxy)methyl]octahydro-5,7β-dimethyl-, [1aR		4249	
1037.	125537-96-4	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 3-(β-*D*-glucopyranosyloxy) octahydro-1a, 5,7b-trimethyl-, [1aS-(1aα,2β,3β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
1038.	125537-95-3	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 4-(β-*D*-glucopyranosyloxy) octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
1039.	105300-10-5	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 5-[(β-*D*-glucopyranosyloxy)methyl]octahydro-1a,7b-dimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
1040.	88848-60-6	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one,6-[(2-O-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]octahydro -1a,5,7b-trimethyl-,[1aS-(1aα,2β,4aβ,5α,6β,7aα,7bα)]-		4249, 4717, 5811b	
1041.	67-56-1	Methanol H_3C-OH	37, 38, 111, 167, 172, 173a, 239, 299, 314, 568b, 605, 639, 643, 645, 722, 916, 1063–1074, 1140, 1348–1350, 1352, 1354, 1365, 1375, 1375a, 1375b, 1377, 1378, 1412–1414, 1416, 1418, 1419, 1422, 1437, 1449, 1495, 1589, 1632, 1741, 1744, 1842, 1875, 2002, 2063, 2079, 2088, 2170, 2180, 2195, 2252, 2270, 2293, 2310, 2313a, 2343, 2394, 2506, 2507, 2520, 2524, 2545, 2570, 2634, 2702, 2703, 2706, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2866, 2939, 2942, 3029, 3048, 3059, 3105, 3132, 3254, 3260, 3266, 3300, 3302, 3308, 3324, 3482, 3493, 3530, 3557, 3583, 3584, 3692, 3880, 3882, 3883, 3901, 3939, 3973, 4005–4007, 4052, 4056, 4162, 4202, 4249, 4257, 4290, 4319, 4733, 5079, 5189, 5359, 5392, 5512, 5554	120, 568b, 1550, 2079, 2293, 2339a, 2394, 2702, 2702a, 2703, 3186, 3188, 3266, 3797, 3974a, 4249, 5079, 5114, 5189, 5306, 5389, 5392, 5811b	1228, 1354, 1375a, 1377, 1378, 2506, 2507, 4052, 4056

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

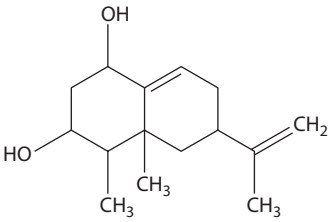
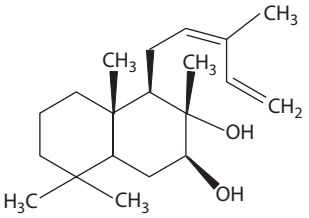
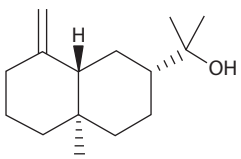
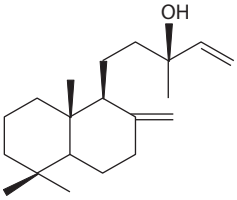
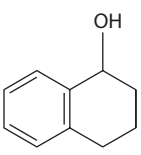
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1042.	79951-97-6	1,2-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl- {11-nor-8-drimanol}		5811, 5811b	
1043.	79886-54-7	1,2-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl-, [1R-(1α,2β,4aβ,8aα)]-		4249, 4949, 5811b	
1044.	37208-05-2	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [1R-(1α,3β,4β,4aα,6α)]- 		1156, 4090, 5811b	
1045.	114393-99-6	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, 3-acetate, [1R-(1α,3β,4)]		4249	
1046.	65513-74-8	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-6-[1-(hydroxymethyl)ethenyl]-4,4a-dimethyl-, (1α,3β,4β,4aα,6α)-		4249	
1047.	27656-76-4	2,3-Naphthalenediol, 1,2α,3β,4,5,6,7,8-octahydro-7α-isopropenyl-1α-methyl-		4249	
1048.	18178-54-6	2,3-Naphthalenediol, 1,2,3,4,5,6,7,8-octahydro-1-methyl-7-(1-methylethenyl)-, [1S-(1α,2β,3α,7β)]- {rishitin}	2601a	1156, 4090, 4249, 4637, 5811b	
1049.	73496-12-5	2,3-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-,[1S-[1α(*E*),2α,3β,4aβ,8aα]]- 		1149, 1149a, 1156, 4090, 4249, 4950	
1050.	102977-87-7	2-Naphthaleneethanol, 3,4-dihydro-1,5,6-trimethyl-		4159b	
1051.	52617-99-9	1-Naphthalenemethanol, decahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [1S-(1α,2β,4aβ,8aα)]-		13, 1661, 4249, 5811b	
1052.	473-15-4	2-Naphthalenemethanol, 1,2α,3,4,4a,5,6,7,8,8aα-decahydro-α,α,4aβ-trimethyl-8-methylene- {β-eudesmol} 		5811, 5811b	
1053.	29484-46-6	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl-, [2S-(2α,4aβ,8aβ)]-		490, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1054.	37574-03-1	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl {*trans*-occidentalol}		5811b	
1055.	473-17-6	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl-, [2R-(2α,4aβ,8aβ)]- {occidentalol}		490, 4249, 5811b	
1056.	117065-22-2	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,6-tetramethyl-, (±)-		5811, 5811b	
1057.	87797-89-5	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,6-tetramethyl-, (R)-		1156, 4090, 4249, 4928	
1058.	5986-36-7	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,8-tetramethyl-, (R)-		4249, 4928, 5811b	
1059.	117065-21-1	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,7,8-tetramethyl-, (±)-		5811, 5811b	
1060.	87797-88-4	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,7,8-tetramethyl-, (R)-		4249, 4928	
1061.	121269-01-0	2-Naphthalenemethanol, 3,4-dihydro-1,5,6-trimethyl-		3547, 4249, 5811b	
1062.	10267-21-7	1-Naphthalenepentanol, decahydro-2-hydroxy-γ,2,5,5,8a-pentamethyl-, [1R-[1α(S*),2β,4aβ,8aα]]		4073b	
1063.		1-Naphthalene-2-pentenol, decahydro-γ,2,5,5,8a-pentamethyl-		4073b	
1064.		1-Naphthalene-2-pentenol, 3,4,4a,5,6,7,8,8a-octahydro-γ,2,5,5,8a-pentamethyl-		4073b	
1065.	596-85-0	1-Naphthalenepropanol, α-ethenyldecahydro-α,5,5,8a-tetramethyl-2-methylene-, [1S-[1α(S*),4aβ,8aα]]- {manool} 		4073b	
1066.	4630-08-4	1-Naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-α,2,5,5,8a-pentamethyl-, [1R-[1α(S*),2β,4aβ,8aα]]- {episclareol}		4073b	
1067.	515-03-7	1-Naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-α,2,5,5,8a-pentamethyl-, [1R-[1α(R*),2β,4aβ,8aα]]- {sclareol}		2308, 2611, 2754, 2755, 4073b	
1068.	57567-06-3	1-Naphthalenepropanol, α-ethenyldecahydro-7-hydroxy-α,5,5,8a-tetramethyl-2-methylene-		4073b	
1069.	529-33-9	1-Naphthalenol, 1,2,3,4-tetrahydro- 	765		
1070.	55591-08-7	1-Naphthalenol, 1,2,3,4-tetrahydro-2,5,8-trimethyl-		2917a	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

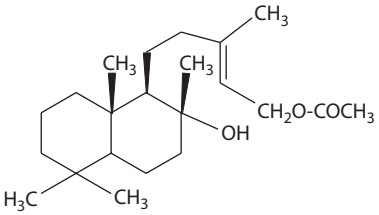
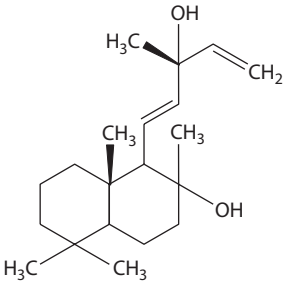
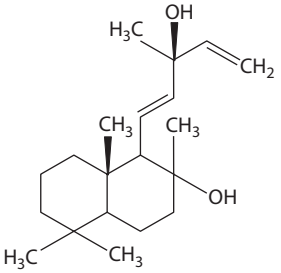
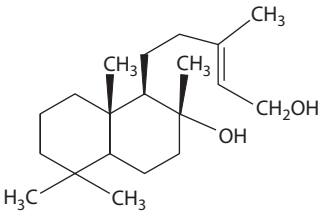
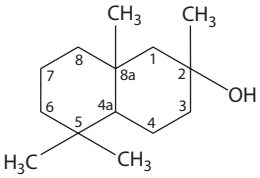
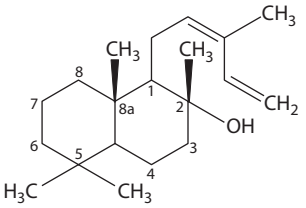
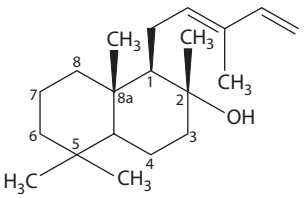
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1071.	30316-22-4	1-Naphthalenol, 1,2,3,4-tetrahydro-3,5,8-trimethyl-	2761, 2762, 2765, 2766, 4249		
1072.	66324-66-1	1-Naphthalenol, 1,2,3,4-tetrahydro-4,5,8-trimethyl-		3547, 4249	
1073.	67494-23-9	1-Naphthalenol, 1,2,3,4-tetrahydro-8-methyl-2-(1-methylethenyl)-, (*Z*)-(±)-		946, 1156, 3547, 4090, 4249	
1074.	31149-06-1	2-Naphthalenol, 1-[5-(acetyloxy)-3-methyl-3-pentenyl]decahydro-2,5,5,8a-tetramethyl-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		1156, 2565, 4090, 4101, 4249	
1075.	66890-73-1	2-Naphthalenol, decahydro-1-(3-hydroxy-3-methyl-1,4-pentadienyl)-2,5,5,8a-tetramethyl-, [1R-[1α(1*E*,3S*),2β,4aβ,8aα]]- 		6, 1149, 1149a, 1156, 4090, 4101	
1076.	66966-02-7	2-Naphthalenol, decahydro-1-(3-hydroxy-3-methyl-1,4-pentadienyl)-2,5,5,8a-tetramethyl -, [1R-[1α(1*E*,3R*),2β,4aβ,8aα]]- 		6, 1149, 1149a, 1156, 4090, 4101	
1077.	10267-31-9	2-Naphthalenol, decahydro-1-(5-hydroxy-3-methyl-3-pentenyl)-2,5,5,8a-tetramethyl-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		1156, 3099, 3613a, 4073b, 4090, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1078.	22343-28-8	2-Naphthalenol, decahydro-1-(5-hydroxy-3-methyl-3-pentenyl)-2,5,5,8a-tetramethyl-, [1R-(1α,2β,4aβ,8aα)]-		4249	
1079.	53163-43-2	2-Naphthalenol, decahydro-1,2,5,5,8a-pentamethyl-, [1R-(1α,2β,4aβ,8aα)]-		13, 1149, 1149a, 1661, 4249, 5811b	
1080.	36211-21-9	2-Naphthalenol, decahydro-2, 5,5,8a-tetramethyl- 		2864a, 5811b	
1081.	49749-17-9	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-, (2α,4aα,8aβ)-(±)-		3547, 4249	
1082.	42569-63-1	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-1,3-pentadienyl)-, [1R-[1α(1*E*,3*E*), 2β,4aβ,8aα]]-	4249, 5811b	4249	
1083.	1616-86-0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-(1α,2β,4aβ,8aα)]- {Z-abienol} 		897, 898, 2338, 2341a, 2786, 2914, 3099, 3607, 3613a, 3621, 3703, 3704, 3706, 4073b, 4090, 4094, 5811b	
1084.	17990-15-7	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-[1α(*E*), 2β,4aβ,8aα]]- 		3099, 3621, 4090, 5811b	
1085.	17990-16-8	2-Naphthalenol,decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-[1α(*Z*), 2β,4aβ,8aα]]-		4249, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

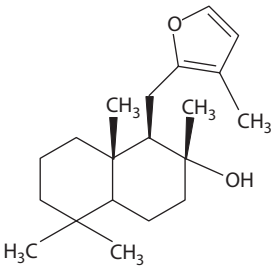
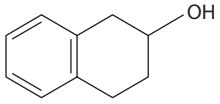
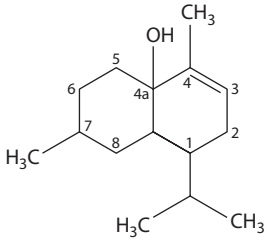
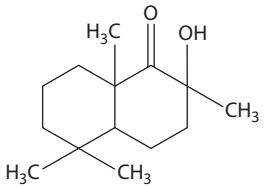
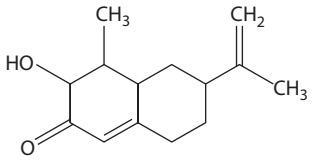
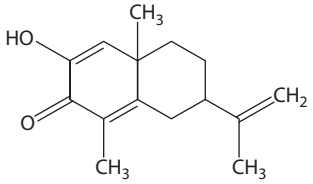
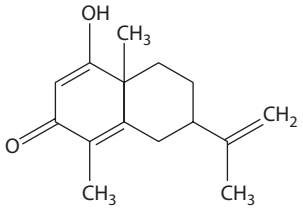
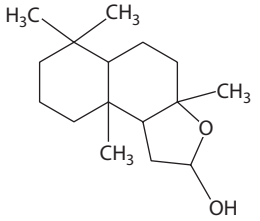
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1086.	62121-32-8	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-[(3-methyl-2-furanyl)methyl]-, [1R-(1α,2β,4aβ,8aα)]- 		1156, 4090, 4101	
1087.	82451-46-5	2-Naphthalenol, decahydro-4a,8,8-trimethyl-3-methylene-4-(3-methyl-2,4-pentadienyl)-, [2S-[2α,4α(*E*), 4aα,8aβ]]-		4073b	
1088.	82458-63-7	2-Naphthalenol, decahydro-4a, 8,8-trimethyl-3-methylene-4-(3-methylene-4-pentenyl)-, [2S-(2α,4α,4aα,8aβ)]-		4073b, 4249, 4819	
1089.	58239-50-2	2-Naphthalenol, decahydro-5,5, 8a-trimethyl-, [2R- (2α,4aα,8aβ)]-		4249	
1090.	530-91-6	2-Naphthalenol, 1,2,3,4-tetrahydro- 	1884, 3746, 3747, 5811b		
1091.	17910-08-6	4a(2*H*)-Naphthalenol, 1,5,6,7,8, 8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1α,4aβ,7α,8aα)]- 		1156, 1256, 4090, 5811b	
1092.	41720-93-8	1(2*H*)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-3-hydroxy-4,4a-dimethyl-6-(1-methylethenyl)-, [3R-(3α,4α,4aβ,6β)]-		4249	
1093.	52811-60-6	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl- 	5811b	3545, 3560, 3561	
1094.	55497-93-3	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [2R-(2α,4aα,8aβ)]-		4249, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

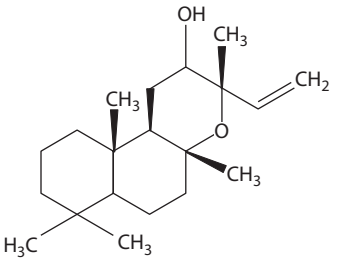
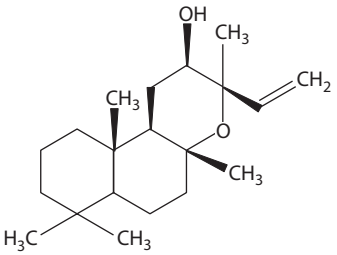
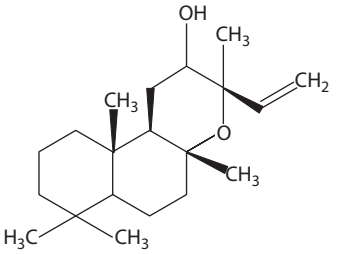
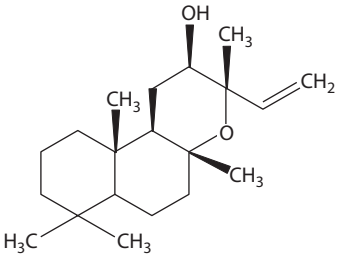
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1095.		2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3-hydroxy-3,4a,8,8-tetramethyl- {2 isomers reported}		3545, 3547, 4249	
1096.	14506-68-4	2(1*H*)-Naphthalenone, 1-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-5,5,8a-trimethyl-, [1R-[1α(R*),4aβ,8aα]]-		4249	
1097.	57567-07-4	2(1*H*)-Naphthalenone, 8-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-4,4,8a- trimethyl-7-methylene-		1248, 4249,4780	
1098.	55051-94-0	2(3*H*)-Naphthalenone, 4,4a,5,6,7, 8-hexahydro-3-hydroxy-4-methyl-6-(1-methylethenyl)-, [3R-(3α,4β,4aβ,6α)]- 		1156, 4090, 4249, 4455, 5811b	
1099.	38044-00-7	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4-hydroxy-1, 4a-dimethyl-7-(1-methylethenyl)-		4249	
1100.	68420-60-0	2(4a*H*)-Naphthalenone, 5,6,7, 8-tetrahydro-3-hydroxy-1, 4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)- 		1156, 3212, 4090	
1101.	38043-97-9	2(4a*H*)-Naphthalenone, 5,6,7, 8-tetrahydro-4-hydroxy-1, 4a-dimethyl-7-(1-methylethenyl)-, (4aR-*cis*)- {1-keto-α-cyperone} 	2761, 2762, 2777	1156, 2389, 3205, 3211, 3219, 4090, 5811b	
1102.	52811-62-8	Naphtho[2,1-*b*]furan-2-ol, dodecahydro-3a,6,6,9a-tetramethyl- {sclaral} 	5811b	2338, 3547	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1103.	56682-25-8	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-,[2R-[2α(R*),3aβ,5aα,9aβ,9bα]]-		6, 7, 1156, 4090	
1104.	56711-38-7	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-,[2R-[2α(S*),3aβ,5aα,9aβ,9bα]]-		6, 7, 1156, 2386, 4086, 4090, 4249	
1105.	56711-39-8	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(S*),3aα,5aβ, 9aα,9bβ]]-		6, 7, 1156, 4086, 4090, 4249	
1106.	56711-40-1	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(R*),3aα,5aβ, 9aα,9bβ]]-		6, 7, 1156, 4086, 4090, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

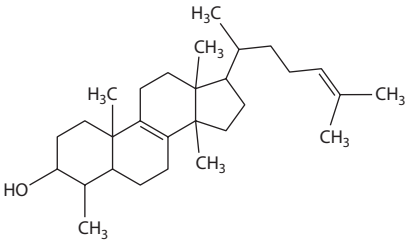
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1107.	59170-14-8	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3β,4aβ,6aα, 10aβ,10bα)]- {labd-14-ene, 8,13-epoxy-12α-hydroxy-; 12α-hydroxy-13-epimanoyl oxide} 	323, 568b, 800, 3251, 3281, 3286, 3971, 5811b	6, 568b, 1156, 1298, 2308, 2386, 3971, 3974a, 4090, 4101	
1108.	64681-69-2	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-,[2R-(2α,3α,4aα,6aβ,10aα,10bβ)]- 		6, 1156, 2308, 2565, 4090, 4101, 4249	
1109.	64681-70-5	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-,[2S-(2α,3α,4aβ,6aα,10aβ,10bα)]- 		6, 1156, 2565, 4090, 4101, 4249	
1110.	67528-84-1	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7, 7,10a-pentamethyl-, [2R-(2α,3β, 4aα,6aβ,10aα,10bβ)]- 		6, 1156, 4090, 4101	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1111.	6624-76-6	1-Nonacosanol $H_3C\text{-}(CH_2)_{27}\text{-}CH_2OH$		3613a	
1112.	52783-43-4	Nonadecanol	3327a, 5811b		
1113.	1454-84-8	1-Nonadecanol $H_3C\text{-}(CH_2)_{17}\text{-}CH_2OH$	172, 812, 3251, 3276, 3302	812, 3613a, 3797, 3973, 3974a	
1114.	63450-36-2	Nonadien-1-ol		5811, 5811b	
1115.	7786-44-9	2,6-Nonadien-1-ol		172a, 174b, 568b, 1053, 3266	
1116.	28069-72-9	2,6-Nonadien-1-ol, (*E,Z*)-		4249	
1117.	56805-23-3	3,6-Nonadien-1-ol		404	
1118.	53046-97-2	3,6-Nonadien-1-ol, (*Z,Z*)-		4249	
1119.	38713-12-1	3,7-Nonadien-1-ol, 4,8-dimethyl- {homogeraniol}		937, 1156, 3547, 4090	
1120.	459-88-1	3,7-Nonadien-1-ol, 4,8-dimethyl-, (*E*)-		4249, 5811b	
1121.	150405-75-7	6,8-Nonadien-2-ol,8-methyl-5-(3-methylbutyl)-		4249	
1122.	40525-38-0	6,8-Nonadien-2-ol, 8-methyl-5-(1-methylethyl)- {solanol}	568b, 1063–1066, 1068–1074, 1371, 1586, 2543, 2545, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3557, 4249, 5811b	537, 568b, 937, 1063–1066, 1068–1074, 1156, 1590a, 2338, 2386, 2389, 2544, 3198, 3215, 3217, 3354, 3547, 3560, 3561, 4090, 4098a, 4249, 5811b	
1123.	64130-24-1	6,8-Nonadien-2-ol, 8-methyl-5-(1-methylethyl)- {solanol isomer}	1063–1066, 1068–1074, 1371, 1586, 2543, 2545, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3557, 4249	537, 937, 1063–1066, 1068–1074, 1156, 1590a, 2338, 2386, 2389, 2544, 3198, 3215, 3217, 3354, 3547, 3560, 3561, 4090, 4098a, 4249, 5811b	
1124.	3937-56-2	1,9-Nonanediol		4098a	
1125.	55023-56-8	2,8-Nonanediol, 5-(1-methylethyl)-	2387, 4249	940, 1149, 1149a, 1156, 1254, 4090, 4098a, 4249, 5811b	2387
1126.		2,7-Nonanedione, 8-hydroxy-8-methyl-5-(1-methylethyl)-		3543, 4249	
1127.	143-08-8	1-Nonanol $H_3C\text{-}(CH_2)_7\text{-}CH_2OH$	172, 568b, 4249, 5811b	568b, 1157, 4098a, 4249	
1128.	628-99-9	2-Nonanol	568b, 4249		
1129.	624-51-1	3-Nonanol	568b, 4249		
1130.	19870-37-2	4-Nonanol, 2,6,8-trimethyl-		568b, 4249	1378
1131.	68-26-8	2,4,6,8-Nonatetraen-1-ol, 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (all-*E*)- {retinol}		2917a	
1132.	55023-53-5	3-Nonene-2,8-diol, 5-(1-methylethyl)-	2545, 2769	940, 1149, 1149a, 1156, 1190, 1254, 3549, 4090, 4098a, 4249, 5811b	
1133.	31502-14-4	2-Nonen-1-ol		1053, 3266, 3370	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

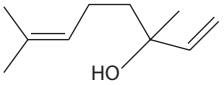
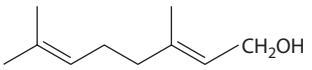
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1134.	10340-23-5	3-Nonen-1-ol, (*Z*)-		404, 2544, 4098a, 4249	
1135.	65017-85-8	2-Nonen-4-one, 8-hydroxy-3-methyl-, (*E*)-		231, 4249	
1136.	122881-64-5	3-Nonen-8-one, 1,2-dihydroxy-2-methyl-5-(1-methylethyl)-		5811, 5811b	
1137.		5-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-		3543, 4249	
1138.	55023-59-1	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-	4249	936, 940, 1149, 1149a, 1156, 1256, 2092, 4090, 4249, 5811b	
1139.	57934-86-8	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (*E*)-(±)-		940, 942, 1156, 4090, 4249	
1140.	60828-13-9	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (6*E*)-		5811, 5811b	
1141.	55023-52-4	6-Nonen-2-one, 8-hydroxy-5-(1-methylethyl)-		940, 942, 1156, 4090, 4249	
1142.	77288-95-0	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [R-[R*,S*-(*E*)]]-		738, 1156, 4090, 4249, 4948	
1143.	77288-96-1	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [S-[R*,R*-(*E*)]]-		738, 1156, 4090, 4249, 4948	
1144.	18444-66-1	19-Norlanosta-1,5,23-triene-3,11,22-trione, 25-(acetyloxy)-2,1 6,20-trihydroxy-9-methyl-, (9β,10α,16α,23*E*)-		4249	
1145.	17278-28-3	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16, 20-trihydroxy-9-methyl-, (3α,9β,10α,16α,23*E*)-		4249	
1146.	89647-62-1	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16, 20-trihydroxy-9-methyl-, (3β,9β,10α,16α,23*E*)-		4249	
1147.	51013-77-5	31-Norlanosterol 		5811	
1148.	557-61-9	1-Octacosanol {montanyl alcohol} H_3C-$(CH_2)_{26}$-CH_2OH	172, 3555, 3608, 4249	1651, 3555, 3608, 3613a, 3755, 4249	
1149.		1-Octacosanol, 26-methyl-		3613a	
1150.		1-Octacosanol, 27-methyl-		3613a	
1151.	506-43-4	9,12-Octadecadien-1-ol, (*Z,Z*)- H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-CH_2OH		4249, 4964	
1152.	554-62-1	1,3,4-Octadecanetriol, 2-amino-, [2S-(2R*,3R*,4S*)]-		4249, 4742	
1153.	1330-70-7	Octadecanoic acid, hydroxy-		2283, 3974a, 4249	
1154.	3155-42-8	Octadecanoic acid, 18-hydroxy- $HOCH_2$-$(CH_2)_{16}$-COOH		3974a, 4249, 4774	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1155.	112-92-5	1-Octadecanol {stearyl alcohol} H_3C-$(CH_2)_{16}$-CH_2OH	172, 812, 3251, 3276, 5811b	812, 2339a, 3613a, 3973, 3974a	
1156.	2490-01-9	1-Octadecanol, 16-methyl-		4249	
1157.	506-44-5	9,12,15-Octadecatrien-1-ol, (*Z,Z,Z*)-	1131–1133		
1158.	104077-09-0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-2-[(1-oxo-9-octadecenyl)oxy]ethyl ester, (*Z,Z,Z*)-		4249	
1159.	104077-10-3	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-		4249	
1160.	104100-34-7	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-1,3-propanediyl ester, (all-*Z*)-		4249	
1161.	104077-06-7	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-3-[(1-oxo-9-octadecenyl)oxy]propyl ester, (*Z,Z,Z*)-		4249	
1162.	104077-07-8	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-		4249	
1163.	104077-11-4	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-		4249	
1164.	104077-12-5	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-		4249	
1165.	104100-35-8	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 2-hydroxy-1,3-propanediyl ester, (all-*Z*)-		4249	
1166.	104077-08-9	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-		4249	
1167.	104077-13-6	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-		4249	
1168.	24753-52-4	9-Octadecenoic acid, 18-hydroxy-, (*Z*)-		4249, 4774, 5811b	
1169.	593-47-5	9-Octadecen-1-ol		4158a	
1170.	66957-95-7	2,7-Octadiene-1,6-diol, 2,6-dimethyl-, [S-(*E*)]-		229, 404, 1156, 4090, 4098a	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1171.	78-70-6	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool} 	317, 568b, 1360, 1375a, 1949, 2761, 2762, 2765, 2766, 3193, 3266, 3302, 3555, 3971, 4249	120, 172a, 174b, 317, 404, 568b, 909, 937, 1053, 1254, 1590a, 1949, 2270, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 2939, 3188, 3205, 3215, 3217, 3219, 3266, 3354, 3370, 3374, 3547, 3555, 3797, 3971, 3973, 3974a, 4098a, 4249, 5079, 5811b	1360, 1375a
1172.	126-91-0	1,6-Octadien-3-ol, 3,7-dimethyl-{*l*-linalool}	5811	5811	
1173.		1,6-Octadien-3-ol, 3,7-dimethyl-, labeled with ^{14}C {linalool-^{14}C}	317	317	
1174.	106-24-1	2,6-Octadien-1-ol, 3,7-dimethyl-, (*E*)-{geraniol} 	568b, 1586, 2761, 2762, 2765–2767, 2775, 3193, 3224, 3266, 3302, 3555, 3557, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1156, 1254, 1256, 2389, 2544, 2611, 2917a, 3215, 3266, 3370, 3555, 3797, 3988, 4090, 4249	
1175.	106-25-2	2,6-Octadien-1-ol, 3,7-dimethyl-, (*Z*)-{nerol}	568b, 3557, 4249	172a, 174b, 568b, 937, 1053, 1254, 1256, 2389, 2544, 3266, 3370, 4249	
1176.		Octanal, 2,7-dimethyl-7-hydroxy-		568b, 4249	
1177.	107-75-5	Octanal, 3,7-dimethyl-7-hydroxy- {hydroxycitronellal}		172a, 174b, 568b, 1053, 3266, 4249	
1178.	20653-90-1	2,3-Octanediol		937, 4249	
1179.	111-87-5	1-Octanol {caprylic alcohol} $H_3C\text{-}(CH_2)_6\text{-}CH_2OH$	172, 568b, 4249, 5811b	172a, 174b, 404, 568b, 1053, 2389, 2544, 2913a, 3266, 3547, 3811a, 3973, 4098a, 4249, 5811b	
1180.	106-21-8	1-Octanol, 3,7-dimethyl-	5811b	568b, 4249, 5811b	
1181.	123-96-6 4128-31-8	2-Octanol	568b, 1360, 1375a, 4249		1360, 1375a
1182.	589-98-0 20296-29-1	3-Octanol		937, 568b, 4098a, 4249	
1183.	78-69-3 57706-88-4	3-Octanol, 3,7-dimethyl- {tetrahydrolinalool}		568b, 1156, 1590a, 2386, 2389, 2544, 4090, 4249, 5811b	
1184.	102488-04-4	2-Octanone, 3,3-dimethyl-7-hydroxy-		5811, 5811b	
1185.	65716-45-2	2-Octanone, 7-hydroxy-3,3-dimethyl-, (±)-		230, 1156, 4090	
1186.	29414-56-0	1,5,7-Octatrien-3-ol, 2,6-dimethyl-	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249		1360, 1375a
1187.	41654-08-4	4-Octenoicacid, 6-ethyl-3-hydroxy-3,7-dimethyl-		4249, 5811b	
1188.		4-Octenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-		1156, 2092, 3547, 4090, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

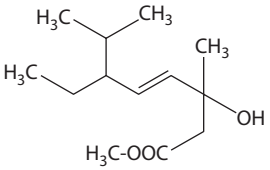
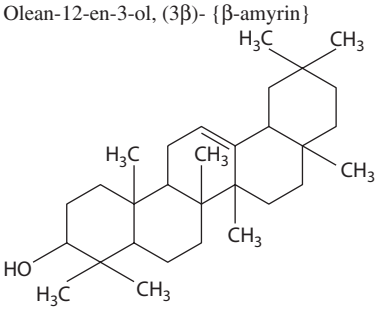
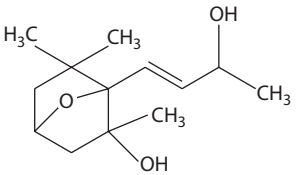
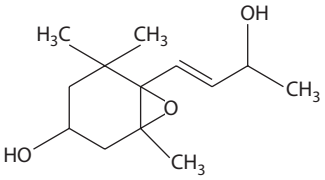
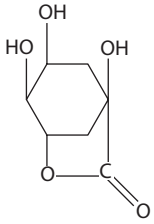
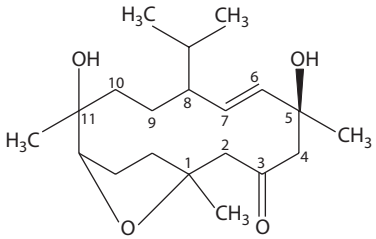
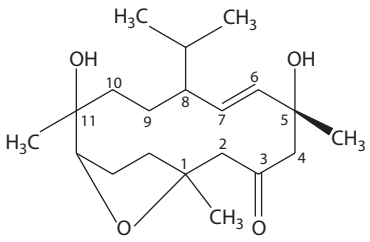
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1189.		4-Octenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-, methyl ester 		404	
1190.	3391-86-4	1-Octen-3-ol		172a, 174b, 568b, 937, 1053, 3266, 3555, 4098a, 4249	
1191.	18409-17-1	2-Octen-1-ol, (*E*)-		4249	
1192.	76649-14-4	3-Octen-2-ol		5811	
1193.	106-22-9	6-Octen-1-ol, 3,7-dimethyl- {*dl*-citronellol}	568b, 2775, 3266, 4249	172a, 174b, 568b, 1053, 1254, 1256, 3266, 3370, 4249, 5811b	
1194.	6812-78-8 141-25-3	7-Octen-1-ol, 3,7-dimethyl- {rhodinol}		172a, 174b, 1053, 3266, 3370	
1195.	508-02-1	Olean-12-en-28-oic acid, 3-hydroxy-, (3β)-		4249	
1196.	471-53-4	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-	3390, 4249		
1197.	559-70-6	Olean-12-en-3-ol, (3β)- {β-amyrin} 	1651, 3484, 3797, 3971, 4249, 5811b	1651, 3470, 3472, 3484, 3493, 3511, 3616, 3755, 3797, 3971, 3973, 3974a, 4249, 5811b	
1198.	73051-73-7	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl- 		1, 234, 1156, 4090, 4249	
1199.	102518-80-9	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-[1 R[1AL]]		5811, 5811b	
1200.	68573-20-6	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl- 		234, 1156, 1251, 4090, 4249, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1201.	72777-88-9	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-		234, 1156, 1251, 4090, 5811b	
1202.	63626-79-9	3-Oxabicyclo[3.3.1]nonan-2-one, 9-hydroxy-5-methyl-	5811, 5811a, 5811b	5811, 5811a, 5811b	
1203.		6-Oxabicyclo[3.2.1]octan-7-one, 6-hydroxy-3-methyl-	568b, 4249		
1204.	72693-08-4	6-Oxabicyclo[3.2.1]octan-7-one, 8-hydroxy-1-methyl-	4249		
1205.	640-06-2	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy- {Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, γ-lactone; quinic acid lactone; quinide} 	1089a, 1364, 1371, 1375, 1375b, 1887a, 2493, 2524a, 2675, 2767, 5811b		
1206.	27783-00-2	6-Oxabicyclo[3.2.1]octan-7-one, 1, 3,4-trihydroxy-, (exo,exo)-	4249, 5811b	4249	
1207.	665-27-0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3, 4-trihydroxy-, [1S-(exo,exo)]-	4249, 5811b		
1208.	98064-77-8	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,11R*, 		4089, 4091, 4249, 5811b	
1209.	98167-33-0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*, 11S*,12S*)]- 		4089, 4098, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

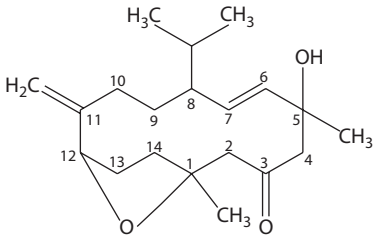
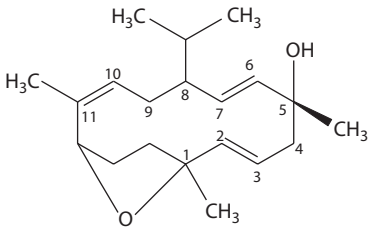
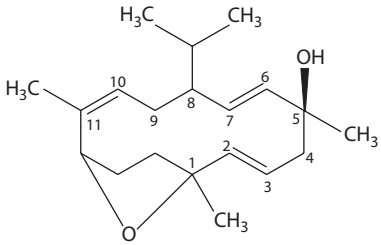
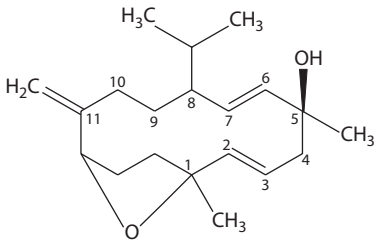
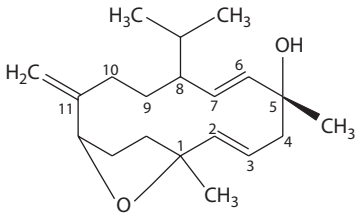
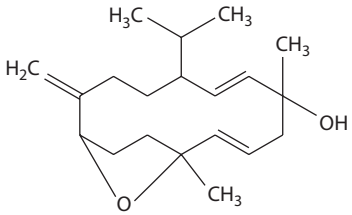
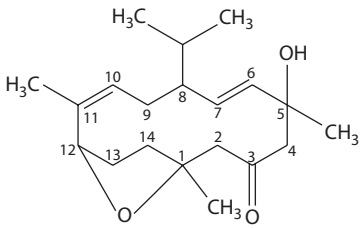
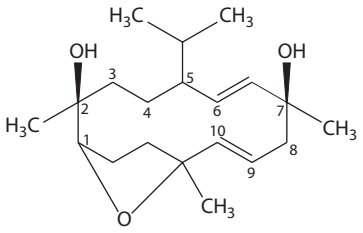
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1210.	98064-76-7	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5-hydroxy-1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,1		943, 3352, 4089, 4091, 4098, 4249, 5811b	
					
1211.	121927-14-8	15-Oxabicyclo[10.2.1]pentadec-6-ene-2,3,5-triol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2S*, 3R*,5S*,6*E*,8*)]		4249	
1212.	57760-48-2	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8S*,10*E*,12S*)]-	568b, 2767, 3361, 4089, 4249	235, 568b, 943, 3352, 3361, 3804, 3973, 3974a, 4089, 4249	
					
1213.	60047-18-9	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)-	2767, 3361, 4089, 4249, 4570a	9, 236, 1149, 1149a, 2386, 2389, 3352, 3361, 3547, 3804, 3973, 3974a, 4089, 4249, 5811b	
					
1214.	57688-98-9	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*, 6*E*,8R*,10S*)]-	327, 1063–1066, 1068–1074, 1586, 2767, 3361, 4249, 5811b	9, 235, 327, 404, 671, 1591, 2389, 2544, 3361, 3973, 3974a, 4089, 5811b	
					

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

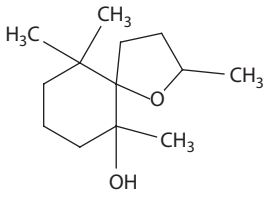
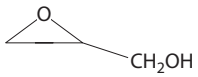
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1215.	57760-47-1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,5R*,6*E*,8S*,12S*)]- 	1063–1066, 1068–1074, 1352, 3361, 4249, 5811b	9, 235, 1352, 1591, 2389, 3222, 3361, 3543, 3545, 3547, 4089, 4249, 5811b	
1216.	60047-16-7	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8- (1-methylethyl)- 	1063–1066, 1068–1074, 1352, 3361	9, 235, 671, 1352, 1591, 3222, 3547	
1217.	102977-88-8	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 5-methyl-11-methylene-8-(1-methylethyl)-		4159b, 5811b	
1218.	58947-96-9	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-2-one, 8-hydroxy-8,12-dimethyl-5-(1-methylethyl)-		4249	
1219.	98064-75-6	15-Oxabicyclo[10.2.1] pentadeca-6,10-dien-3-one, 5-hydroxy-1,5,11-trimethyl- 8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,10*E*, 		3219, 3971, 4089, 4091, 5811b	
1220.	66890-76-4	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol, 2,8,12-trimethyl-5-(1-methylethyl)-, [1S-(1R*,2S*,5R*,6*E*,8R*,10*E*,12S*)]- 		235, 327, 404, 1156, 3219, 3547, 3971, 4089, 4090, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1221.	66966-04-9	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol, 2,8,12-trimethyl-5-(1-methylethyl)-, [1S-(1R*,2R*,5R*,6*E*,8R*,10*E*,12S*)]-		235, 404, 1156, 3219, 3547, 3971, 4084, 4089, 4090, 4249, 4573	
1222.	119613-99-9	15-Oxabicyclo[12.1.0]pentadec-9-en-5-one, 11,13-dihydroxy-1,11-dimethyl-8-(1-methylethyl)-,[1S-(1R*,8R*,9*E*,11R*,13S*,14S*)]-		4249, 5811b	
1223.	98064-73-4	15-Oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one, 8-hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,8R*,9*E*,11R*,		9, 12, 235, 236, 1156, 3971, 4089–4091, 5811b	
1224.	152209-53-5	15-Oxabicyclo[12.1.0] pentadeca-4,9-diene-6,8-diol, 11-(1-hydroxy-1-methylethyl)-4,8,14-trimethyl-, [1S-(1R*,4*E*,6S*,8R*,9*E*,11S*,14R*)]-		4249	
1225.	70969-36-7	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-		4249	
1226.	75281-93-5	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,6S*,8S*,9*E*,11R*,14R*)]-		4100, 4249	
1227.	75281-99-1	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,6S*,8R*,9*E*,11R*,14R*)]-		227, 236, 4249, 5811b	
1228.	75282-00-7	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1R-(1R*,4*E*,6R*,8S*,9*E*,11S*,14R*)]-		4089, 4249, 5811b	
1229.	62498-80-0	15-Oxabicyclo[9.3.1]pentadeca-2,6-diene-5,12-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8R*,11S*,12S*)]-		12, 4089, 4249	
1230.	72962-43-7	β-Homo-7-oxaergostan-6-one, 2,3,22,23-tetrahydroxy-,(2α,3α,5α,22R,23R,24S)-		429c, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

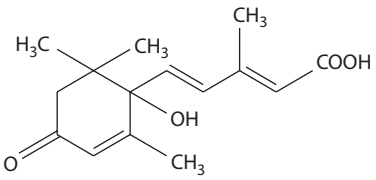
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1231.	65620-50-0	1-Oxaspiro[4.5]decane, 6-hydroxy-2,6,10,10-tetramethyl- {6-hydroxydihydrotheaspirane} 		1053, 3266	
1232.	77341-24-3	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-		5811, 5811b	
1233.	77288-97-2	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-, [2α(αS*,δR*),3α]-		4249, 4948	
1234.	77288-94-9	Oxiranebutanol, 3-(1-hydroxyethyl)-α-methyl-δ-(1-methylethyl)-		4249, 4948, 5811b	
1235.	61892-62-4	2,3-Oxiranedimethanol, monopropanoate	568b, 3553, 4249, 5811b		
1236.	556-52-5	Oxiranemethanol {glycidol} 	568b, 3553, 4249, 5811b		
1237.	51297-34-8	Oxiranemethanol, 3-(1-ethyl-2-methylpropyl)-α,α-dimethyl-		1660, 4249, 5811b	
1238.	9046-40-6	Pectic acid		120, 925, 2270, 2947c, 3492, 3973, 4249, 5079, 5114, 5189, 5306, 5419	
1239.		Pectic acid, labeled with ^{14}C {pectic acid-^{14}C}		2764	
1240.		Pectic acid, calcium magnesium salt		1971, 5777	
1241.	65028-58-2	Pectic acid, magnesium salt		2939	
1242.	9000-69-5	Pectin		120, 172, 174b, 176, 248, 344a, 385, 385a, 535, 722, 1063–1074, 1077, 1263, 1289, 1361, 1435a, 1887, 1933a, 2070, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2851, 2939, 2947c, 3029, 3042, 3059, 3266, 3305, 3372, 3429, 3450, 3468, 3551, 3651, 3665a, 3702, 3767, 3797, 3871, 3973, 3974a, 3974b, 4151, 4249, 4279, 4396, 4999, 5079, 5114, 5189, 5234, 5306, 5344, 5811b, 5831	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1243.		Pectin, labeled with ^{14}C {pectin-^{14}C}		2864	
1244.	9047-18-1	Pectinic acid		120, 344a, 925, 1263, 2270, 2337, 2338, 3702, 3973, 3974b, 5079	
1245.	129074-11-9	Pentacosanol	3327a		
1246.	26040-98-2	1-Pentacosanol H_3C-$(CH_2)_{23}$-CH_2OH		3612, 3613a, 3755, 4249	
1247.	63785-24-0	1-Pentacosanol, 24-methyl- $(H_3C)_2$═CH-$(CH_2)_{22}$-CH_2OH		3973, 3974a, 4249, 4964	
1248.	102673-27-8	4,9-Pentadecadienal, 6-(acetyloxy)-8-hydroxy-4, 8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4*E*,6R*,8R*,9*E*,11S*)]-		4249	
1249.	95360-16-0	4,9-Pentadecadienal, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4*E*,6R*, 8S*,9*E*,11S*)]-		4249	
1250.	102734-47-4	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4, 8-dimethyl-11-(1-methylethyl)-14-oxo-		5811b	
1251.	70898-33-8 102734-49-6	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-{isomer}	2722	943, 2098, 2722, 4089, 4249, 5811, 5811b	
1252.	102734-50-9	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, methyl ester, [6R-(4*E*,6R*,8S*,9*E*,11S*)]-		3973, 3974a	
1253.	102734-51-0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, methyl ester, [6R-(4*E*,6R*,8R*,9*E*,11S*)]-		3973, 3974a	
1254.	152209-55-7	6,11-Pentadecadien-2-one, 8,10,15-trihydroxy-8,12-dimethyl-5-(1-methylethyl)-, [5S-(5R*,6*E*,8R*,10S*,11*E*)]-		4249	
1255.	629-76-5	1-Pentadecanol H_3C-$(CH_2)_{13}$-CH_2OH	172, 568b, 4249, 5811b	568b, 4098a, 4249, 4964, 5811b	
1256.	20194-48-3	1-Pentadecanol, 14-methyl- $(H_3C)_2$═CH-$(CH_2)_{12}$-CH_2OH		4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

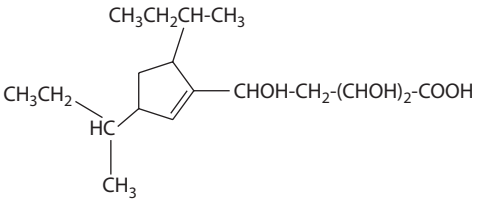
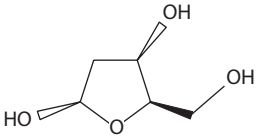
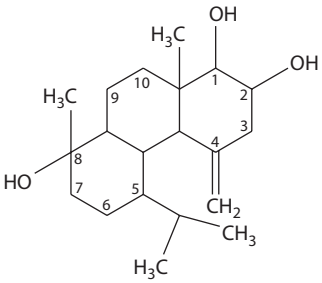
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1257.	21293-29-8 14375-45-2	2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-, [S-(*Z,E*)]- {abscisic acid} 		1156, 1206a, 2864a, 3216, 3218, 3973, 4090, 5811b	
1258.	4949-20-6	2,4-Pentadien-1-ol $H_2C{=}CH\text{-}CH{=}CH\text{-}CH_2OH$	4249	4249	
1259.		Pentanedioic acid, 2,3,4-trihydroxy- $HOOC\text{-}(CHOH)_3\text{-}COOH$		1971, 4249	
1260.	3174-67-2	1,3-Pentanediol	568b, 1371, 3553, 4249		
1261.		1,4-Pentanediol, 3-[2-(2-hydroxyethyl)-1,3,3-trimethylcyclohexyl]-	2601a		
1262.	107-41-5	2,4-Pentanediol, 2-methyl-	568b, 1375, 1375b, 1586, 2767, 3553, 3557, 4249	568b, 937, 4249	
1263.		Pentanenitrile, 2-hydroxy-	1067		
1264.		Pentanenitrile, 3-hydroxy-4-methyl-	1364		
1265.		1,2,5-Pentanetriol, 3-methyl-	2767, 4249		
1266.	96937-52-9	Pentanoic acid, hydroxy-methyl-	3741, 3743, 4249, 4897, 5811b		
1267.	617-31-2	Pentanoic acid, 2-hydroxy-		2337a, 2796, 3797, 3973, 3974a, 4249	
1268.	488-15-3	Pentanoic acid, 2-hydroxy-3-methyl-		2092, 2796, 3973, 3974a, 4249, 5811b	
1269.	498-36-2	Pentanoic acid, 2-hydroxy-4-methyl-		2337a, 2796, 3797, 3973, 3974a, 4249	
1270.	54031-97-9	Pentanoic acid, 2-hydroxy-4-oxo-		4249, 4845	
1271.	150-96-9	Pentanoic acid, 3-hydroxy-3-methyl-		3797, 3973, 3974a, 4249	
1272.	5980-21-2	Pentanoic acid, 3-hydroxy-4-methyl-		3797, 3973, 3974a, 4249	
1273.	150-97-0	Pentanoic acid, 3,5-dihydroxy-5-methyl- {mevalonic acid}		3973	
1274.	41654-03-9	Pentanoic acid, 4-hydroxy-3-methyl-		2092, 4249, 5811b	
1275.	67920-51-8	Pentanoic acid,5-(acetylamino)-2-hydroxy-,(±)-		2796, 4249, 4817a	
1276.	63316-30-3	Pentanoic acid,5-(acetylamino)-2-hydroxy-,(R)-		2796, 4249, 4817a, 5811b	
1277.	63316-29-0	Pentanoic acid, 5-amino-2-hydroxy-, (R)-		5811, 5811b	
1278.	16814-81-6	Pentanoic acid, 5-amino-2-hydroxy-, (S)-		2796, 4249	
1279.	63316-28-9	Pentanoic acid, 5-amino-3-hydroxy-		2796, 4249, 4869	
1280.		Pentanoic acid, 5-hydroxy-3-(1-methylethyl)-		2033	
1281.	66274-27-9	Pentanoic acid, 5-hydroxy-4-oxo-, methyl ester	3904, 4249, 5811b		3404
1282.	526-91-0 D 4172-43-4 4172-44-5 L 17828-56-7	Pentanoic acid, 2,3,4,5-tetrahydroxy- $HOCH_2\text{-}(CHOH)_3\text{-}COOH$		926, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1283.	71-41-0	1-Pentanol {amyl alcohol} H_3C-$(CH_2)_3$-CH_2OH	172, 568b, 4249, 5811b	404, 568b, 937, 1053, 1590a, 2282, 2339a, 3186, 3188, 3266, 3547, 3555, 3973, 4249	
1284.	6570-87-2	1-Pentanol, 3,4-dimethyl-		404	
1285.	105-30-6	1-Pentanol, 2-methyl-		568b, 2339a, 4249	
1286.	589-35-5	1-Pentanol, 3-methyl-		404, 568b, 2339a, 2939, 3547, 3797, 3974a, 4249	
1287.	626-89-1	1-Pentanol, 4-methyl-		404, 568b, 1157, 2339a, 4249	
1288.	6032-29-7	2-Pentanol		568b, 4249	
1289.	590-36-3	2-Pentanol, 2-methyl-		568b, 1157, 3550, 3973, 4249	
1290.	565-60-6	2-Pentanol, 3-methyl-		568b, 4249	
1291.	108-11-2	2-Pentanol, 4-methyl-	568b, 1365, 1371, 2545, 2775, 3410, 4249	568b, 2339a, 4249	
1292.	584-02-1	3-Pentanol		404	
1293.	565-67-3	3-Pentanol, 2-methyl-	568b, 4249		
1294.	77-74-7	3-Pentanol, 3-methyl-	2775, 4249		
1295.		3-Pentanol, 1-phenyl-	2767		
1296.	64502-89-2	2-Pentanone, 1-hydroxy- H_3C-$(CH_2)_2$-CO-CH_2OH	5811b		3402, 3404, 4249
1297.	4161-60-8	2-Pentanone, 4-hydroxy- H_3C-CHOH-CH_2-CO-CH_3	2769, 3557, 4249	2339a	
1298.	123-42-2	2-Pentanone, 4-hydroxy-4-methyl- {diacetone alcohol} $(H_3C)_2$═C(OH)-CH_2-CO-CH_3	568b, 1378, 2767, 2769, 2773, 3397, 3555, 3559, 4249, 5770, 5811b	568b, 2356, 4249, 4867, 5811b	1378
1299.	1071-73-4	2-Pentanone, 5-hydroxy-	568b, 4249	568b, 4249	
1300.	1567-93-7	2-Pentanone, 5-hydroxy-3-methyl-	2774, 4249		
1301.	66309-84-0	2-Pentanone, 5-hydroxy-4-methyl-	2570, 2769, 4249		
1302.	101758-45-6	2-Pentene-1,4-diol, 5-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-3-methyl-, [1α(3*E*,4S*),2β,4a		4249	
1303.	616-25-1	1-Penten-3-ol	314, 568b,4249	568b, 1550, 2339a, 3186, 3188, 4249	
1304.	2088-07-5	1-Penten-3-ol, 2-methyl-	4249, 4570a	4249	
1305.	1576-95-0	2-Penten-1-ol, (*Z*)		2339a	
1306.	87563-33-5	2-Penten-1-ol, 3-methyl-5-(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1S-[1α(*E*),4aβ,8aα]]-		4249	
1307.	87585-55-5	2-Penten-1-ol, 3-methyl-5-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [4aS-[1(*E*),4aα,8aβ]]-		4249	
1308.	39161-19-8	3-Penten-1-ol		5811, 5811b	
1309.	763-89-3	3-Penten-1-ol, 4-methyl-		2339a	
1310.	4325-82-0	3-Penten-2-ol, 4-methyl-	1140, 4249, 5770		
1311.	60026-13-3	4-Penten-2-ol, 5-(tetrahydro-2-methyl-2-furanyl)-		2544, 4249	
1312.	72692-98-9	Pentitol, 2,3-dideoxy-3-methyl-	4249		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1313.	61989-60-4	Pentonic acid, 2,3-anhydro-, γ-lactone	4249, 5811b		
1314.	491-14-5	Pentonic acid, 5-C-[3,5-bis(1-methylpropyl)-1-cyclopenten-1-yl]-4-deoxy- 	4249	4249	
1315.	9473-19-9	*D*-erythro-Pentonic acid, 3-deoxy-, γ-lactone	4249	4249	
1316.	5803-57-6	Pentonic acid, 5-deoxy-, γ-lactone	4249, 5811b		
1317.	116001-96-8	Pentosan		2154, 2947c, 5079. 5194, 5234	
1318.		Pentose		1971, 5079, 5189, 5306, 5344, 5777	
1319.	533-67-5	*D*-erythro-Pentose, 2-deoxy- {deoxyribose} 		1351, 3079, 3973, 3974a, 4249, 5811b	
1320.	488-84-6	*D*-erythro-2-Pentulose {xylulose} = *D*-ribulose 488-84-6 $HOCH_2$-CO-$(CHOH)_2$-CH_2OH		429b, 4249, 4712	
1321.	24218-00-6	*D*-erythro-2-Pentulose, 1,5-bis(dihydrogen phosphate)		4249	
1322.	111924-41-5	1,2,8-Phenanthrenetriol, tetradecahydro-8, 10a-dimethyl-4-methylene-5-(1-methylethyl)- 		4249	
1323.	3690-05-9	Phenol, 4-(3-hydroxy-1-propenyl)- (coumaryl alcohol)		1102, 2338	
1324.	537-33-7	Phenol, 4-(3-hydroxy-1-propenyl)-2,6-dimethoxy- {sinapyl alcohol}		1102, 2338,3973, 4249, 4438a, 5811b	
1325.	458-35-5	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy- {coniferyl alcohol}	596, 1879, 1881, 1883, 1884, 3712, 3828, 4249, 5811b	1102, 2338, 3973	
1326.	32811-40-8	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-,(*E*)-		1879, 4249	
1327.	69056-21-9	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-,(*Z*)-		1879, 4249, 5811b	
1328.	31105-03-0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
1329.		Pheophorbide, hydroxysolanesyl		5517	
1330.		Pheophytin, 10-hydroxy-		5517	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

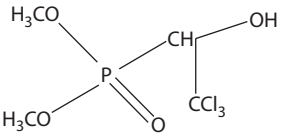
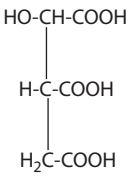
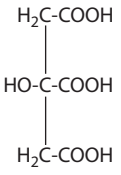
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1331.	52-68-6	Phosphonic acid, 2,2,2-trichloromethyl-1-hydroxyethyl-, dimethyl ester {Trichlorphon®; Dipterex®} 	1333	1333, 2650a, 3380, 3633, 3973, 3977, 4271a	
1332.	25322-68-3	Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-		2543, 4249	
1333.	145-13-1	Pregn-5-en-20-one, 3-hydroxy-, (3β)-		429c, 4249, 4613	
1334.		*L*-Proline, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
1335.		*L*-Proline, hydroxy-		5907	
1336.	18610-59-8	*L*-Proline, 1-hydroxy-		1063–1066, 1068–1074, 1351, 2337, 2394a, 2597a, 3491, 3797, 3973, 3974a, 4224, 4226	
1337.	62137-28-4	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-		4249, 4429	
1338.	62137-29-5	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-L-arabinofuranosyl)oxy]-, *trans*-		4249, 4429	
1339.	51-35-4	*L*-Proline, 4-hydroxy-, *trans*-		120, 1305a, 5811b	
1340.	30310-80-6	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}		486, 3300, 3947, 3948, 5811b	
1341.	367-47-5	Propanal, 2,3-dihydroxy- {glyceraldehyde} $HOCH_2$-CH_2OH-CH═O	1238, 5811b	3973, 5811b	
1342.	142-10-9	Propanal, 2,3-dihydroxy-, 3-phosphate		555b	
1343.	2134-29-4	Propanal, 3-hydroxy-	5034		
1344.	997-10-4	Propanal, 2-oxo-3-hydroxy- {reductone} $HOCH_2$-CO-CH═O		3797	
1345.	4464-20-4	Propanedial, dihydroxy- $(HO)_2$═C═$(CH═O)_2$		4249, 4946	
1346.	80-69-3	Propanedioic acid, hydroxy- HO-CH═$(COOH)_2$		4249, 4950a	
1347.	57-55-6	1,2-Propanediol {propylene glycol} H_3C-CHOH-CH_2OH	167, 173a, 174e, 239, 409, 568b, 627, 966, 1350, 1352, 1354, 1360, 1364, 1371, 1373, 1375, 1375a, 1375b, 1382, 1427, 1437, 1445, 1586, 1603, 1944, 1963, 2144, 2300, 2387, 2410, 2543, 2545, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 3190, 3255, 3266, 3302, 3308, 3410, 3551, 3553, 3557, 3559, 3603, 3797, 3835, 3876, 3992, 4249, 4259, 4337, 5770, 5811b	172a, 174b, 320, 568b, 569, 570, 27, 830a, 858, 865, 974, 1024, 1053, 1294, 1295, 383, 2009, 2188, 2195, 2196, 2246, 2313a, 2788, 2790, 2917a, 2939, 3163, 3264, 3266, 3370, 3549, 3550, 3551, 3603, 3707, 3797, 3974a, 4249, 4259, 4337, 5009, 5639, 5811b, 5817	1354, 1360, 1375a, 2387
1348.	627-69-0	1,2-Propanediol, 1-acetate H_3C-CHOH-CH_2-OOC-CH_3	568b, 2543, 2773, 3553, 3559, 4249, 4319, 5811b	568b, 2389, 2544, 3905, 4249, 5811b	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1349.	6214-01-3	1,2-Propanediol, 2-acetate H_3C-CH(OOC-CH_3)-CH_2OH	568b, 3553, 3557, 4249	568b, 2389, 2544, 3905, 4249	
1350.	96-24-2	1,2-Propanediol, 3-chloro- Cl-CH_2-CHOH-CH_2OH	568b, 1375, 1375b, 1586, 2570, 2767, 3255, 3553, 3557, 4249, 5811b		
1351.	10602-14-9	1,2-Propanediol, 1-(dihydrogen phosphate)		429b, 4249, 4570	
1352.	20390-21-0	1,2-Propanediol, 3-(furfuryloxy)-	586b, 1586, 2767, 3553, 4249		
1353.	115888-33-0	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl)-, [2S-[2α(S*),8α,8aβ]]-		4249	
1354.	99694-82-3	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl)-, [2R-[2α(S*),8β,8aα]]-		4249	
1355.	115788-21-1	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-3-hydroxy-8,8a-dimethyl-2-naphthalenyl)-, [2S-[2α(S*),3α,8β,8aα]]-		4249	
1356.	115788-20-0	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-5-hydroxy-8,8a-dimethyl-2-naphthalenyl)-, [2R-[2α(R*),5α,8]		4249	
1357.	54541-18-3	1,2-Propanediol, 2-propanoate	568b, 3553, 4249, 5811b		
1358.	504-63-2	1,3-Propanediol {trimethylene glycol} $HOCH_2$-CH_2-CH_2OH	568b, 3553, 3557, 4249, 5811b	568b, 2246, 2788, 2790, 4249, 5811b	
1359.	126-30-7	1,3-Propanediol, 2,2-dimethyl-	568b, 1360, 1375a, 2761, 2762, 2765, 2766, 4249		1360, 1375a
1360.	78-97-7	Propanenitrile, 2-hydroxy- H_3C-CHOH-CN	568b, 1067, 1360, 1371, 1375a, 2543, 2545, 2679, 2761, 2762, 2775, 2777, 3410, 3553, 4249, 5811b		1360, 1375a
1361.	75-86-5	Propanenitrile, 2-hydroxy-2-methyl- $(H_3C)_2$═COH-CN	568b, 3553, 4249, 5770, 5811b		
1362.	30810-51-6	1,2,3-Propanetricarboxylic acid, 1-hydroxy- {isocitric acid} 		120, 3973, 5811b	
1363.	77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid} 	2079, 3029, 3302, 3324, 3555, 5079, 5447, 5811b	69, 120, 172a, 256, 305, 385, 543a, 555, 634, 677b, 826a, 835, 836, 838, 839, 963, 840, 1053, 1063–1066, 1068–1074, 1289, 1305a, 1330, 1332, 1333, 1548, 1923, 1933a, 1982, 2014, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2374, 2529,	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
				2532, 2688, 2761–2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3052, 3107, 3194, 3266, 3353, 3370, 3476, 3486, 3555, 3660, 3655b, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 3974b, 3976, 4249, 4275, 5079, 5108, 5109, 5126, 5244, 5381, 5389, 5419, 5477, 5478, 5745, 5749, 5753, 5764, 5811b, 5832, 5896, 5909	
1364.	58308-53-5	1,2,3-Propanetricarboxylic-1,3-$^{14}C_2$ acid, 2-hydroxy-, labeled with ^{14}C {citric acid-^{14}C}	2763, 4249	2763, 4249	
1365.	813-94-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, calcium salt		5079, 5189, 5342	
1366.	3609-96-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, dipotassium salt		4249, 4560	
1367.	3344-18-1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, magnesium salt		5079, 5189, 5342	
1368.		1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monomethyl ester	1375a, 1377		1375a, 1377
1369.	18996-35-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monosodium salt		4249, 4760, 5548	
1370.	68-04-2	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, sodium salt	5811b	174b, 1053, 3266, 4249, 5548	
1371.	866-84-2	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, potassium salt	5811b	174b, 3266, 4249, 5811b	
1372.	77-93-0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester {triethyl citrate}	3190, 3992	172a, 174b, 1053, 2386, 3266, 4249	
1373.	6100-05-6	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripotassium salt, monohydrate		5079, 5189, 5342, 5548	
1374.	56-81-5	1,2,3-Propanetriol {glycerol} $HOCH_2$-CHOH-CH_2OH	50, 167, 172, 173a, 174e, 409, 568b, 607, 627, 636, 723, 849, 966, 1089a, 1209, 1218, 1332, 1333, 1348, 1350, 1352, 1354, 1364, 1373, 1375, 1375a, 1375b, 1378, 1382, 1427, 1450, 1586, 1603, 1819, 1842, 1882, 1887a, 1944, 1963, 2079, 2144, 2170, 2270, 2300, 2380, 2387, 2410, 2493, 2524a, 2545, 2547, 2570, 2601a, 2691–2695, 2767, 2774, 2799a, 2857, 2939, 3190, 3255, 3266, 3302, 3308, 3454, 3551, 3553, 3557, 3559, 3603, 3835, 3876, 3992, 3999, 4103, 4249, 4319, 4337, 5034, 5079, 5189, 5286, 5512, 5811b	120, 172a, 174b, 300–302, 310, 311, 319, 568b, 627, 830a, 858, 865, 1053, 1124, 1024, 1221, 1294–1296, 1332, 1383, 1819, 1933a, 2079, 2188, 2192, 2196, 2270, 2313a, 2380, 2481, 2547, 2761, 2762, 2765, 2766, 2788, 2790, 2789, 2913, 2939, 3163, 3266, 3370, 3551, 3603, 3689, 3707,	50, 1354, 1375a, 1378, 2387

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

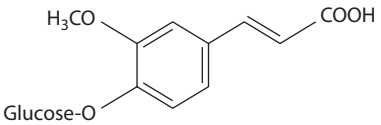
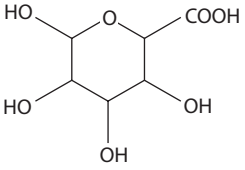
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
				3797, 3813, 3876, 3973, 3974a, 4103, 4249, 4337, 5009, 5079, 5180, 5228, 5286, 5388, 5679, 5682, 5692, 5811b, 5817, 5836	
1375.	63346-81-6	1,2,3-Propanetriol, labeled with ^{13}C {glycerol-^{13}C}		5028, 5583	
1376.	4254-13-1	1,2,3-Propanetriol, labeled with ^{14}C {glycerol-^{14}C}	300–302, 310, 319	300–302, 310, 319	
1377.	61892-59-9	1,2,3-Propanetriol, 1-acetate 2-formate	568b, 3553, 4249, 5811b		
1378.	25395-31-7	1,2,3-Propanetriol, diacetate {diacetin}	568b, 1063–1066, 1068–1074, 1371, 1375, 1375b, 1586, 2543, 2601a, 2765–2767, 2773, 3553, 4249, 4570a	568b, 3905, 4249, 4751	
1379.	29860-16-0	1,2,3-Propanetriol, 1,2-diacetate {1,2-diacetin}	568b, 4249	568b, 4249, 5811b	
1380.	105-70-4	1,2,3-Propanetriol, 1,3-diacetate {1,3-diacetin}	568b, 4249	568b, 4249	
1381.	57-03-4	1,2,3-Propanetriol, 1-(dihydrogen phosphate)		429b	
1382.	927-20-8	1,2,3-Propanetriol, 1-(dihydrogen phosphate), magnesium salt (1:1)		429b, 4249, 4975	
1383.	17603-42-8	1,2,3-Propanetriol, 1-(dihydrogen phosphate), sodium salt		4249, 4908a	
1384.	1335-34-8	1,2,3-Propanetriol, mono(dihydrogen phosphate), potassium salt		4249, 4908a	
1385.	106-61-6 26446-35-5	1,2,3-Propanetriol, monoacetate {monoacetin}	568b, 1350, 1354, 1360, 1371, 1375a, 1375, 1375a, 1375b, 1586, 2543, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 3255, 3553, 3557, 4249, 4570a, 5811, 5811b	568b, 2389, 2544, 4249, 5811, 5811b	1354, 1360, 1375a
1386.	72692-68-3	1,2,3-Propanetriol, monoformate	4249, 4810		
1387.		1,2,3-Propanetriol, phosphatidyl-		3973	
1388.	11046-98-3	1,2,3-Propanetriol, propanoate	5811, 5811a, 5811b		
1389.	62244-24-0	1,2,3-Propanetriol, 1-propanoate, (R)-	3553, 4249		
1390.	473-81-4	Propanoic acid, 2,3-dihydroxy- {glyceric acid} $HOCH_2$-CHOH-COOH	1882, 1886, 4249, 5811b	120, 2892b, 2939, 3797, 3974a, 4249, 5811b	
1391.	6000-40-4	Propanoic acid, 2,3-dihydroxy-, (R)-		4249	
1392.	65644-56-6	Propanoic acid, 2,3-dihydroxy-, calcium salt		5811b	
1393.	50-21-5 598-82-3	Propanoic acid, 2-hydroxy- {lactic acid} H_3C-CHOH-COOH	126b, 172, 237, 568b, 1099, 1235, 1364, 1445, 1674, 1842, 1882, 2133, 2493, 2582, 2767, 2939, 3053, 3059, 3060, 3061, 3255, 3266, 3302, 3308, 3384, 3394, 3496, 3553, 3557, 3559, 4249, 5512, 5811b	120, 172a, 174b, 568b, 722, 1053, 1279, 2079, 2917a, 2939, 3052, 3053, 3060, 3266, 3486, 3797, 3973, 3974a, 4131, 4249, 5079, 5447, 5811b	3393, 3402, 3405
1394.	97-73-4	Propanoic acid, 2-hydroxy-, anhydride		4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1395.	138-22-7	Propanoic acid, 2-hydroxy-, butyl ester {butyl lactate}	5811		
1396.	97-64-3	Propanoic acid, 2-hydroxy-, ethyl ester {ethyl lactate} $H_3C\text{-}CHOH\text{-}COO\text{-}C_2H_5$	568b, 1371, 1884, 2761, 2762, 2765, 2766, 2777, 3266, 3553, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370	
1397.	547-64-8	Propanoic acid, 2-hydroxy-, methyl ester $H_3C\text{-}CHOH\text{-}COO\text{-}CH_3$	1371, 2761, 2762, 2765, 2766, 2777, 3410, 4249		3404
1398.	72-17-3 16595-31-6	Propanoic acid, 2-hydroxy-, sodium salt $H_3C\text{-}CHOH\text{-}COO\text{-}Na$		3476, 4249, 5811, 5811b	
1399.	16039-53-5	Propanoic acid, 2-hydroxy-, zinc salt		5811b	
1400.	594-61-6	Propanoic acid, 2-hydroxy-2-methyl- $(H_3C)_2{=}COH\text{-}COOH$		1948, 2337a, 4249	
1401.	820-11-1	Propanoic acid, 2-hydroxy-3-(phosphonooxy)-		429b, 4249, 4634, 5811b	
1402.	503-66-2	Propanoic acid, 3-hydroxy- $HO\text{-}(CH_2)_2\text{-}COOH$	568b, 1364, 1371, 1882, 3255, 3394, 3553, 4249, 5811b	120, 568b, 3974a, 4249	3393
1403.	4835-90-9	Propanoic acid, 3-hydroxy-2,2-dimethyl- {hydroxypivalic acid} $HOH_2C\text{-}C(CH_3)_2\text{-}COOH$		2917a	
1404.	80657-57-4	Propanoic acid, 3-hydroxy-2-methyl-, methyl ester	568b, 4249		
1405.		Propanoic acid, 3-hydroxy-2-methylamino-, propyl ester	3553, 4249		
1406.	1113-60-6	Propanoic acid, 3-hydroxy-2-oxo- $HOH_2C\text{-}CO\text{-}COOH$		1971, 2939, 3797, 4634, 5777, 5811	
1407.	2553-59-5	Propanoic acid, 3-hydroxy-2-(phosphonooxy)-		429b, 4634	
1408.	71-23-8	1-Propanol $H_3C\text{-}CH_2\text{-}CH_2OH$	172, 568b, 1140, 1375a, 1377, 1412, 1413, 1416, 2559, 2559a, 4249, 5811b	568b, 2339a, 3217, 3973, 4249, 4807, 5811b	1375a, 1377
1409.	110053-58-2	1-Propanol, 2,2-bis(1-hydroxypropoxy)- $HOCH_2\text{-}C(CH_3){=}(OCH_2CH_2CH_2OH)_2$	3553, 5811, 5811a, 5811b		
1410.	78-83-1	1-Propanol, 2-methyl- {isobutyl alcohol} $(H_3C)_2{=}CH\text{-}CH_2OH$	1140, 1416, 3266, 3302, 3797, 4249, 5811b	172a, 174b, 174b, 1053, 2282, 2339a, 3266, 3370, 4249	
1411.	108-61-2	1-Propanol, 2,2′-oxybis- $[HOCH_2\text{-}CH(CH_3)]_2{=}O$	3553, 4249, 5811b		
1412.	2396-61-4	1-Propanol, 3,3′-oxybis- $(HOCH_2\text{-}CH_2\text{-}CH_2)_2{=}O$	3553, 4249		
1413.	67-63-0	2-Propanol	568b, 1140, 1375, 1375b, 1378, 1419, 3254, 3882, 4249, 5811b	568b, 1550, 1600, 1601, 2339a, 4249	1378
1414.	110-98-5	2-Propanol, 1,1′-oxybis- $(CH_3\text{-}CHOH\text{-}CH_2)_2{=}O$	3553, 4249, 5811b		
1415.	110053-57-1	2-Propanol, 1,1-bis(2-hydroxypropoxy)- $CH_3\text{-}CHOH\text{-}CH{=}(OCH_2CHOHCH_3)_2$	3553, 5811, 5811a, 5811b		
1416.	127-00-4	2-Propanol, 1-chloro-	3559, 4249		
1417.		2-Propanol, 2-(2-ethyl-1, 3-dimethylcyclopenten-2-yl)-		2917a	
1418.	107-98-2	2-Propanol, 1-methoxy-		3905, 4249	
1419.	75-65-0	2-Propanol, 2-methyl- {*tert*-butanol}	3265	2386, 4249	
1420.	1321-48-8	1-Propanone, 1-phenyl-3-hydroxy-	1586		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1421.	116-09-6	2-Propanone, 1-hydroxy- {acetol} H_3C-CO-CH_2-OH	568b, 1063–1066, 1068–1074, 1360, 1371, 1375a, 2337, 2493, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3397, 3410, 3553, 3555, 3557, 3559, 4249, 5811b	404, 568b, 1590a, 2337, 2339b, 2389, 2544, 2917a, 3549, 3555, 4249, 5811b	1360, 1375a, 2244, 3401, 3402, 3404, 3405
1422.	57-04-5	2-Propanone, 1-hydroxy-3-(phosphonooxy)-		429b	
1423.	96-26-4	2-Propanone, 1,3-dihydroxy-	1371, 4249		
1424.		2-Propanone, 1-[2-hydroxy-5-(1-methylethyl)-2-methyl-1-cyclopentyl]-		3547, 4249	
1425.	50672-03-2	2-Propanone, 1-[5-(hydroxymethyl)-2-furanyl]-	568b, 1375, 3553, 4249, 5811b		
1426.	636-38-4	2-Propenal, 2,3-dihydroxy- HOCH═CHOH-CH═O		3797, 4249	
1427.	17093-82-2	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]- {1-*O*-caffeoylglucose}		3797, 3974a, 4402	
1428.	7196-71-6 14364-12-6	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-methoxyphenyl]- {1-*O*-feruloylglucose} 		3797, 3974a, 4249, 4402, 5811, 5811b	
1429.	14364-05-7	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)phenyl]-		2023, 4249	
1430.	107-18-6	2-Propen-1-ol {allyl alcohol} H_2C═CH-CH_2OH	37, 38, 172, 299, 568b, 1365, 2559, 2559a, 3255, 3530, 3553, 4249, 5811b	38, 568b, 3633, 4249	3401
1431.	104-54-1	2-Propen-1-ol, 3-phenyl- {cinnamyl alcohol}	336, 568b, 4249	172a, 174b, 336, 568b, 1053, 1254, 1256, 3266, 3370, 3547, 4249	
1432.	4407-36-7	2-Propen-1-ol, 3-phenyl-, (*E*)-		429b	
1433.	551-68-8	*D*-Psicose HOCH_2-CO-$(CHOH)_3$-CH_2OH		3667, 4249	
1434.	56159-42-3	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-		4249, 4603	
1435.	38477-23-5	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-		4249, 4603	
1436.	54538-20-4	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-		4249, 4620	
1437.	9046-38-2	2-Pyrancarboxylicacid, 3, 4,5,6-tetrahydroxytetrahydro- {oxane-2-carboxylicacid, 3,4,5,6-tetrahydroxy-; *D*-galacturonan} 		5811, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

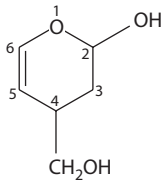
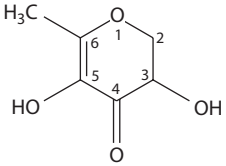
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1438.	70898-35-0	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro-6-hydroxy-3-oxo-	1378	2939, 3797, 4249	1378
1439.		2*H*-Pyran-4-methanol, 3,4-dihydro-2-hydroxy- 	3553		
1440.	61892-96-4	2*H*-Pyran-6-methanol, 3,4-dihydro-3-hydroxy-	568b, 3553, 4249		
1441.	19752-84-2	2*H*-Pyran-3-ol, tetrahydro-	568b, 3553, 4249, 5811b		3405
1442.		2*H*-Pyran-2-one, 4,5-dihydro-3-hydroxy-	1375, 3553, 3557, 4249		
1443.	55100-07-7	2*H*-Pyran-2-one, 5,6-dihydro-4-hydroxy-		3430, 5811b	
1444.	73850-01-8	2*H*-Pyran-2-one, hydroxy ethyl-	4097, 4249, 5811, 5811a, 5811b		
1445.		2*H*-Pyran-2-one, hydroxy-methyl-	3746, 3747		
1446.	496-64-0	2*H*-Pyran-2-one, 3-hydroxy-	1375a, 1377, 5811b	3973	1375a, 1377, 4249
1447.	73692-69-0	2*H*-Pyran-2-one, 3-hydroxy-6-methyl-		3430	
1448.		2*H*-Pyran-2-one,tetrahydro-3,4-epoxy-5-hydroxy-	1375a (0), 1377 (0)		1375a, 1377
1449.	5058-01-5	2*H*-Pyran-2-one, tetrahydro-3-hydroxy-	1586, 2543, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3553, 3557, 5811b		3401, 3402, 3404
1450.	61892-56-6	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-	1351, 3553, 4249		
1451.	503-48-0 110053-65-1	2*H*-Pyran-2-one,tetrahydro-4-hydroxy-4-methyl-	5811b	323, 4249	
1452.	33691-73-5	2*H*-Pyran-2-one, tetrahydro-5-hydroxy-	568b, 1360, 1375, 1375b, 1586, 2570, 2767, 2777, 3553, 3557, 4249, 5811b		
1453.	90-80-2	2*H*-Pyran-2-one, tetrahydro-6-hydroxymethyl, 3,4, 5-trihydroxy {gluconic acid, δ-lactone}	1360, 4249		
1454.	121197-11-3	2*H*-Pyran-3(4*H*)-one,dihydro-4-(hydroxymethyl)-	4249	5811b	
1455.	28564-83-2	4*H*-Pyran-4-one, 2,3-dihydro-3, 5-dihydroxy-6-methyl- 	568b, 1089a, 1134, 1138, 1351, 1352, 1360, 1375, 1375a, 1375b, 1882, 1887a, 2337, 2493, 2524a, 2543, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2857, 3394, 3397, 3553, 3557, 3828, 4249, 5811b	568b, 2339b, 2917a, 3549, 4249, 5811b	1360, 1375a, 3402, 3405
1456.	6380-97-8	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-2-(hydroxymethyl)-	3553, 4249	3430, 5811b	
1457.	38877-21-3	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-6-methyl-	1134, 1138, 4249		
1458.	131524-09-9	4*H*-Pyran-4-one, 2,6-diethyl-3-hydroxy-	90b, 4249, 5811b		
1459.	4940-17-4	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-	90b, 4249, 5811b		
1460.	131524-16-8	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-6-methyl-	90b, 4249, 5811b		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1461.	4940-11-8	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy- {ethylmaltol}	90b, 568b, 3266, 4249, 5811b	172a, 174b, 568b, 1053, 3219, 3266, 3370, 4249	
1462.	131524-08-8	4*H*-Pyran-4-one,2-ethyl-3-hydroxy-5,6-dimethyl-	90b, 4249, 5811b		
1463.	131524-04-4	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5-methyl-	90b, 4249, 5811b		
1464.	22639-24-3	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-6-methyl-	90b, 4249, 5811b		
1465.	61892-88-4	4*H*-Pyran-4-one, 2-hydroxy-3-methyl-	3410, 3553, 4249		
1466.	61892-87-3	4*H*-Pyran-4-one, 2-hydroxy-5-methyl-	1351, 1352, 3553, 4249		
1467.		4*H*-Pyran-4-one, 2-hydroxymethyl-3,5,6-trihydroxy-	1375a (0), 1377 (0), 4249		1375a, 1377
1468.		4*H*-Pyran-4-one, 2-methyl-3,5,6-trihydroxy-	1375a (0), 1377 (0)		1375a, 1377
1469.	29943-42-8	4*H*-Pyran-4-one, 2,3,5,6-tetrahydro- = 4*H*-Pyran-4-one, tetrahydro-	568b, 4249		
1470.	488-18-6	4*H*-Pyran-4-one, 3,5-dihydroxy-	568b, 1351, 1375a, 1377, 1586, 2769, 4249		1375a, 1377
1471.		4*H*-Pyran-4-one, 2,5-dihydroxy-3-methyl-	1351, 1352		
1472.	61892-86-2	4*H*-Pyran-4-one, 3,5-dihydroxy-2,6-dimethyl-	568b, 1375, 1375b, 2767, 3553, 3557, 4249		
1473.	1073-96-7	4*H*-Pyran-4-one, 3,5-dihydroxy-2-methyl- {5-hydroxymaltol}	568b, 1089a, 1351, 1352, 1360, 1375, 1375a, 1375b, 1377, 1882, 1856, 1887a, 2524a, 2761, 2762, 2765–2767, 2777, 3394, 3410, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 3430, 4249, 5811b	1360, 1375a, 1377, 3402, 3404, 3405
1474.		4*H*-Pyran-4-one,3,5-dihydroxymethyl-2,6-dimethyl-	1375, 1375b, 2767, 4249		
1475.	496-63-9	4*H*-Pyran-4-one, 3-hydroxy-	568b, 1351, 1352, 1375, 1375a, 1375b, 1377, 1586, 2767, 3553, 3557, 4249, 5811b		1375a, 1377, 3401, 3402, 3404, 3405, 4249
1476.	40311-00-0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylethyl)-	90b, 4249, 5811b		
1477.	4940-18-5	4*H*-Pyran-4-one,3-hydroxy-2-(1-methylpropyl)-	90b, 4249, 5811b		
1478.	131524-11-3	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylbutyl)-	90b, 4249, 5811b		
1479.	76015-10-6	4*H*-Pyran-4-one,3-hydroxy-2-(2-methylpropyl)-	90b, 4249, 5811b		
1480.	131524-12-4	4*H*-Pyran-4-one, 3-hydroxy-2-(3-methylbutyl)-	90b, 4249, 5811b		
1481.	131524-05-5	4*H*-Pyran-4-one, 3-hydroxy-2,5,6-trimethyl-	90b, 4249, 5811b		
1482.	131524-02-2	4*H*-Pyran-4-one, 3-hydroxy-2,5-dimethyl-	90b, 4249, 5811b		
1483.	2298-99-9	4*H*-Pyran-4-one, 3-hydroxy-2,6-dimethyl-	90b, 4249, 5811b		
1484.		4*H*-Pyran-4-one, 3-hydroxy-methyl-	1582		
1485.	118-71-8	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}	568b, 1131, 1351, 1352, 1375, 1375a, 1375b, 1377, 1378, 1586, 1881, 1884, 2570, 2767, 2777, 3266, 3397, 3553, 3555, 3557, 4249, 5811b	172a, 174d, 568b, 965, 1053, 1590a, 2337, 2339b, 2386, 2389, 2544, 2917a, 3266, 3430, 3543, 3555, 3560, 3561, 5811b	1375a, 1377, 1378, 3401, 3402, 3404, 3405

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

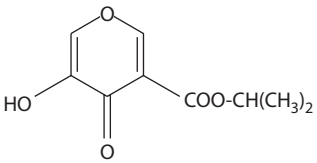
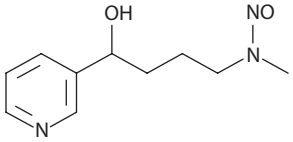
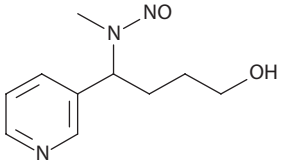
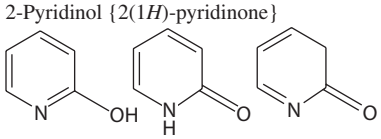
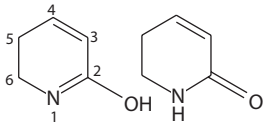
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1486.	131524-10-2	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-6-propyl-	90b, 4249, 5811b		
1487.	131524-13-5	4*H*-Pyran-4-one, 3-hydroxy-2-pentyl-	90b, 4249, 5811b		
1488.	4940-16-3	4*H*-Pyran-4-one, 3-hydroxy-2-propyl-	90b, 4249, 5811b		
1489.	42508-10-1	4*H*-Pyran-4-one, 3-hydroxy-5-methyl-	568b, 4249		
1490.	131524-07-7	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylethyl)-	90b, 4249, 5811b		
1491.	131524-14-6	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylpropyl)-	90b, 4249, 5811b		
1492.	131524-15-7	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(2-methylpropyl)-	90b, 4249, 5811b		
1493.	40861-87-8	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-propyl-	90b, 4249, 5811b		
1494.	131524-03-3	4*H*-Pyran-4-one, 5-hydroxy-2,3-dimethyl-	90b		
1495.	644-46-2	4*H*-Pyran-4-one, 5-hydroxy-2-methyl- = 4*H*-pyran-4-one, 3-hydroxy-6-methyl- {allomaltol}	568b, 1351, 1352, 1364, 2601a, 3553, 4249, 5811b		
1496.	131524-06-6	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-methyl-	90b, 4249, 5811b		
1497.	131524-17-9	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-propyl-	90b, 4249, 5811b		
1498.	499-78-5	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-	1375a (0), 1377 (0)	2544, 4249	1375a, 1377
1499.		4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-, (1-methylethyl) ester 	1375a (0), 1377 (0)		1375a, 1377, 4249
1500.	61892-91-9	Pyrazinebutanol, 3-methyl-	568b, 2767, 4249		
1501.	6705-31-3	Pyrazineethanol	568b, 2570, 2767, 3553, 4249, 5811b	568b, 3649, 4249	
1502.	61892-92-0	Pyrazineethanol, 3-methyl-	568b, 2767, 3553, 4249	568b, 3649, 4249	
1503.	61892-93-1	Pyrazineethanol, 6-methyl-	568b, 2767, 3553, 4249, 4407	568b, 3649, 4249	
1504.	6705-33-5	Pyrazinemethanol	2767, 3255, 3553, 4249		
1505.	61892-95-3	Pyrazinemethanol, 5-methyl- = Pyrazinemethanol, 3-methyl-	568b, 3553, 3559, 4249	568b, 3649, 4249	
1506.		Pyrazinepentanol		3553, 4249	
1507.		Pyrazinol, 3-methyl-	1351, 1587a, 3553	3649	
1508.	5716-15-4 21422-41-3	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt		3636, 4249, 5811b	
1509.		Pyridine, 2-(1-hydroxy-1-pentyl)-	568b, 4249		
1510.	4754-27-2	Pyridine, 3-(1-hydroxyethyl)-	568b, 4249		
1511.	123676-95-9	Pyridine, 3-[1-[(hydroxy-1-oxooctyl)oxy]-2-pyrrolidinyl]-		2567, 4249, 5811b	
1512.	25429-24-7	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, monohydroxy derivative, (S)-	568b, 3553, 3559, 4249	554, 568b, 3444, 4249	
1513.	17945-79-8	2-Pyridinebutanol	3553		
1514.	103-74-2	2-Pyridinemethanol	568b, 4249		

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1515.	59578-66-4 76014-81-8	3-Pyridinebutanol, δ-(methylnitrosoamino)-{NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-; 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-} 	24, 25, 59, 486, 991, 1565, 1571a, 1573a, 1584, 1702, 1751, 3184, 3256, 3300, 5585	469, 486, 507a, 728, 995, 1562a, 1565, 1571a, 1573a, 1584, 1702, 1771, 3943b, 3973, 4236, 4249, 5577	
1516.	133201-37-3	3-Pyridinebutanol, δ-(methylnitrosoamino)-{iso-NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-} 	59, 486, 508, 1584, 1702, 1751, 3256, 3943a, 3944–3946, 4249	486, 1562a, 1584, 1679, 1702, 3943a, 3944–3946, 3947, 3948, 3973, 4236, 5577	
1517.	70898-36-1	3-Pyridinebutanol, δ-amino-		4249	
1518.	58-56-0	3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride		429b	
1519.	100-55-0	3-Pyridinemethanol		2917a, 4249	
1520.	85352-99-4	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-, 1-oxide		4249	
1521.	5264-15-3	4-Pyridinebutanol	568b, 4249, 5811b		
1522.	60655-87-0	Pyridinium,1-α-*L*-arabinopyranosyl-3-carboxy-		4249	
1523.	35323-45-6	Pyridinium, 3-carboxy-1-β-*D*-glucopyranosyl-, hydroxide {trigonelline}		1858a, 4249	
1524.	535-83-1	Pyridinium, 3-carboxy-1-methyl-, hydroxide, inner salt		3973	
1525.	27341-45-3	Pyridinol	167, 1586, 1963, 4249, 5034		
1526.	51025-25-3	Pyridinol, dimethyl-	1586, 2767		
1527.		Pyridinol, methyl-	1371, 1375, 1375b, 2543, 2773, 2775, 2777, 3410, 3557	3550	
1528.	142-08-5 72762-00-6	2-Pyridinol {2(1*H*)-pyridinone} 	568b, 1124a, 1375, 1375b, 1586, 2724, 2767, 2773, 3553, 3557, 4249, 5811b		
1529.	61892-76-0	2-Pyridinol, 5-acetyl-3,4-dihydro-{2(1*H*)-pyridinone, 5-acetyl-3,4-dihydro-}	568b, 3553, 4249		
1530.	57147-25-8	2-Pyridinol, 3,4-dihydro- {2(1*H*)-pyridinone, 3,4-dihydro-}	2543, 2775, 3553, 3559, 4249		
1531.	61892-77-1	2-Pyridinol, 3,6-dihydro- {2(1*H*)-pyridinone, 3,6-dihydro-}	568b, 2570, 3553, 4249		
1532.	6052-73-9	2-Pyridinol, 5,6-dihydro- {2(1*H*)-pyridinone, 5,6-dihydro-; 2-piperidone, 3,4-dehydro-} 	568b, 1371, 1371, 1375, 1375b, 1586, 2387, 2545, 2570, 2761, 2762, 2765–2767, 2775, 3255, 3397, 3398, 3410, 3553, 3557, 3559, 4249, 5811b	568b, 2386, 2389, 2544, 3491, 3550, 4249	2387

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

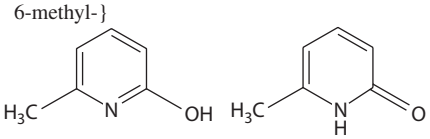
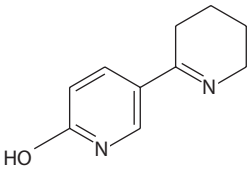
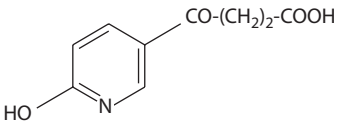
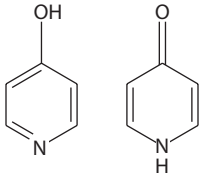
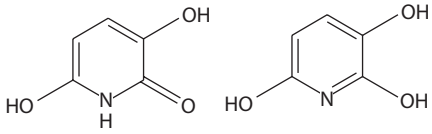
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1533.		2-Pyridinol, 5,6-dihydro-3,6,6-trimethyl- {2(1*H*)-pyridinone, 5,6-dihydro-3,6,6-trimethyl-}		939, 4249	
1534.	72692-83-2	2-Pyridinol, dimethyl- {2(1*H*)-pyridinone, dimethyl-}	3553, 4249		
1535.	6456-92-4	2-Pyridinol, 1,3-dimethyl- {2(1*H*)-pyridinone, 1,3-dimethyl-}	3559, 4249		
1536.	36330-90-2 95907-02-1	2-Pyridinol, 3,4-dimethyl- {2(1*H*)-pyridinone, 3,4-dimethyl-}	568b, 3553, 4249		
1537.	3718-67-0	2-Pyridinol, 3,5-dimethyl- {2(1*H*)-pyridinone, 3,5-dimethyl-}	568b, 1371, 3553, 4249, 5811b		
1538.	53428-02-7	2-Pyridinol, 3,6-dimethyl- {2(1*H*)-pyridinone, 3,6-dimethyl-}	568b, 3553, 4249, 5811b		
1539.	16115-08-5	2-Pyridinol, 4,6-dimethyl- {2(1*H*)-pyridinone, 4,6-dimethyl-}	568b, 3553, 4249, 5811b		
1540.	27992-31-0	2-Pyridinol, 5,6-dimethyl-	5811, 5811a, 5811b		
1541.		2-Pyridinol, 3-ethyl- {2(1*H*)-pyridinone, 3-ethyl-}	568b, 4249		
1542.	62003-48-9	2-Pyridinol, 5-ethyl- {2(1*H*)-pyridinone, 5-ethyl-}	568b, 4249		
1543.	61892-99-7	2-Pyridinol, 6-ethyl- {2(1*H*)-pyridinone, 6-ethyl-}	568b, 2767, 4249		
1544.	1003-56-1 91914-04-4	2-Pyridinol, 3-methyl- {2(1*H*)-pyridinone, 3-methyl-}	568b, 3553, 3559, 4249, 5811b		
1545.	91914-05-5	2-Pyridinol, 4-methyl- {2(1*H*)-pyridinone, 4-methyl-}	568b, 4249		
1546.	1003-68-5 91914-06-6	2-Pyridinol, 5-methyl- {2(1*H*)-pyridinone, 5-methyl-}	568b, 2543, 3553, 4249, 5811b		
1547.	3279-76-3	2-Pyridinol, 6-methyl- {2(1*H*)-pyridinone, 6-methyl-} 	568b, 1360, 1371, 1375a, 1586, 2761, 2762, 2765–2767, 2773, 2775, 3410, 3553, 4249, 5811b		1360, 1375a
1548.	19006-81-6	2-Pyridinol, 4-phenyl- {2(1*H*)-pyridinone, 4-phenyl-}	642, 4249	642, 4249	
1549.		2-Pyridinol, 5-(2,3,4,5-tetrahydropyridinyl)- 		1101, 4249	
1550.		2-Pyridinol-5-butanoic acid, γ-oxo- {2(1*H*)-pyridinone-5-butanoic acid, γ-oxo-} 		1101, 4249	
1551.		2-Pyridinol-5-pentanoic acid, δ-oxo- {2(1*H*)-pyridinone-5-pentanoic acid, δ-oxo-}		1101, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1552.	109-00-2	3-Pyridinol	568b, 1099, 1360, 1371, 1375, 1375a, 1375b, 1445, 1582, 1586, 1882, 2091a, 2133, 2228, 2493, 2543, 2570, 2601a, 2724, 2761, 2762, 2765–2767, 2773–2775, 2777, 2857, 2876, 2939, 3255, 3302, 3308, 3397, 3398, 3488, 3491, 3501, 3553, 3557, 3797, 4249, 5811b	5811b	1360, 1375a
1553.		3-Pyridinol, alkyl-	1582, 1583, 3491, 3559, 4249		
1554.	27296-76-0	3-Pyridinol, 2,4-dimethyl-	568b, 3553, 4249, 5811b		
1555.	1122-43-6	3-Pyridinol, 2,6-dimethyl-	568b, 1371, 2767, 3410, 3553, 4249, 5811b		
1556.	27296-77-1	3-Pyridinol, 4,6-dimethyl-	568b, 3553, 4249, 5811b		
1557.	61893-00-3	3-Pyridinol, 5,6-dimethyl-	3553, 4249		
1558.	61893-02-5	3-Pyridinol, 2-ethyl-	568b, 1364, 1371, 1586, 2543, 2767, 2773, 2775, 3410, 3553, 4249	568b, 3561, 4249	
1559.		3-Pyridinol, 5-ethyl-	3553, 4249		
1560.	51834-96-9	3-Pyridinol, 6-ethyl-	568b, 3255, 4249		
1561.	42451-07-0	3-Pyridinol, 6-ethyl-2-methyl-	568b, 3410, 3553, 4249, 5811b		
1562.	61893-01-4	3-Pyridinol, 6-ethyl-4-methyl-	568b, 3553, 4249		
1563.	40222-77-3	3-Pyridinol, 6-hydroxymethyl- {2-pyridinemethanol, 5-hydroxy-}	568b, 3553, 4249, 5811b		
1564.	91491-14-4	3-Pyridinol, methyl-	1375, 1375b, 2570, 2775, 3410, 4249, 5811b		
1565.	1121-25-1	3-Pyridinol, 2-methyl-	568b, 1586, 2570, 2767, 3410, 3553, 4249, 5811b	568b, 3561, 4249	
1566.	1121-19-3	3-Pyridinol, 4-methyl-	568b, 1586, 3255, 3553, 3557, 4249, 5811b		
1567.	42732-49-0	3-Pyridinol, 5-methyl-	568b, 1586, 2767, 3553, 4249, 5811b		
1568.	1121-78-4	3-Pyridinol, 6-methyl-	568b, 1371, 1375, 1375b, 1582, 1583, 2570, 2767, 2775, 3410, 3491, 3553, 4249, 4407, 5811b		
1569.	14159-68-3	3-Pyridinol, 2-propyl-	568b, 3553, 4249		
1570.	61893-03-6	3-Pyridinol, 4-propyl-	3553, 4249		
1571.	61893-04-7	3-Pyridinol, 5-propyl-	3553, 4249		
1572.	108-96-3 626-64-2	4-Pyridinol {4(1*H*)-pyridinone} 	568b, 2387, 4249, 4407		2387
1573.	39954-19-3	2(1*H*)-Pyridinone, 3,6-dihydroxy- {2,3,6-pyridinetriol} 		1101, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

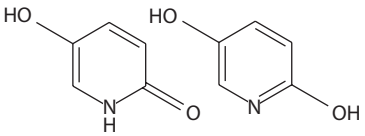
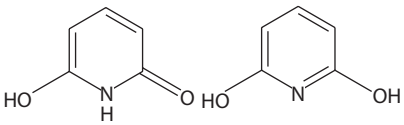
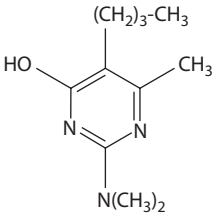
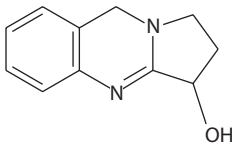
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1574.	5154-01-8	2(1*H*)-Pyridinone, 5-hydroxy-{2,5-pyridinediol} 		1101, 4249, 4918	
1575.	626-06-2	2(1H)-Pyridinone, 6-hydroxy-{2,6-pyridinediol} 		1101, 4249, 4918	
1576.	40316-88-9	2(1*H*)-Pyridinone, 3-(1-methyl-2-pyrrolidinyl)-2-{2-pyridinol, 3-(1-methyl-2-pyrrolidinyl)-} {nicotone}	2224, 2228, 2724, 3308, 4249	2226, 4249, 4572	
1577.	50609-61-5	4*H*-Pyrido[1,2-*a*]pyrimidine-3-acetic acid, 9-hydroxy-4-oxo-, ethyl ester	2601a		
1578.	3303-26-2	Pyrido[3,2-*d*]pyrimidin-4-ol, 2-methyl-		2917a	
1579.	5221-53-4	Pyrimidine, 5-butyl-2-dimethylamino-4-hydroxy-6-methyl- {Dimetherimol®} 		3633, 4249	
1580.		Pyrimidine, 2,5-dimethyl-6-hydroxy-	3553, 4249		
1581.	88070-43-3	Pyrimidine, 5-hydroxy-4-phenyl-	2601a, 4249		
1582.	34939-17-8	2(1*H*)-Pyrimidinone, 4,5-dimethyl- = 2-pyrimidinol, 4,5-dimethyl-	3553, 4249		
1583.	67383-34-0 3059-71-0	4(1*H*)-Pyrimidinone, 2,5-dimethyl- = 6-pyrimidinol, 2,4-dimethyl-	3553, 5811, 5811a, 5811b		
1584.	6622-92-0	4(1*H*)-Pyrimidinone, 2,6-dimethyl- = 6-pyrimidinol, 2,5-dimethyl-	3553, 4249		
1585.	34916-78-4	4(1*H*)-Pyrimidinone, 5,6-dimethyl- = 6-pyrimidinol, 4,5-dimethyl-	3553, 4249		
1586.	16858-16-5	4(1*H*)-Pyrimidinone, 6-methyl-2-propyl- = 6-pyrimidinol, 4-methyl-2-propyl-	3559, 4249		
1587.		Pyrrole, hydroxymethyl-	1586, 4249		
1588.		1*H*-Pyrrole-1-acetic acid, 2-formyl-5-hydroxymethyl-α-(2-methylpropyl)-	2337, 4249		
1589.		1*H*-Pyrrole-2-acetaldehyde, α-hydroxy-	1587		
1590.	29813-44-3	1*H*-Pyrrole-2-carboxaldehyde, 5-(hydroxymethyl)-1-methyl-	568b, 1587, 4249, 5811b	404, 568b, 4249	
1591.	61892-73-7	1*H*-Pyrrole-2,5-dione, 3-(hydroxymethyl)-	3553, 4249		
1592.	61892-71-5	1*H*-Pyrrole-2,5-dione, 3,4-bis(hydroxymethyl)-1-methyl-	568b, 3553, 4249	568b, 2544, 3186, 4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1593.	61892-72-6	1*H*-Pyrrole-2,5-dione,3-ethyl-4-(hydroxymethyl)-	3553, 4249	2544, 3186, 4249	
1594.	72692-82-1	1*H*-Pyrrolemethanol	1586, 4249		
1595.	115849-82-6	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		4249	
1596.	115849-79-1	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		4249	
1597.	116353-95-8	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotetradecyl)-2-(3-pyridinyl)-		4249	
1598.	115849-84-8	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
1599.	120042-33-3	Pyrrolidine, 1-(3-hydroxy-14-methyl-1-oxopentadecyl)-2-(3-pyridinyl)-		4249	
1600.	115849-80-4	Pyrrolidine, 1-(3-hydroxy-1-oxododecyl)-2-(3-pyridinyl)-		4249	
1601.	120042-32-2	Pyrrolidine, 1-(3-hydroxy-1-oxohexadecyl)-2-(3-pyridinyl)-		4249	
1602.	120042-34-4	Pyrrolidine, 1-(3-hydroxy-1-oxopentadecyl)-2-(3-pyridinyl)-		4249	
1603.	115849-85-9	Pyrrolidine, 1-(3-hydroxy-1-oxotetradecyl)-2-(3-pyridinyl)-		4249	
1604.	115849-83-7	Pyrrolidine, 1-(3-hydroxy-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
1605.	77829-17-5	Pyrrolidine, 1-(6-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		994, 2566, 2567, 3973, 4236, 4249, 5811b	
1606.	77829-18-6	Pyrrolidine, 1-(7-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		994, 2566, 2567, 3973, 4236, 4249, 5811b	
1607.	61892-97-5	2-Pyrrolidinemethanol, 5-methyl-	5811, 5811a, 5811b		
1608.	28115-37-9	2-Pyrrolidinemethanol, 5-methyl-, *cis*-	568b, 2767, 4249		
1609.	14498-44-3	2-Pyrrolidinepropanol, 1-methyl-	2387		2387
1610.	18366-19-3	2,5-Pyrrolidinedione, 3-hydroxy- (S)	2767, 3553, 4249		
1611.	6159-55-3	Pyrrolo[2,1-b]quinazolin-3-ol, 1,2,3,9-tetrahydro- {*l*-peganin, *l*-vasicin} 		3763, 5079	
1612.		Quinoline, 5-amino-2-hydroxymethyl-6-methoxy-		2917a	
1613.	5328-43-8	Rhamnitol $H_3C\text{-}(CHOH)_4\text{-}CH_2OH$		3669	
1614.		Rhamnitol, 2,4-di-*O*-methyl-		3669	
1615.		Rhamnitol, 3,4-di-*O*-methyl-		3669	
1616.		Rhamnitol, 3-*O*-methyl-		3669	
1617.		Rhamnitol, 2,3,4-tri-*O*-methyl-		3669	
1618.	39280-21-2	(1→2)-*L*-Rhamno-(1→4)-α-*D*-galacturonan		5811, 5811b	
1619.	488-81-3	Ribitol [pentahydroxypentane]	5580		

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

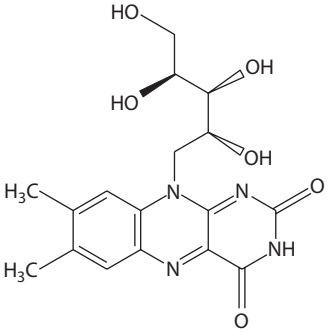
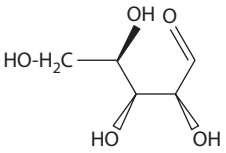
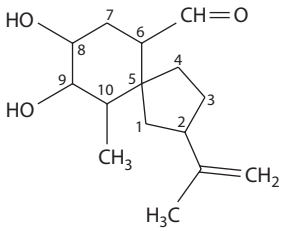
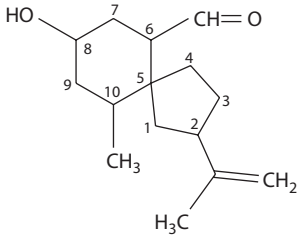
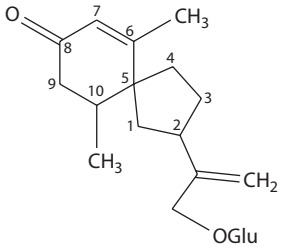
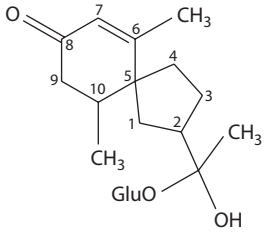
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1620.	83-88-5	Riboflavin 		120, 1941, 2270, 3973, 4249, 5079	
1621.	146-17-8	Riboflavin 5′-(dihydrogen phosphate)		4249, 4956	
1622.	106777-19-9	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-		429b, 4249	
1623.	27442-42-8	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-, 5-(dihydrogen phosphate)		429b, 4249	
1624.	3615-55-2	Ribose, 5-(dihydrogen phosphate)		429b, 4249, 4670	
1625.	50-69-1	*D*-Ribose 	5580	120, 344a, 2939, 3075, 3254, 3797, 3973, 3974a, 4249, 5811b	
1626.	24259-59-4	*L*-Ribose		3075	
1627.	129990-04-1	Saponin B, from tobacco		120, 2153a, 2153b, 2270, 2939, 5079	
1628.	6898-95-9	Serine $HO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 2858, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1063–1066, 1068–1074, 1223, 1305a, 1351, 1493, 1918, 1919, 2048, 2270, 2337, 2338, 2339b, 2445a, 2453, 2532, 2597a, 2795, 2911a, 2911c, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c 5079, 5699, 5827, 5831, 5881, 5896, 5905, 5907	
1629.	35688-48-3	*D*-Serine, *N*-(carboxyacetyl)-		2048, 4249, 4728	
1630.	56-45-1	*L*-Serine		3973, 5811b	
1631.	5692-15-9	*L*-Serine, labeled with ^{14}C		4249, 4940	
1632.	142785-07-7	*L*-Serine, *L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1633.	146440-48-4	*L*-Serine, *L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		4249	
1634.	55784-90-2	Spiro[4.5]decane-6-carboxaldehyde, 8,9-dihydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,9α,10β]]- 		1156, 4090, 4249, 4608	
1635.	35951-50-9	Spiro[4.5]decane-6-carboxaldehyde,8-hydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*), 6β,8β,10β]]- 		1156, 4090, 4249, 4637	
1636.	62574-27-0	Spiro[4.5]dec-6-en-8-one, 2-[1-[(β-*D*-glucopyranosyloxy) methyl]ethenyl]-6,10-dimethyl- 		77, 1156, 4090, 4249	
1637.	62574-29-2	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl- 		77, 1156, 4090, 4249	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

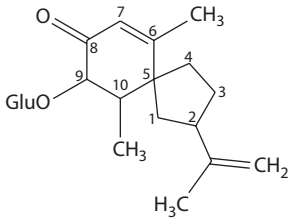
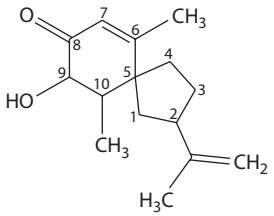
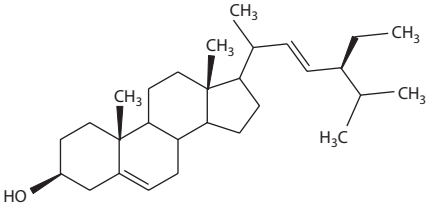
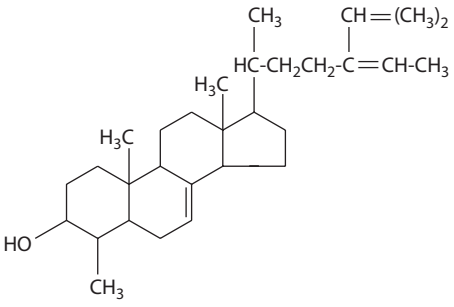
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1638.	62623-87-4	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-		77, 1156, 4090, 4249	
1639.		Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethenyl)-		4249, 4611	
1640.		Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethyl)- {isomer}		4249, 4611	
1641.	18444-79-6	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethylidene)-, (5R-*cis*)-		3547, 4249	
1642.	62574-25-8	Spiro[4.5]dec-6-en-8-one, 9-(β-*D*-glucopyranosyloxy)-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]- 		77, 1156, 4090, 4249	
1643.	62623-88-5	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]- 		1156, 4090, 4249, 4717	
1644.	117407-01-9	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6, 10-dimethyl-2-(1-methylethenyl)- {spirovetivan A}		5811, 5811b	
1645.	117332-54-4	Spiro[4.5]dec-6-en-8-one,2-[1-(hydroxymethyl)ethenyl]-6-methyl- {spirovetivan B}		5811, 5811b	
1646.	9005-25-8	Starch	5811b	69, 120, 248, 385, 385a, 420, 535, 677b, 722, 963, 1063–1066, 1068–1074, 1266, 1267, 1289, 1329, 1330, 1333, 1933a, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2394a, 2395, 2529, 2543, 2545, 2688, 2761, 2762, 2764–2766, 2914, 2939, 2947c, 3059, 3087, 3334, 3372, 3450,	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Starch (cont.)		3551, 3592, 3797, 3871, 3973, 3974a, 3974b, 4249, 4261, 4262, 4275, 5079, 5108, 5109, 5126, 5189, 5194, 5298, 5344, 5449, 5468, 5767, 5811b, 5831, 5843, 5866, 5896	
1647.	39341-47-4	Starch, labeled with ^{13}C {starch-^{13}C}		976a, 4249, 4720	
1648.	70226-57-2	Starch, labeled with ^{14}C {starch-^{14}C}		2764	
1649.	83-48-7	Stigmasta-5,22-dien-3-ol, (3β,22*E*)- {stigmasterol} 	167, 172, 239, 612, 705, 765, 966, 1099, 1100, 1352, 1360, 1375a, 1437, 1586, 1651, 1842, 2176, 2178, 2570, 2601a, 2767, 2799a, 2900, 2939, 3059, 3251, 3255, 3302, 3391, 3484, 3555, 3557, 3608, 3741, 3797, 3876, 3999, 4249, 4319, 4336, 4354, 5811b	114, 120, 435, 832, 838, 907a, 214, 1291, 1329, 1352, 1433, 1560, 1651, 2178, 2338, 2400, 2939, 3059, 3072, 3219, 3263, 3268, 3269, 3291, 3346, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3555, 3604, 3605, 3608, 3611, 3616, 3755, 3797, 3867, 3920, 3924, 3973, 3973, 3974a, 3974b, 3984, 4249, 4336, 5628, 5682, 5811b	1360, 1375a
1650.	28949-66-8	Stigmasta-5,24-dien-3-ol, (β)-		5811, 5811b	
1651.	18472-36-1	Stigmasta-5,24(28)-dien-3-ol, (3β)-	429c, 2312a, 5811b	429c, 2312a, 5811b	
1652.	17605-67-3	Stigmasta-5,24(28)-dien-3-ol, (3β,24*E*)-	429c, 5811b	5811b	
1653.	481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3β,24*Z*)-		429c	
1654.	2364-23-0	Stigmasta-5,25-dien-3-ol, (3β,24S)-		429c, 5811b	
1655.	12002-39-0	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-{sitosterols}		5811, 5811b	
1656.	7212-91-1	Stigmasta-7,24(28)-dien-3-ol, (3β,5α)-		429c	
1657.	23290-26-8	Stigmasta-7,24(28)-dien-3-ol, (3β,5α,24*Z*)-		429c, 5811b	
1658.	39006-52-5	Stigmasta-7,24(28)-diene-3-ol, 4-methyl- (3β,4α,5α,24*E*)		5811, 5811b	
1659.	474-40-8	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α,24*Z*)- {α-sitosterol} 	1375, 1375b, 2939, 3302, 3555, 3557, 3797, 3999	2939, 3098, 3555, 3797, 4249, 4820, 5811b	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

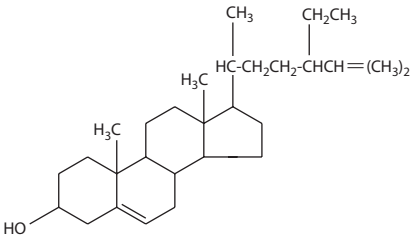
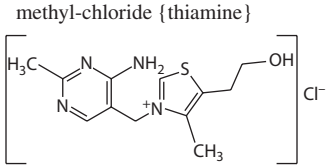
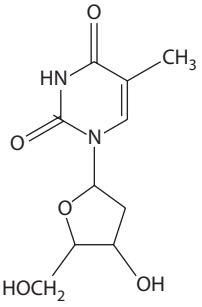
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1660.	120056-15-7	Stigmasta-7,24(28)-dien-3-ol,4-methyl-,(3β,5α)-	273, 429c		
1661.	11040-28-1	Stigmasta-7,24(28)-dien-3-ol,4-methyl-,(3β,5α)-	429c	429c	
1662.	34347-65-4	Stigmasta-8,14-dien-3-ol, (3β,5α)-		429c	
1663.	159169-57-0	Stigmasta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c	
1664.	34350-85-1	Stigmasta-8,14,24(28)-trien-3-ol, (3β,5α)-		429c	
1665.	159169-58-1	Stigmasta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-		429c	
1666.	83-46-5	Stigmast-5-en-3-ol, (3β)- {β-sitosterol} 	172, 278, 705, 765, 1099, 1100, 1352, 1360, 1375, 1375a, 1375b, 1586, 1651, 1842, 1933, 2176, 2570, 2767, 2939, 3059, 3251, 3255, 3257, 3265, 3268, 3302, 3308, 3391, 3423, 3484, 3557, 3608, 3741, 3797, 3999, 4249, 4319, 5512, 5811b	114, 116, 120, 722, 832, 838, 907a, 214, 1291, 1329, 1352, 1647, 1651, 2338, 2400, 2939, 3059, 3072, 3219, 3263, 3268, 3269, 3291, 3346, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3604, 3605, 3608, 3611, 3616, 3755, 3797, 3867, 3920, 3924, 3974a, 4249, 5628, 5811b, 5860	1360, 1375a
1667.	83-47-6	Stigmast-5-en-3-ol, (3β, 24*S*))- {γ-sitosterol}	765, 2176, 2601a	1080, 2400, 3059, 3346, 3973, 5811b	
1668.	6869-99-4	Stigmast-7-en-3-ol, (3β)-		278, 429c, 4249, 5811b	
1669.	521-03-9	Stigmast-7-en-3-ol, (3β,5α)-		429c, 4249, 4820	
1670.	4736-56-5	Stigmast-22-en-3-ol (3β,5α,22*Z*,24S)-		5811, 5811b	
1671.	1401-55-4	Tannins {tannic acid}		120, 1053, 2270, 2154, 2939, 2947c, 3266, 3708, 3973, 4249, 5079, 5126, 5381	
1672.	506-51-4	1-Tetracosanol $H_3C\text{-}(CH_2)_{22}\text{-}CH_2OH$	172, 812, 3251, 3276, 3302, 3299, 3555, 3797, 5811b	1651, 3613a, 3755, 4249, 4444	
1673.	63785-29-5	1-Tetracosanol, 22-methyl-		3613a, 4249, 4964	
1674.		1-Tetracosanol, 23-methyl-		3613a	
1675.	69521-46-6	Tetracosen-1-ol		4249, 4964	
1676.	1961-72-4	Tetradecanoic acid, 3-hydroxy- $H_3C\text{-}(CH_2)_{10}\text{-}CHOH\text{-}CH_2\text{-}COOH$		3547, 4249	
1677.	112-72-1	1-Tetradecanol $H_3C\text{-}(CH_2)_{12}\text{-}CH_2OH$	172, 568b, 4249	568b, 2339a, 4098a, 4249, 4964	
1678.	50313-71-8	1-Tetradecanol, 12-methyl-		4249, 4964	
1679.	150405-77-9	2,6,11,13-Tetradecatetraen-1-ol, 3,7,13-trimethyl-10-(1-methylethyl)-		4249	
1680.	59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-chloride {thiamine} 		120, 1941, 2270, 4249, 5079, 17B10	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1681.	67-03-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-chloride, monohydrochloride {thiamine hydrochloride}		1053, 3266, 4249	
1682.	72-19-5	*L*-Threonine H_3C-CHOH-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3555, 3797, 4249, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1305a, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5811b, 5827, 5831, 5881	
1683.	32190-57-1	*L*-Threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]-		3819a, 4249	
1684.		*L*-Threonine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337	
1685.	50-89-5	Thymidine 		3973, 4249	
1686.	99-20-7	Trehalose		3075	
1687.	593-50-0	1-Triacontanol		3613a	
1688.	3133-01-5	1-Tricosanol H_3C-(CH_2)$_{21}$-CH_2OH	172, 812, 3276, 3302, 3299, 3797, 4249, 5811b	812, 3299, 3613a, 3755, 3797, 3973, 3974a, 4249, 5811b	
1689.	63907-54-0	1-Tricosanol, 22-methyl- $(H_3C)_2$═CH-(CH_2)$_{20}$-CH_2OH		4249, 4964	
1690.	472-97-9	Tricyclo[6.3.1.02,5]dodecan-1-ol, 4,4,8-trimethyl-, [1R-(1α,2α,5β,8β)]-		3217, 4249	
1691.	129777-24-8	3,7-Tridecadiene-2,12-dione, 6-hydroxy-6-methyl-9-(1-methylethyl)-		2544, 4249	
1692.	112-70-9	1-Tridecanol H_3C-(CH_2)$_{11}$-CH_2OH	172, 568b, 3559, 4249	568b, 4098a, 4249, 4964	
1693.	21987-21-3	1-Tridecanol, 12-methyl- $(H_3C)_2$═CH-(CH_2)$_{10}$-CH_2OH		4249, 4964	

(*continued*)

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

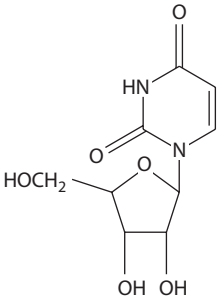
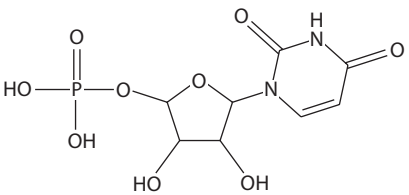
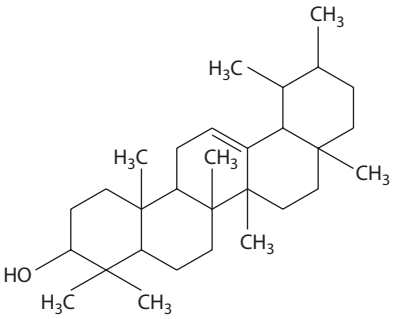
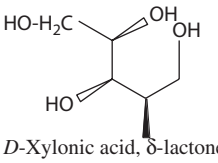
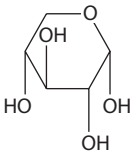
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1694.	60026-14-4	3-Tridecene-2,8-diol, 4,8,12-trimethyl- $(H_3C)_2$═CH-$(CH_2)_3$-C(OH) (CH_3)-$(CH_2)_3$-C(CH_3)═CH-CHOH-CH_3		1156, 2389, 2544, 4090, 4249	
1695.	34393-22-1	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
1696.	53837-34-6	5,9-Undecadien-2-ol, 6,10-dimethyl-	2769	5811b	
1697.	65017-84-7 133561-45-2	5,8-Undecadien-2-one, 6,10-dimethyl-10-hydroxy- (*E,E*)-		231, 1156, 4090, 4098a, 4249, 5811	
1698.	74233-43-5	5,10-Undecadien-2-one, 6,10-dimethyl-9-hydroxy-		5811b	
1699.	152209-56-8	6,10-Undecadien-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-2-methyl-2-furanyl)-		4249	
1700.	112-42-5	1-Undecanol H_3C-$(CH_2)_9$-CH_2OH	172, 568b, 1364, 4249	568b, 2356, 3547, 4098a, 4249	
1701.	38713-13-2	2-Undecanol, 6,10-dimethyl- H-[CH_2-CH(CH_3)-(CH2)2]$_2$-CH_2-CHOH-CH_3		937, 1156, 2339a, 4090, 4249, 5811b	
1702.	129777-22-6	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-, (*E*)-		4249, 5811b	
1703.	133561-48-5	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-		5811, 5811b	
1704.	29093-90-1	5-Undecen-2-one, 10-hydroxy-6,10-dimethyl-		4249, 5811b	
1705.	160115-56-0	6-Undecen-2-one, 10-(acetyloxy)-8,11-dihydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-5-hydroxy-2-methyl-2-furanyl)-		4249	
1706.	58-96-8	Uridine 		3973, 4249	
1707.	133-89-1	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-glucopyranosyl ester		4249, 4489, 4580	
1708.	3616-06-6	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester		429b, 4249	
1709.	19253-25-9	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester		4249, 4458	
1710.	58-97-9	5′-Uridylic acid 		429b, 4249, 4474	
1711.	94414-19-4	Urs-12-en-28-oicacid,3,23-dihydroxy-,(3β,4α)-		4249	

TABLE 2.5 (continued)
Alcohols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1712.	77-52-1	Urs-12-en-28-oic acid, 3-hydroxy-, (3β)-		429b	
1713.	638-95-9	Urs-12-en-3-ol, (3β)- {α-amyrin}	3484, 4249	3470, 3472, 3484, 3493, 3616, 4249, 5811b	
					
1714.		*L*-Valine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
1715.	12001-76-2	Vitamin B		950a, 1971, 4249	
1716.	9014-63-5	Xylan		842, 2070, 2850, 2939, 3371, 3666, 3797, 3973, 3974a, 4249, 5811b	
1717.		Xylan, 4′-*O*-methylglucuronyloxy-		4249, 4584	
1718.	87-99-0	Xylitol	5580	3075	
					
1719.	82796-87-0	*D*-Xylonic acid, δ-lactone	4249		
1720.	58-86-6 25990-60-7	Xylose	2145, 2939, 3302, 4249, 5580, 5811, 5811a, 5811b	120, 2070, 2270, 3079, 3797, 3973, 3974a, 4249, 5768, 5785, 5811, 5811a, 5811b	
					
1721.	31178-70-8	α-*D*-Xylose		3075, 3667, 3973, 3974a, 4249	
1722.	31178-71-9	β-*D*-Xylose		3667, 3973, 3974a, 4249	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke.

Relative to the low level of cholesterol {1a}, tobacco usually contains substantial levels of several phytosterols (campesterol {Ib}, β-sitosterol {Ic}, stigmasterol {Id}, and ergosterol {Ie}) structurally similar to cholesterol. Phytosterols {Ib}, {Ic}, and {Id} differ slightly from cholesterol in the structure of the long side chain, whereas ergosterol {Ie} not only differs slightly from cholesterol in the structure of its long side chain but also has an extra double bond at the 7 position (Figure 2.4). They are present in tobacco in both the free and bound form (as glycosides and esters), and they are transferred as such to mainstream smoke (MSS). The sterols constitute about 0.2% of the tobacco weight.

In the late 1950s/early 1960s, Rodgman proposed that the tobacco phytosterols—campesterol, β-sitosterol, stigmasterol, ergosterol—might generate compounds analogous to the tumorigenic 4-cholesten-3-one {Va} and 3,5-cholestadiene

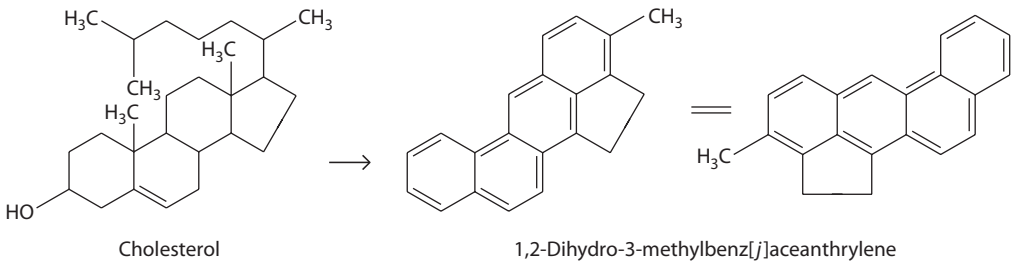


FIGURE 2.3 Theoretical conversion of cholesterol to 1,2-dihydro-3-methylbenz[*j*]aceanthrylene. *Sterol*, R =; Ia, cholesterol -$(CH_2)_3$-$CH(CH_3)_2$; Ib, campesterol -$(CH_2)_2$-$CH(CH_3)$-$CH(CH_3)_2$; Ic, β-sitosterol -$(CH_2)_2$-$CH(C_2H_5)$-$CH(CH_3)_2$; Id, stigmasterol -CH═CH-$CH(C_2H_5)$-$CH(CH_3)_2$; Ie, ergosterol[a] -CH═CH-$CH(CH_3)$-$CH(CH_3)_2$; II, 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene); III, chrysene; IV, Diels hydrocarbon; Va, 4-cholesten-3-one; Vb, 4-campesten-3-one; Vc, β-4-sitosten-3-one; Vd, stigmasten-3-one; Ve, ergostadien-3-one; VIa, 3,5-cholestadiene; VIb, 3,5-campestadiene; VIc, β-3,5-sitostadiene; VId, 3,5-stigmastadiene; VIe, 3,5,7-ergostatriene; [a]Ergosterol has a double bond at the 7-position.

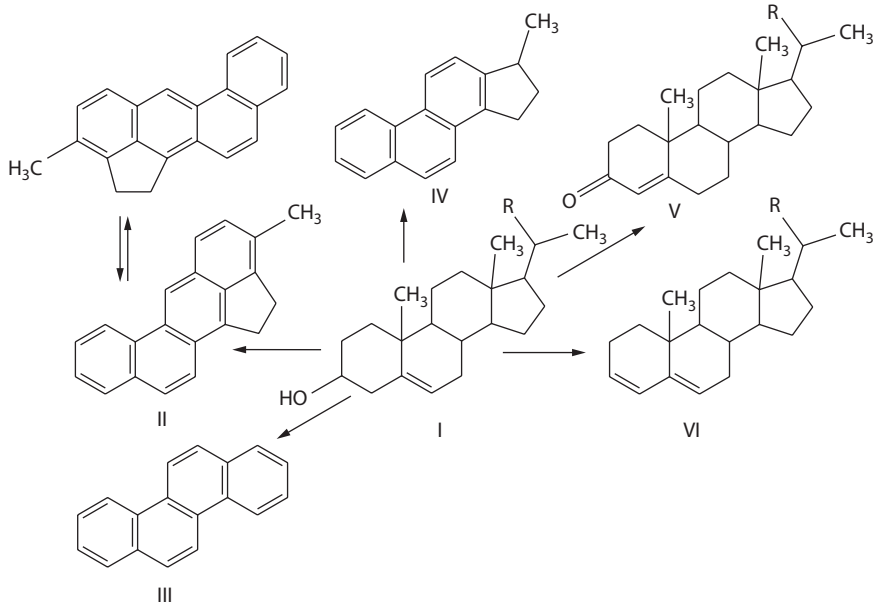


FIGURE 2.4 Possible sterol degradation products.

{VIa} generated from cholesterol, i.e., 4-campesten-3-one {Vb}, 3,5-campestadiene {VIb}, β-4-sitosten-3-one {Vc}, 3,5-sitostadiene {VIc}, 4-stigmasten-3-one {Vd}, 3,5-stigmastadiene {VId}, ergosten-3-one {Ve}, 3,5,7-ergostatriene {VIe} on thermal degradation of these tobacco phytosterols or their esters during the smoking process. These campesterol-, β-sitosterol-, stigmasterol-, and ergosterol-related compounds might also be mouse-skin tumorigens as are their cholesterol counterparts. For nearly a decade, Rodgman and Cook (3286) were unsuccessful in their periodic efforts to isolate any of these phytosteryl ketones or dienes from CSC and identify them. However, Benner et al. (273) did subsequently identify two of these 3,5-dienes, 3,5-campestadiene {VIb} and 3,5-stigmastadiene {VId}, in tobacco smoke, see also Eatough et al. (1099, 1100).

In 1939, the PAHs anthracene, phenanthrene, and B[*a*]P were reported as components of a tobacco-related material by Roffo (3323, 3325, 3326) and his son (3316–3318). In discussions of tobacco smoke, the Roffo findings are generally disregarded because the three PAHs they reported were not detected in tobacco smoke but were identified in a destructive distillate of tobacco. However, Roffo did report another finding that led to much research both within and outside the tobacco industry. Roffo (3327) reported that comparison of the destructive distillate of tobacco with the destructive distillate of an ethanol-extracted tobacco indicated that the PAH content, particularly B[*a*]P, and the specific tumorigenicity of the extracted tobacco destructive distillate were reduced from those of the destructive distillate from the control tobacco. Roffo speculated that the precursors of the tumorigenic PAH components of his distillates were ethanol-soluble phytosterols. Eventually his prediction, as far as it went, was found to be true for cigarette MSS (327, 398). In July 1954, Rodgman—a newly hired scientist at RJRT R&D—described the findings of the Roffos (3316–3318, 3323, 3325, 3327) to two colleagues who were previously

TABLE 2.6
Studies on Identification of Phytosterols and Phytosteryl Derivatives in Tobacco and Tobacco Smoke

	Identification in Tobacco of		Identification in Tobacco Smoke of		
Year	Phytosterols	Derivatives of Phytosterols	Phytosterols	Derivatives of Phytosterols	Pyrolysis Studies on Sterols or Their Inclusion in a Smoked Cigarette
1913	Traetta-Mosca (3942b)				
1928					Kennaway and Sampson (2080)
1935	Kobel and Neuberg (2153a)		Schürch and Winterstein (3562)		
1937	Shmuk (3656a)				
1939					Veldstra (4042a)
1942	Roffo (3327)				
1943	Venkatarao et al. (4042b)				
1949					Falk et al. (1171)
1955	Khanolkar et al. (2087)	(G)[a] Khanolkar et al. (2087)			
1957			Kosak et al. (2178), Rodgman and Chappell (3268)		
1958	Rowland (3346); Dymicky and Stedman (1079); Grossman and Stedman (1433)	(G) Dymicky and Stedman (1079)	Carruthers and Johnstone (612)		Wynder et al. (4355), Rodgman and Cook (3269)
1959	Dymicky and Stedman (1080, 1082)	(G) Dymicky and Stedman (1080, 1081)		(E) Rodgman et al. (3296)	Wynder et al. (4356)
1960	Stedman and Rusaniwskyj (3808)				
1961	Giles (1291), Reid (3097)		Sakaguchi and Kobashi (3391)	(G) Kallianos et al. (2018)	
1963		(G) Kallianos et al. (2019)		(G) Kallianos et al. (2019)	
1965	Ehrhardt et al. (1117)				
1968	Cheng et al. (690)				
1971			Grunwald et al. (1434)		
1972	Davis (907a)				
1974/5	Schmeltz et al. (3484)		Schmeltz et al. (3484)		
1976	Tancogne and Chouteau (3867), Lotti et al. (2400)				
1977	Davis (909), Menser et al. (2531), Tojib et al. (3920), Tancogne (3866)				
1978	Severson et al. (3612)				
1979					Severson et al. (3616)
1984					Chopra and Al-Kubaisi (705)
1998					Forehand and Moldoveanu (1214)
2000					Britt et al. (435)
2001					Britt et al. (433)

[a] (G), glucosides, (E), esters.

TABLE 2.7
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

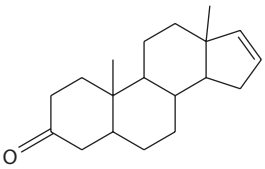
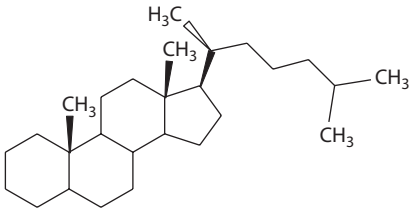
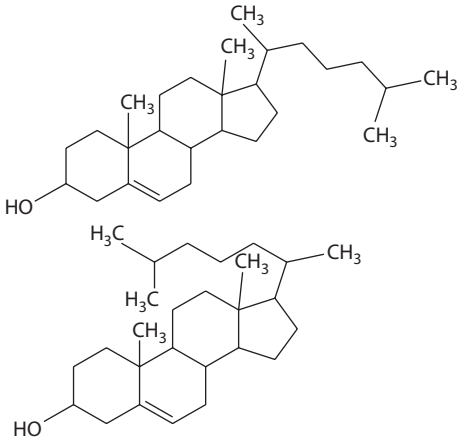
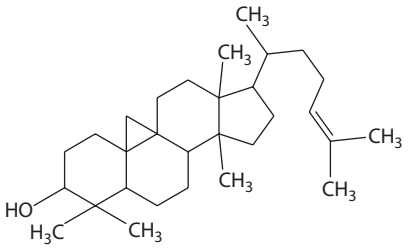
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	18339-16-7	5α-Androst-16-en-3-one {androstenone} 		5811	
2.	119973-28-3	Chol-3-ene, 23-methyl-, (5α)-	273, 429c		
3.	747-90-0	Cholesta-3,5-diene	273, 2601a, 3263		
4.		Cholesta-3,5-diene, 24-ethyl-	1099, 1100, 3255		
5.	481-21-0	Cholestane, (5α)- {coprostane} 		429c, 3867, 4249	
6.	80-97-7	Cholestan-3-ol (3β) {dihydrocholesterol}		5811, 5811b	
7.		Cholesta-3,5,22-triene, 24-methyl-	1099, 1100, 3255		
8.	96443-01-5	Cholest-4-en-3-ol, 4-methyl- (3α)	2601a		
9.	57-88-5	Cholest-5-en-3-ol (3β)- {cholesterol} 	126a, 126b, 172, 237, 1099, 1100, 1171, 1352, 1360, 1373, 1375a, 1434, 1445, 1586, 1651, 1674, 1842, 1933, 2080, 2570, 2601a, 2767, 2939, 3255, 3257, 3265, 3484, 3557, 3608, 3741, 4249, 5079, 5108, 5109, 5189, 5300, 5413, 5811b	832, 840, 907a, 1076a, 1171, 1329, 1352, 1651, 1933a, 2080, 2338, 2400, 2939, 3072, 3263, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3608, 3755, 3797, 3867, 3920, 3973, 3974a, 4249, 5079, 5242, 5811b, 4A03, 4A04, 4A05, 25A54, 25A58	1360, 1375a
10.	604-35-3	Cholest-5-en-3-ol (3β)-, acetate {cholesteryl acetate}	5811a, 5811b		
11.	2645-22-4	Cholest-5-en-3-ol (3β)-, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {cholesteryl linolenate}		433	
12.	303-43-5	Cholest-5-en-3-ol (3β)-, 9-octadecenoate, [3β(*Z*),22*E*]- {cholesteryl oleate}		433	
13.	35602-69-8	Cholest-5-en-3-ol (3β)-, octadecanoate, (3β,22*E*)- {cholesteryl stearate}		433	
14.	474-77-1	Cholest-5-en-3-ol, (3α)- {epicholesterol}		429c	
15.	1253-88-9	Cholest-5-en-3-ol, 4,4-dimethyl-, (3β)-		429c, 4249	
16.	6036-58-4	Cholest-7-en-3-ol, (3β)-		429c, 4249, 4820	

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
17.	481-25-4	Cholest-7-en-3-ol, 4-methyl-, (3β,4α,5α)-		429c, 4249	
18.	6062-47-1	Cholest-8-en-3-ol, 14-methyl-, (3β,5α)-		429c	
19.	5241-24-7	Cholest-8-en-3-ol, 4,4-dimethyl-, (3β,5α)-		429c	
20.	5241-22-5	Cholest-8-en-3-ol, 4-methyl-, (3β,4α,5α)-		429c	
21.	100017-41-2	Cholest-9(11)-en-3-ol, 14-methyl-, (3β,5α)-		429c	
22.	60485-38-3	9,19-Cyclocholest-24-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c	
23.	34443-88-4	9,19-Cycloergost-24(28)-en-3-ol,14-methyl-,(3β,5α)-		429c	
24.	469-39-6	9,19-Cycloergost-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)- {cycloeucalenol}		429c, 3098, 4249, 4429, 5811b	
25.	34347-58-5	9,19-Cycloergostan-3-ol, 14-methyl-, (3β,5α,9β)-		429c	
26.	59780-40-4	9,19-Cycloergostan-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-		429c	
27.	4657-58-3	9,19-Cyclolanostan-3-ol, (3β)-		4249, 4686	
28.	26955-76-0	9,19-Cyclolanostan-3-ol, 24,25-epoxy-, (3β)-		4249, 4686, 5811b	
29.	1449-09-8	9,19-Cyclolanostan-3-ol, 24-methylene-, (3β)-		3098, 4249	
30.	469-38-5	9,19-Cyclolanost-24-en-3-ol, (3β)- {cycloartenol} 	663, 1651, 3608	1117, 1651, 3098, 3608, 3616, 4249, 5811b	
31.	25692-13-1	9,19-Cyclolanost-24-en-3-ol, 24-methyl-, (3β)-		4484, 4249	
32.		9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3β,24*S*)-	4249	4249 (?)	
33.	511-61-5	9,19-Cyclolanost-25-en-3-ol, 24-methyl-,(3β,24*S*)-		4249	
34.	124713-05-9	9,19-Cyclolanost-5-en-3-ol, 24-methylene-, (3β)-		1651	
35.	50906-50-8	9,19-Cyclostigmast-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24*Z*)-		429c	
36.	119973-29-4	26,27-Dinorergosta-3,5-diene	273	429c	
37.	119973-31-8	26,27-Dinorergosta-3,5,22-triene, (22*E*)-	273	429c	
38.	119973-30-7	26,27-Dinorergost-3-ene, (5α)-	273	429c	
39.	474-60-2	Ergostan-3-ol, (3β,5α,24*R*)- {campestanol}		5811, 5811b	
40.	20304-54-5	Ergost-4-en-3-ol, (24*R*)- {campest-7-en-3-β-ol}		5811, 5811b	
41.	474-62-4	Ergost-5-en-3-ol, (3β,24*R*)- {campesterol}	172, 1099, 1100, 1352, 1360, 1375a, 1586, 1651, 1744, 1842, 2018, 2019, 2570, 2601a, 2767, 3059, 3255, 3308, 3484, 3557, 3608, 5512, 5811, 5811b	832, 838, 907a, 082, 1329, 1352, 1651, 2018, 2019, 2338, 2400, 2939, 3059, 3072, 3435, 3476, 3484, 3493, 3511, 3608, 3755, 3797, 3867, 3920, 3973, 3974a, 5811, 5811b	1360, 1375a

(*continued*)

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

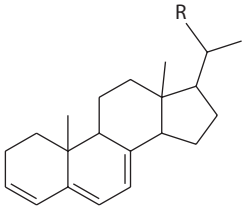
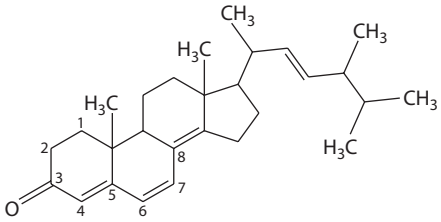
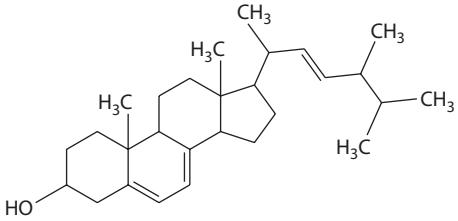
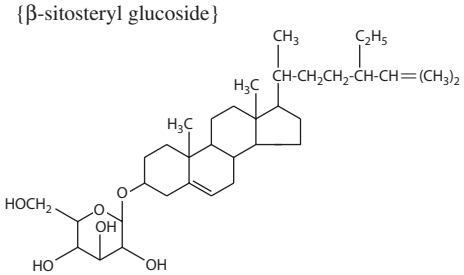
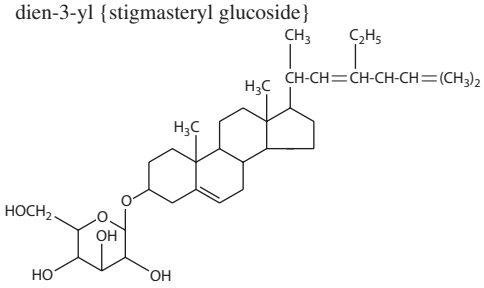
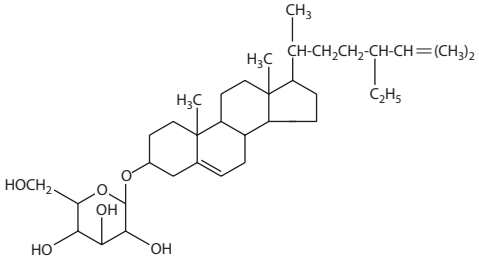
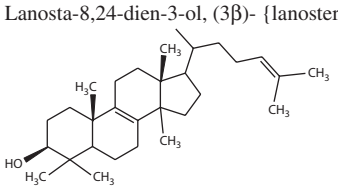
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
42.	26047-31-4	Ergost-7-en-3-ol, (3β)-		429c	
43.	17105-75-8	Ergost-7-en-3-ol, (3β,24ξ)-	273, 429c		
44.	33860-48-9	Ergost-8-en-3-ol, 14-methyl-, (3β,5α)-		429c	
45.	16910-33-1	Ergost-8-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c, 4479	
46.	70116-48-2	Ergost-8-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-		429c	
47.	77327-07-2	Ergosta-3,5,7-triene, (24ξ)-	273, 278, 1099, 1100		
		 R = -$(CH_2)_2$-$CH(CH_3)$-$CH(CH_3)_2$			
48.	19254-69-4	Ergosta-4,6,8(14),22-tetraen-3-one, (22*E*)-		334, 3866, 4249	
					
49.	474-67-9	Ergosta-5,22-dien-3-ol, (3β,22*E*)-		429c, 2400, 5811b	
50.	474-63-5	Ergosta-5,24(28)-dien-3-ol, (3β)-		429c, 1971, 5777, 5811, 5811b	
51.	52936-69-3	Ergosta-5,25-dien-3-ol, (3β)-		429c	
52.	57-87-4	Ergosta-5,7,22-trien-3-ol, (3β,22*E*)- {ergosterol}	3059	334, 1080, 3867, 3973, 3974a, 5811b	
					
53.	21490-25-5	Ergosta-7,24(28)-dien-3β-ol, 4β-methyl-		429c, 3098, 4249	
54.	474-68-0	Ergosta-7,24(28)-dien-3-ol, (3β,5α)-		429c, 4249, 4431	
55.	1176-52-9	Ergosta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α)-		429c, 4249, 4851, 5811b	
56.	74635-33-9	Ergosta-8,14,24(28)-trien-3-ol,4-methyl-,(3β,4α,5α)-		429c, 4249, 1971	
57.	23839-47-6	Ergosta-8,14-dien-3-ol, (3β,5α)-		429c	
58.	33886-74-7	Ergosta-8,24(28)-dien-3-ol, 14-methyl-, (3β,5α)-		429c	
59.	16910-32-0	Ergosta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c, 5811b	
60.	80736-41-0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22*R*, 23*R*,24*S*)-		429c	
61.	121468-15-3	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3β,5α,22*R*,23*R*,24*S*)-		429c	
62.	92751-21-8	Ergostan-6-one, 3,22,23-trihydroxy-, (3β,5α, 22*R*,23*R*,24*S*)-		429c	

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
63.	87734-68-7	Ergostan-6-one, 3,22,23-trihydroxy-, (3α,5α,22*R*, 23*R*,24*S*)-		429c	
64.	7073-61-2	β-*D*-Glucopyranoside, (3β)-cholest-5-en-3-yl {cholesteryl glucoside}	648, 1434, 4249, 4534	390, 4249	
65.	32214-82-7	β-*D*-Glucopyranoside, (3β)-ergost-5-en-3-yl {campesteryl glucoside}	648, 2018, 2019, 2079, 3308, 3667, 4249	2018, 2019, 4249, 5777	
66.	474-58-8 20431-48-5	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl {β-sitosteryl glucoside} 	648, 2018, 2019, 2939, 3296, 3302, 3308, 4249	1079, 2018, 2019, 2270, 2939, 3296, 3302, 3346, 3349, 4249	
67.	19716-26-8	β-*D*-Glucopyranoside, (3β,22*E*)-stigmasta-5,22-dien-3-yl {stigmasteryl glucoside} 	648, 908, 2018, 2019, 2939, 3296, 3302, 3308, 4249, 4534	908, 2018, 2019, 3302, 3346, 3349, 4249	
68.	51064-38-1	β-*D*-Glucopyranoside, (3β,24*S*)-stigmast-5-en-3-yl {γ-sitosteryl glucoside} 	2018	120, 2087, 3346, 4249	
69.		Hexacosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl hexacosanoate}	1230	1230	
70.	79-62-9	Lanost-8-en-3-ol, (3β)-		4249, 4686	
71.	6890-88-6	Lanost-8-en-3-ol, 24-methylene-, (3β)-		4249, 4431	
72.	26409-08-5	Lanost-9(11)-en-3-ol, 24,25-epoxy-, (3β)-		429c, 4249, 4868	
73.	79-63-0	Lanosta-8,24-dien-3-ol, (3β)- {lanosterol} 		1117, 4249, 4480	

(*continued*)

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

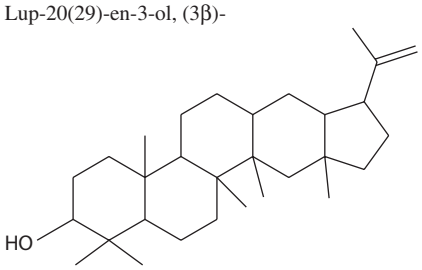
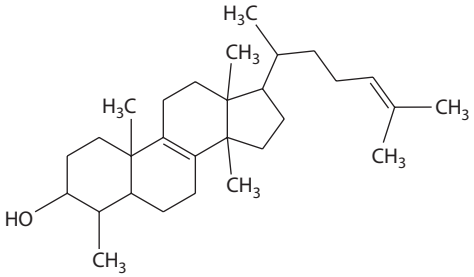
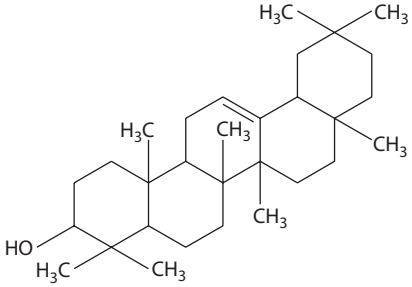
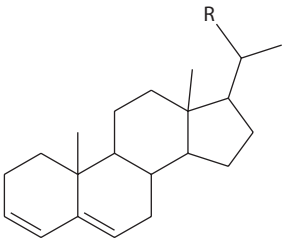
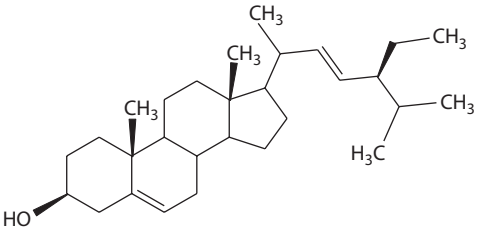
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
74.	67493-77-0	Lanostane-3,7,11-triol, 3,7-diacetate, (3β,7β,11β)-		4249, 4497	
75.	70898-27-0	Lanostane-3,7-diol, (3β,7β)-		4249, 4497	
76.	545-47-1	Lup-20(29)-en-3-ol, (3β)- 		1157a, 3098, 4249	
77.	18444-66-1	19-Norlanosta-1,5,23-triene-3,11,22-trione, 25-(acetyloxy)-2,16,20-trihydroxy-9-methyl-, (9β,10α,16α,23*E*)-		4249	
78.	17278-28-3	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3α, 9β,10α,16α,23*E*)-		4249	
79.	89647-62-1	19-Norlanosta-5,23-diene-2,11, 22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3β,9β,10α,16α,23*E*)-		4249	
80.	51013-77-5	31-Norlanosterol 		5811	
81.		Octacosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl octacosanoate)	1230	1230	
82.	508-02-1	Olean-12-en-28-oic acid, 3-hydroxy-, (3β)-		4249	
83.	471-53-4	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-	3390, 4249		
84.	559-70-6	Olean-12-en-3-ol, (3β)- {β-amyrin} 	1651, 3484, 3797, 3971, 4249	1651, 3470, 3472, 3484, 3493, 3511, 3616, 3755, 3797, 3971, 3973, 3974a, 4249, 5811b	
85.	72962-43-7	β-homo-7-Oxaergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22*R*,23*R*,24*S*)-		429c, 4249	
86.	57-83-0	Pregn-4-ene-3,20-dione		429c, 4249, 4613	
87.	145-13-1	Pregn-5-en-20-one, 3-hydroxy-, (3β)-		429c, 4249, 4613	
88.	32378-60-2	Pregnan-20-one, 3-[(1-oxohexadecyl)oxy]-, (3β,5α)-		429c, 4249, 4613	

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
89.	79897-80-6	Stigmasta-3,5-diene, (24ξ)-  R = -CH═CH-CH(C_2H_5)-CH(CH_3)$_2$	273, 1099, 1100, 3263		
90.	28949-66-8	Stigmasta-5,24-dien-3-ol, (β)-		5811, 5811b	
91.	83-48-7	Stigmasta-5,22-dien-3-ol, (3β,22*E*)- {stigmasterol} 	167, 172, 239, 612, 705, 765, 966, 1099, 1100, 1352, 1360, 1375a, 1437, 1586, 1651, 1744, 1842, 2176, 2178, 2570, 2601a, 2767, 2799a, 2900, 2939, 3059, 3251, 3255, 3302, 3391, 3484, 3555, 3557, 3608, 3741, 3797, 3876, 3999, 4249, 4319, 4336, 4354, 5512, 5811b	114, 120, 435, 832, 838, 907a, 214, 1291, 1329, 1352, 1433, 1560, 1651, 2178, 2338, 2400, 2939, 3059, 3072, 3219, 3263, 3268, 3269, 3291, 3346, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3555, 3604, 3605, 3608, 3611, 3616, 3755, 3797, 3867, 3920, 3924, 3973, 3973, 3974a, 3974b, 3984, 4249, 4336, 5628, 5682, 5811b	
92.	71607-87-9	Stigmasta-5,22-dien-3-ol, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {stigmasteryl linolenate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
93.	71278-15-4	Stigmasta-5,22-dien-3-ol, 9,12-octadecadienoate, [3β(9*Z*,12*Z*),22*E*]- {stigmasteryl linoleate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
94.	31615-93-7	Stigmasta-5,22-dien-3-ol, 9-octadecenoate, [3β(*Z*),22*E*]- {stigmasteryl oleate}	3251, 3296, 4249	2939, 3296, 4249	
95.	20242-97-1	Stigmasta-5,22-dien-3-ol, dodecanoate, (3β,22*E*)- {stigmasteryl laurate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
96.	2308-84-1	Stigmasta-5,22-dien-3-ol, hexadecanoate, (3β,22*E*)- {stigmasteryl palmitate}	3251, 3296, 4249	2939, 3296, 4249	
97.	23838-16-6	Stigmasta-5,22-dien-3-ol, octadecanoate, (3β,22*E*)- {stigmasteryl stearate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
98.	20242-98-2	Stigmasta-5,22-dien-3-ol, tetradecanoate, (3β,22*E*)- {stigmasteryl myrsitate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
99.	28949-66-8	Stigmasta-5,24-dien-3-ol, (β)-		5811, 5811b	
100.	18472-36-1	Stigmasta-5,24(28)-dien-3-ol, (3β)-	429c, 2312a, 5811b	429c, 2312a, 5811b	
101.	17605-67-3	Stigmasta-5,24(28)-dien-3-ol, (3β,24*E*)-	429c, 5811b	5811b	
102.	481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3β,24*Z*)-		429c	
103.	2364-23-0	Stigmasta-5,25-dien-3-ol, (3β,24*S*)-		429c, 5811b	
104.	12002-39-0	Stigmasta-7,24(28)-dien-3-ol, 4-methyl- {sitosterols}		5811, 5811b	

(*continued*)

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

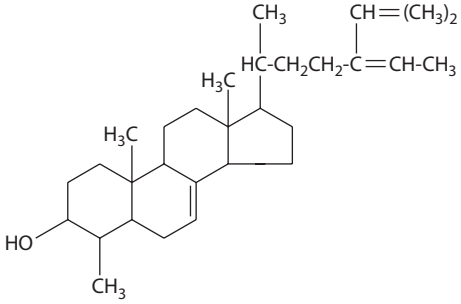
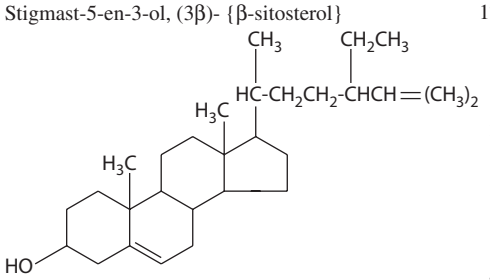
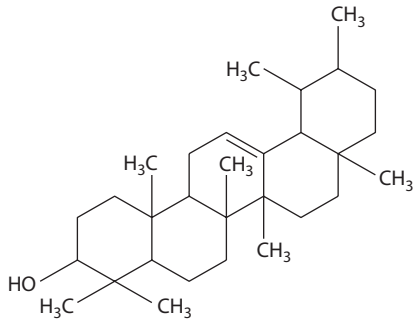
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
105.	7212-91-1	Stigmasta-7,24(28)-dien-3-ol, (3β,5α)-		429c, 5811b	
106.	23290-26-8	Stigmasta-7,24(28)-dien-3-ol, (3β,5α,24*Z*)-		429c, 5811b	
107.	39006-52-5	Stigmasta-7,24(28)-diene-3-ol, 4-methyl- (3β,4α,5α,24*E*)		5811, 5811b	
108.	474-40-8	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α,24*Z*)- {α-sitosterol} 	1375, 1375b, 2939, 3302, 3555, 3557, 3797, 3999	2939, 3098, 3555, 3797, 4249, 4820	
109.	120056-15-7	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,5α)-	273, 429c		
110.	11040-28-1	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,5α)-	429c	429c	
111.	34347-65-4	Stigmasta-8,14-dien-3-ol, (3β,5α)-		429c	
112.	159169-57-0	Stigmasta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3β,4α,5α)-		429c	
113.	102491-96-3	Stigmasta-3,5,22-triene, (22*E*)-	1098, 5811b	429c	
114.	81531-12-6	Stigmasta-3,5,22-triene, (22*E*,24ξ)-	273, 2601a	429c	
115.	86709-50-4	Stigmasta-3,5,24(28)-triene	273	429c	
116.	34350-85-1	Stigmasta-8,14,24(28)-trien-3-ol, (3β,5α)-		429c	
117.	159169-58-1	Stigmasta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-		429c	
118.	83-46-5	Stigmast-5-en-3-ol, (3β)- {β-sitosterol} 	172, 278, 705, 765, 1099, 1100, 1352, 1360, 1375, 1375a, 1375b, 1586, 1651, 1744, 1842, 1933, 2176, 2570, 2767, 2939, 3059, 3251, 3255, 3257, 3265, 3268, 3302, 3308, 3391, 3423, 3484, 3557, 3608, 3741, 3797, 3999, 4249, 4319, 5512, 5811b	114, 116, 120, 722, 832, 838, 907a, 214, 1291,1329, 1352, 1647, 1651, 2338, 2400, 2939, 3059, 3072, 3219, 3263, 3268, 3269, 3291, 3346, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3604, 3605, 3608, 3611, 3616, 3755, 3797, 3867, 3920, 3924, 3974a, 4249, 5628, 5811b, 5860	1360, 1375a
119.	83-47-6	Stigmast-5-en-3-ol, (3β, 24*S*))- {γ-sitosterol}	765, 2176, 2601a	1080, 2400, 3059, 3346, 3973, 5811b	
120.	3177-92-2	Stigmast-5-en-3-ol, 9,12,15-octadecatrienoate, [3β(9*Z*,12*Z*,15*Z*)]- {β-sitosteryl linolenate}	3251, 3296, 4249	3296, 4249	
121.	3577-13-7	Stigmast-5-en-3-ol, 9,12-octadecadienoate, [3β(*Z*,*Z*)]- {β-sitosteryl linoleate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	

TABLE 2.7 (continued)
Phytosterols, Their Derivatives, and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
122.	3712-16-1	Stigmast-5-en-3-ol, 9-octadecenoate, [3β(*Z*)]- {β-sitosteryl oleate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
123.	41005-65-6	Stigmast-5-en-3-ol, dodecanoate, (3β)- {β-sitosteryl laurate}	3251, 3296, 4249	3296, 4249	
124.	2308-85-2	Stigmast-5-en-3-ol, hexadecanoate, (3β)- {β-sitosteryl palmitate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
125.	34137-25-2	Stigmast-5-en-3-ol, octadecanoate, (3β)- {β-sitosteryl stearate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
126.	10473-40-2	Stigmast-5-en-3-ol, tetradecanoate, (3β)- {β-sitosteryl myristate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
127.	6869-99-4	Stigmast-7-en-3-ol, (3β)-		278, 429c, 4249, 5811b	
128.	521-03-9	Stigmast-7-en-3-ol, (3β,5α)-		429c, 4249, 4820	
129.	4736-56-5	Stigmast-22-en-3-ol (3β,5α,22*Z*,24*S*)-		5811, 5811b	
130.		Tetracosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl tetracosanoate}	1230	1230	
131.		Triacontanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl triacontanoate}	1230	1230	
132.	94414-19-4	Urs-12-en-28-oic acid, 3,23-dihydroxy-, (3β,4α)-		4249	
133.	77-52-1	Urs-12-en-28-oic acid, 3-hydroxy-, (3β)-		429b	
134.	638-95-9	Urs-12-en-3-ol, (3β)- {α-amyrin}	3484, 4249	3470, 3472, 3484, 3493, 3616, 4249, 5811b	



unaware of them. He particularly emphasized the organic-solvent extraction of tobacco to remove PAH precursors. The discussion resulted within a week of one of the colleagues proposing an extraction method for removal of the phytosterols from tobacco (114). A few months later, Rodgman initiated a lengthy study of the effect of organic-solvent extraction on the PAH content of its MSS (3240–3242, 3246, 3251). All of the extractions of different tobacco types and blends with different organic solvents and the fabrication of the cigarettes from the extracted and control tobaccos were conducted by Ashburn (116, 117).

Two major mechanisms were proposed for the pyrogenesis of PAHs in tobacco smoke: (1) PAHs are formed by degradation of organic tobacco components to simpler molecules and/or free radicals during the pyrolysis processes occurring in the burning cigarette, followed by recombination of these simpler fragments to yield PAHs (the degradation–combination mechanism) [cf. Badger et al. (142–144) and earlier papers]. (2) PAHs are formed unimolecularly by cyclization, dehydration, aromatization, ring expansion, etc., of high-molecular-weight tobacco components such as the phytosterols, the tetradecacyclic duvanes, long-chained saturated and unsaturated hydrocarbons, alcohols, and esters (the aromatization reaction) [Rodgman and Cook (3269, 3286)].

Obviously, the mechanism of formation of PAHs is not an either-or situation. Experimental data indicate that both mechanisms are operative in PAH formation in the burning cigarette. Evidence for unimolecular aromatization was provided by pyrolysis data and by MSS PAH data from cigarettes "spiked" with phytosterols (3269, 3286). The relatively large

increase in the levels of chrysene and methylcyclopentaphenanthrene (Diels' hydrocarbon) vs. those for B[*a*]P and other tetra- and pentacyclic PAHs is more readily explained by the unimolecular aromatization of the tetracyclic sterol than by the degradation–recombination mechanism. The formation of several PAHs (chrysene, picene, several cyclopentaphenanthrenes, etc.) from various sterols had been reported by Diels, Ruzicka, and their colleagues in the 1920s and 1930s [see historical summary by Fieser and Fieser (1949)]. Early research on PAHs in roasted and/or grilled meats evolved from the theory that cholesterol when heated would generate the highly potent tumorigen 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene). As noted previously, sterols in tobacco include cholesterol plus much higher levels of several phytosterols whose structures differ only slightly from that of cholesterol. In 1959, Wynder et al. in an addendum to their publication (4356) reported that the pyrolysis of tobacco phytosterols at 720°C and 850°C gave B[*a*]P and other PAHs plus low levels of alkyl derivatives of phenanthrene, pyrene, and chrysene.

Much of the early research on the isolation and identification of phytosterol and their derivatives from tobacco and tobacco smoke is summarized and referenced in the 1959 review by Johnstone and Plimmer (1971) and the 1968 review by Stedman (3797).

Table 2.6 chronicles many of the reported studies on phytosterols and their derivatives in tobacco and tobacco smoke plus the studies on the pyrolysis of phytosterols. Table 2.7 lists the 134 phytosterols and phytosteryl derivatives identified in tobacco and tobacco smoke. Of these 123 components, 54 have been reported as tobacco smoke components, 123 as tobacco components, and 43 in both tobacco and tobacco smoke.

3 Aldehydes and Ketones

The publication in the early 1950s of the results of several retrospective studies on association between cigarette smoking and respiratory tract cancer, particularly lung cancer, and the study on induction of skin carcinoma in a susceptible strain of mice painted with massive doses of cigarette tar for the better part of their life span [Wynder et al. (4306a)] triggered intensive interest in the composition of cigarette mainstream smoke (MSS). Because the cigarette smoke condensate (CSC) (or total particulate matter [TPM]), the phase of the smoke aerosol reported to be the mouse-skin tumorigen, embodied the particulate phase of the cigarette smoke aerosol, considerable effort was devoted to defining its composition with emphasis on the presence in it of tumorigenic polycyclic aromatic hydrocarbons (PAHs), particularly benzo[*a*]pyrene (B[*a*]P). This effort was conducted by research groups both within and outside of the tobacco industry.

However, because knowledge of the composition of tobacco smoke was so sketchy in the mid-1950s, several research groups initiated the detailed examination of the tobacco smoke aerosol to define not only its physical characteristics but also the composition of its vapor phase. For most of the balance of the 1950s, the results from the composition studies of cigarette smoke vapor phase received little attention compared to that directed at the particulate-phase composition results.

In 1954, Kosak (2170) published a list of components reported to be present in tobacco smoke. His list is shown in Table 3.1. The aldehydes listed included formaldehyde, acetaldehyde, acrolein (2-propenal), butyraldehyde (butanal), benzaldehyde, and 2-furaldehyde. In several instances, Kosak questioned whether the analytical data reported were sufficient to define unequivocally the identity of the smoke component. The ketones listed by Kosak included 3-pentanone (diethyl ketone), 4-heptanone (di-*n*-propyl ketone), 17-tritriacontanone (dipalmityl ketone), 2,3-butanedione (biacetyl), and "higher" ketones.

Because the low-molecular-weight aldehydes such as formaldehyde, acetaldehyde, propionaldehyde (propanal), acrolein (propenal), and butyraldehyde (butanal) and ketones such as acetone, methyl ethyl ketone (2-butanone), and diethyl ketone (3-pentanone) in cigarette MSS occur primarily in the vapor phase, their identification and analysis in the 1950s and 1960s were facilitated by conversion to less volatile compounds. Many of these low-molecular-weight carbonyl compounds form stable compounds with various derivatizing agents, and in many instances, the derivative formation is almost quantitative. The use of Girard T (trimethylamine) or Girard P (pyridine) reagent to derivatize tobacco smoke carbonyl compounds was described by Seligman (3581) and Resnik and Seligman (3108). The derivatives were separated by paper chromatography and identified from their mass spectra. A reagent that proved to be an excellent one to derivatize tobacco MSS aldehydes, ketones, and keto acids was 2,4-dinitrophenylhydrazine. Individual hydrazones were isolated by various chromatographic means (column chromatography, paper chromatography, and eventually HPLC) and their levels estimated spectrophotometrically. Another ingenious use of 2,4-dinitrophenylhydrazine was the following: The less stable Girard T or Girard P derivatives were decomposed and the carbonyl compounds released were converted to the highly stable 2,4-dinitrophenylhydrazones for identification and quantitation. Subsequently, the 2,4-dinitrophenylhydrazine procedure was adapted to the investigation of carbonyl compounds in tobacco, in its headspace vapors, in sidestream smoke (SSS), and in environmental tobacco smoke (ETS).

A third reagent used for the estimation of aliphatic aldehydes in tobacco smoke was 3-methylbenzothiazolone hydrazone hydrochloride [Weaving (4155), Davis and Sneade (915)].

Table 3.2 summarizes some of the studies on low-molecular-weight carbonyl components of tobacco smoke in which various derivatizing reagents were used, the derivatives formed were separated by a variety of techniques (column, paper, TLC, HPLC) and identified and estimated by spectral means (UV, IR, mass, colorimetry).

The results of many of these studies provided quantitative data on the per cigarette MSS yield of several carbonyl compounds of interest.

As the interest in the overall composition of tobacco smoke escalated in the 1950s and 1960s, the potential of the utilization of gas chromatography to examine and define the vapor-phase composition was examined. For example, Seligman et al. (3584) in their gas chromatographic study of the components of a synthetic mixture comprising 17 compounds known to be present in tobacco smoke demonstrated the feasibility that the 17 diverse compounds could be successfully separated by gas chromatography. Among the 17 standard compounds, ranging from methane to water, were acetaldehyde, propionaldehyde, and acetone. Subsequent to the successful separation of the compounds, the identity of each was confirmed by mass spectroscopy.

As a requisite and adjunct to their study of selective filtration of tobacco smoke components and the effect of carbon filters on cigarette MSS composition, Laurene et al. (2305) developed and described a gas chromatographic analysis of acetaldehyde, acrolein, and acetone in cigarette MSS. In addition to the analytical methodology, Laurene et al. also provided data on the MSS yields of acetaldehyde, acetone, and acrolein from 65 mm nonfiltered cigarettes containing individual tobacco types (flue-cured or burley or Oriental tobacco) or a blend of all three (50 mm of the tobacco rod

TABLE 3.1
Tobacco Smoke Components Listed by Kosak (2170)

Class	Component	Class	Component	Class	Component
Hydrocarbons	Hentriacontane (?)	Ketones	3-Pentanone	Acids	Formic acid
	Acetylene		4-Heptanone		Acetic acid
	"Unsaturated hydrocarbons"		17-Tritriacontanone (?)		Butyric acid
			2,3-Butanedione		Valeric acid
	Azulene		"Higher" ketones (?)		Caproic acid
	Phenanthrene (?)				C_7 and C_8 aliphatic acids (?)
	Anthracene (?)				Succinic acid (?)
	Benzopyrene (?)				Fumaric acid (?)
	"Condensed aromatics" (?)				Citric acid (?)
					Benzoic acid (?)
					Phenolic acids (?)
Alcohols and Phenols	Methanol	Alkaloids	Nicotine	Miscellaneous components	Levoglucosan[b]
	Glycerol		Pyridyl ethyl ketone		"Phytosterol" (?)
	Diethylene glycol		Myosmine		$C_{10}H_{14}O$ (a furan ?)
	Ethylene glycol		Nicotyrine		"Resins" (?)
	Phenol (?)		α-Socratine[a]		"Resin acids" (?)
	Catechol (?)		β-Socratine[a]		
			γ-Socratine[a]		
			Obelin[a]		
			Lohitam[a]		
			Anodmin[a]		
			Lathraein[a]		
			Poikiline[a]		
			Gudham[a]		
Aldehydes	Formaldehyde	Other N-containing components	Pyrrole (?)	Inorganic components	Ammonia
	Acetaldehyde		"Pyrroles" (?)		Carbon monoxide
	Butyraldehyde		"*N*-Methyl-pyrrolidines" (?)		Carbon dioxide
	Acrolein (?)		Pyridine		Hydrogen cyanide
	Benzaldehyde		"Picoline" (?)		Hydrogen sulfide
	2-Furaldehyde (?)[c]		"Lutidine" (?)		Thiocyanic acid (?)
			"Collidine" (?)		Oxygen
			"Pyridine bases" (?)		Arsenic[d]
			Methylamine (?)		"Acetates" (?)
			"Chlorophyll degradation products" (?)		"Chlorides" (?)
			"Uric acids" (?)		"Cyanides" (?)
					"Nitrates" (?)

[a] Subsequent study demonstrated this component was not a well-defined compound but an artifact, a mixture, or an ammonium salt [see discussion by Johnstone and Plimmer (1971)].
[b] 1,6-Anhydro-β-*D*-glucopyranose.
[c] The question mark indicates that Kosak did not consider the evidence in the literature to be definitive proof of the identity of the component.
[d] Probably present as As_2O_3.

smoked). The effect of a charcoal filter tip on the MSS levels of these carbonyl compounds was also determined. Their data are summarized in Table 3.3.

Modifications of gas chromatographic methods to determine vapor-phase carbonyl compounds in cigarette MSS continued for more than three decades, e.g., Miyake and Shibamoto (2564).

In Figure 3.1 is shown the approximate composition of MSS from a cigarette that delivers about 22.5 mg of wet total particulate matter (WTPM) and 17.6 mg of FTC "tar." Excluding carbon monoxide and carbon dioxide, acetaldehyde is the vapor-phase component usually found at the highest level in cigarette MSS.

The nonfiltered cigarette MSS yield of acetaldehyde ranged from 18 [Huynh et al. (1853a)] to 2815 µg/cig [Miyake and Shibamoto (2564)]. The acetone yield was slightly less than 50% of the acetaldehyde yield. Acrolein is the next most plentiful aldehyde, followed by formaldehyde, 2-furaldehyde, and crotonaldehyde. Per cigarette formaldehyde MSS yields ranged from 3.4 µg for filtered cigarettes to 283 µg in nonfiltered cigarettes [Schaller et al. (3427), Miyake and Shibamoto (2564)].

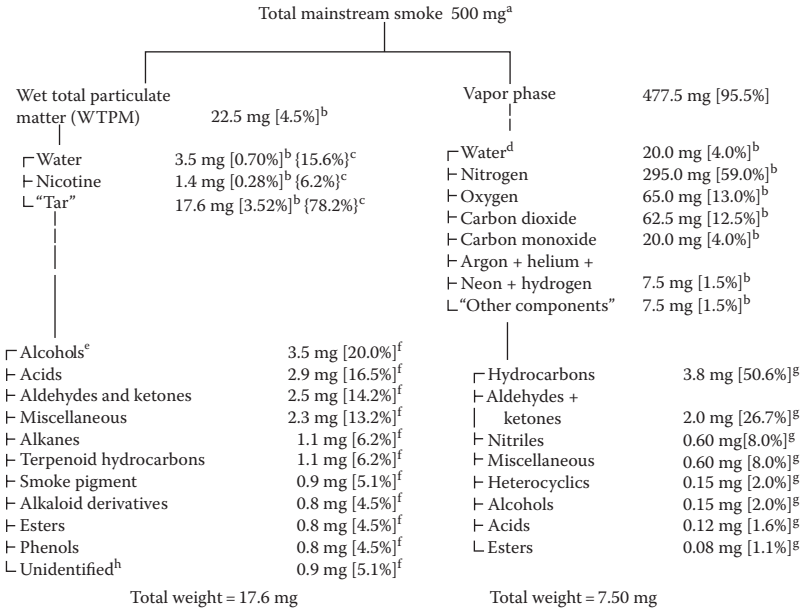
TABLE 3.2
Studies on Low-Molecular-Weight Carbonyls in Tobacco and Tobacco Smoke: Derivatizing Agents

Description	Reference
Girard T or Girard P reagent	
Aldehydes and ketones in cigarette MSS separated by conversion to Girard T or Girard P derivatives; derivatives separated by paper chromatography	Seligman (3581)
Girard T or Girard P derivatives of cigarette MSS aldehydes and ketones were characterized my mass spectroscopy	Resnik and Seligman (3108)
4-Nitrophenylhydrazine (4-NPH)	
To isolate and identify the low boiling aldehydes and ketones in cigarette MSS, they were derivatized with *p*-nitrophenylhydrazine	Sakuma et al. (3396)
2,4-Dinitrophenylhydrazine (2,4-DNPH)	
Classification of the structures of various carbonyl compounds from the UV and IR spectra of their 2,4-DNPH derivatives	Jones et al. (1977a)
Cigarette MSS aldehydes and ketones, regenerated from Girard T or Girard P derivatives, were characterized by conversion to their 2,4-DNPH derivatives	Seligman (3581)
2,4-DNPH derivatives of tobacco smoke carbonyls were separated by paper and column chromatography	Seligman and Edmonds (3582)
Various keto acids in tobacco seeds were identified from their 2,4-DNPH derivatives	Glock and Jensen (1312)
Levels of mono- and dicarbonyl components of cigarette MSS were estimated by spectrophotometry of their 2,4-DNPH derivatives	Harrow et al. (1540)
The levels of low-molecular-weight aldehydes and ketones in cigarette MSS were estimated from their 2,4-DNPH derivatives	McRae and Mold (2525) Mold and McRae (2591)
After removal of other oxidizable material, the glycerol content of tobacco could be estimated by oxidation of the glycerol and conversion of its oxidation product to its 2,4-DNPH derivative	Martin et al. (2581)
Examination of 2,4-DNPH derivatives from tobacco and smoke revealed presence of several keto acids	Glock (1310)
Carbonyl components of cigar MSS were characterized by IR, UV, x-ray diffraction, and paper chromatography of their 2,4-DNPH derivatives	Schepartz and Ogg (3438)
Examination of the 2,4-DNPH derivatives of tobacco smoke carbonyls revealed the presence of several dicarbonyl compounds	Halter et al. (1491)
Identification of dicarbonyl components of tobacco smoke via their 2,4-DNPH derivatives	Martin (2469)
To aid in identification of aldehydes and ketones in tobacco smoke and in cellulose smoke, over 90 2,4-DNPH derivatives were prepared to serve as melting point and spectral standards	Fredrickson et al. (1238)
Carbonyl components in cigar MSS identified after 2,4-DNPH derivative formation, followed by exchange reaction of 2,4-DNPH derivatives with α-ketoglutaric acid	Schepartz and McDowell (3436)
α-Ketoglutaric acid exchange procedure applied to identification of low-molecular-weight carbonyl components of tobacco	Stephens et al. (3817)
2,4-DNPH derivatives of low-molecular-weight carbonyl components of tobacco smoke were separated by TLC	Lindsey et al. (2369)
2,4-DNPH derivatives previously prepared (1238) were used to characterize carbonyl components in cigarette smoke	Frederickson et al. (1239)
Instead of α-ketoglutaric acid, oxalic acid and *p*-dimethylaminobenzaldehyde were used in exchange release of low-molecular-weight smoke carbonyl components from their 2,4-DNPH derivatives	Jones and Monroe (1978a)
2,4-DNPH derivatives of cigarette smoke carbonyls separated by gas chromatography	Donzel (1049)
Formaldehyde level of cigarette MSS estimated by HPLC of its 2,4-DNPH derivative	Hodge and Mansfield (1670) Mansfield et al. (2456)
The levels of C_1 through C_4 aldehydes and ketones in cigarette MSS were estimated by HPLC of their 2,4-DNPH derivatives	Canon and Frank (591)
2,4-DNPH derivatives of acrolein (propenal) and acetone from tobacco smoke were separated by HPLC	Manning et al. (2452)
The level of 5-hydroxymethyl-2-furaldehyde in tobacco and tobacco smoke was estimated via its 2,4-DNPH derivative	Perini and Bell (2930)
Volatile, low-molecular-weight carbonyl components of the headspace from tobacco and from MSS were quantitated through their 2,4-DNPH derivatives	Brunnemann et al. (500)
Development of method to determine formaldehyde in cigarette SSS; method applicable to other low-molecular-weight carbonyl components of SSS	Bell et al. (243)
Low-molecular-weight carbonyl compounds in ETS were collected as their 2,4-DNPH derivatives	DeLuca (929)
3-Methylbenzothiazolone hydrazone hydrochloride	
Aliphatic aldehydes in MSS were estimated by derivative formation, followed by colorimetry	Weaving (4155)
Aliphatic aldehydes in MSS were estimated by derivative formation, followed by colorimetry. Analysis refined to permit estimation of acrolein (propenal)	Davis and Sneade (915)
Aldehyde and ketone derivatization	
Review of compounds used to derivatize aldehydes and ketones in tobacco smoke	Green and Rodgman (1373)

TABLE 3.3
Analysis of Cigarette MSS by Gas Chromatography

Cigarette Sample[a]	Puffs/cig, avge	Acetaldehyde, µg/cig	Acetone, µg/cig	Acrolein, µg/cig
Flue-cured, nonfiltered	9.3	856	372	83
Burley, nonfiltered	7.3	847	533	57
Oriental, nonfiltered	11.0	726	385	54
Tobacco blend, nonfiltered	8.0	832	440	75
Tobacco blend, carbon filtered	8.0	208	42	11

[a] 50 of 65 mm tobacco rod smoked during analysis.



Note: The properties of the cigarette studied were as follows: 85-mm filtered cigarette; 68-mm, tobacco rod; 17-mm triacetin-plasticized cellulose acetate filter tip; cased commercial American blend.

[a] It is now estimated that over 5000 components have been identified in MSS from tobacco cigarettes. Some components such as water, the simple phenols, hydrogen cyanide,and the volatile N-nitrosamines are found in both the vapor and particulate phases of cigarette MSS. Hence the total of the number in the two phases appears to exceed the number in the whole.

[b] Value in brackets represents percent of Total Mainstream Smokweight, 500 mg.

[c] Value in parentheses represents percent of WTPM, 22.5 mg.

[d] Much of this water is contributed by the air drawn through the cigarette during puffing (35-mL puff, 1-s duration, 1 puff/min, total puffs = 10) in a laboratory whose atmosphere is controlled to the specifications proposed by the FTC; namely, temperature = 25°C, relative humidity (RH) = 60%.

[e] This class of compounds includes added humectants (glycerol, propylene glycol) transferred from the tobacco rod to the MSS. The transferred humectants constitute about 10%–12% of the FTC "Tar."

[f] Value in brackets represents percent of FTC "tar" weight, 17.6 mg.

[g] Value in brackets represents percent of "other components" weight, 7.5 mg.

[h] There have been various estimates of the number of unidentified components present in extremely small amounts in the FTC "tar." Several investigators have estimated the number of unidentified components to range from 5 to 20 times the number of identified components, i.e., from about 20,000 to 100,000.

FIGURE 3.1 Approximate composition of cigarette MSS. *Note*: The properties of the cigarette studied were as follows: 85-mm filtered cigarette; 68-mm, tobacco rod; 17-mm triacetin-plasticized cellulose acetate filter tip; cased commercial American blend. [a]It is now estimated that over 5000 components have been identified in MSS from tobacco cigarettes. Some components such as water, the simple phenols, hydrogen cyanide, and the volatile *N*-nitrosamines are found in both the vapor and particulate phases of cigarette MSS. Hence the total of the number in the two phases appears to exceed the number in the whole; [b]Value in brackets represents percent of Total Mainstream Smoke weight, 500 mg; [c]Value in parentheses represents percent of WTPM, 22.5 mg; [d]Much of this water is contributed by the air drawn through the cigarette during puffing (35-mL puff, 1-s duration, 1 puff/min, total puffs = 10) in a laboratory whose atmosphere is controlled to the specifications proposed by the FTC; namely, temperature = 25°C, relative humidity (RH) = 60%; [e]This class of compounds includes added humectants (glycerol, propylene glycol) transferred from the tobacco rod to the MSS. The transferred humectants constitute about 10%–12% of the FTC "*Tar*"; [f]Value in brackets represents percent of FTC "tar" weight, 17.6 mg; [g]Value in brackets represents percent of "Other Components" weight, 7.5 mg; [h]There have been various estimates of the number of unidentified components present in extremely small amounts in the FTC "tar." Several investigators have estimated the number of unidentified components to range from 5 to 20 times the number of identified components, i.e., from about 20,000 to 100,000.

Because of the extreme differences between the levels of various components in cigarette smoke, levels that vary from mg/cig for nitrogen, carbon dioxide, and carbon monoxide to pg/cig for several *N*-heterocyclic amines (Trp-P-1 and Trp-P-2), a logarithmic plot of the levels of specific MSS components was found to be a convenient way to compare their deliveries. In Figure 3.2, a truncated form of the original logarithmic plot presented by Green and Rodgman (1373), are shown the cigarette MSS yields of several of the most plentiful vapor-phase aldehydes and acetone.

Table 3.4, modified and updated from similar tables presented by Chortyk and Schlotzhauer (722) and by Baker (171a), summarizes the major precursor relationships proposed and/or demonstrated to date between tobacco leaf components and tobacco smoke components. These proposals are based in part on the results of a great variety of pyrolysis studies. In some cases, the validation of the proposals is based on the results obtained by addition of leaf components to tobacco and assessing the effect on the levels of specific MSS components when the "spiked" tobacco

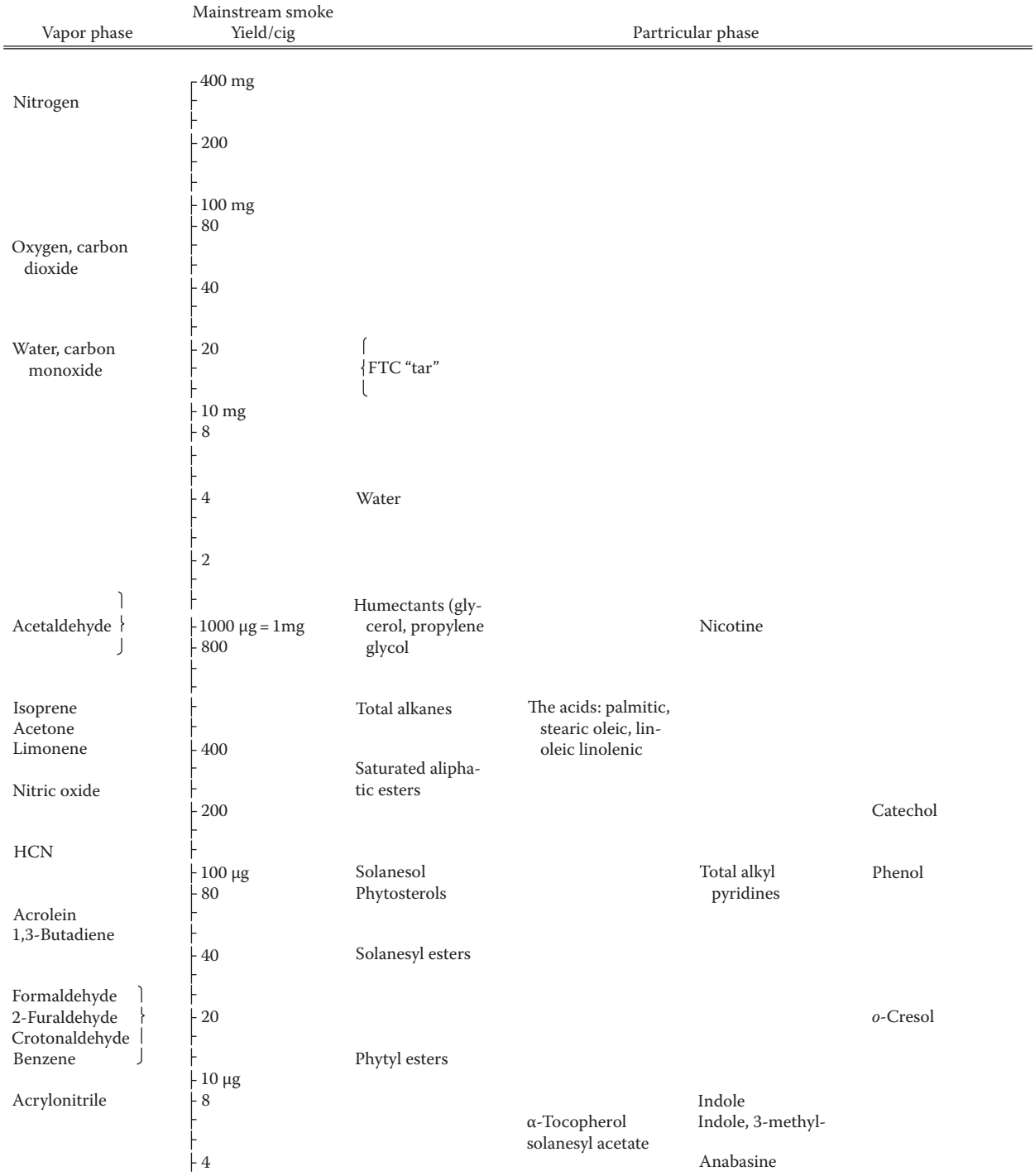


FIGURE 3.2 Cigarette MSS components: logarithmic plot.

TABLE 3.4
Precursors in Tobacco of Aldehydes and Ketones in Tobacco

Aldehydes and Ketones	Precursors	References
Formaldehyde, acetaldehyde, 2-propenal (acrolein), acetone, α,β-dicarbonyls, furaldehydes	Sugars	Gager et al. (1264, 1265) Higman et al. (1647) Houminer and Patai (1835) Johnson et al. (1960)
	Polysaccharides (cellulose, starch, and/or pectin)	Fredrickson (1228) Fredrickson et al. (1238) Newell and Best (2764) Zamorani et al. (4398c)
	Lignin	Martin et al. (2468a) Scheijen and Boon (3428)
	Pectins	Newell and Best (2764) Scheijen et al. (3429)
C_1–C_5 Aldehydes C_3–C_4 Ketones 2-Furancarboxaldehyde	Pectin	Squire and Waymack (3779a)
Acetaldehyde Propanal Propanal, 2-methyl- (isobutyraldehyde) 2-Propenal 2-Butenal (crotonaldehyde) 2-Furancarboxaldehyde 2-Furancarboxaldehyde, 5-methyl- 2-Butanone 3-Buten-2-one	Cellulose	Kato et al. (2046) Sakuma et al. (3401, 3402, 3404, 3045) Wakeham and Silberman (4104) Yamazaki and Saito (4369)
	Triglycerides	Kitamura (2111a)
Formaldehyde Acetaldehyde Acetone 2-Propenal	Glycerol	Doihara et al. (1023, 1024)
2-Propenal	Glycerol	Harbin and Laurene (1497) Kröller (2192, 2196) Kobashi et al. (2144) Wynder and Hoffmann (4337)
2-Propenal	Polysaccharides Lignin	Burton (535) Fagerson (1170a) Kaburaki et al. (2003) Kato (2042) Kato et al. (2043, 2046)
Aromatic aldehydes: Benzaldehyde, 3,4-dihydroxy- (protocatechualdehyde), Benzaldehyde, 4-hydroxy- Benzaldehyde, 4-hydroxy-3-methoxy- (vanillin), Benzaldehyde, 3,5-dimethoxy-4-hydroxy- (syringaldehyde)	Lignin	Kato et al. (2043) Martin et al. (2468a) Yang and Wender (4378)
	Direct transfer from tobacco; however, lignin is the most likely precursor of many aromatic aldehydes as well as many aromatic acids in tobacco	Wender and Yang (4163) Yang and Wender (4378, 4379)

is actually smoked in a cigarette and its MSS composition is compared to that of the MSS from the control tobacco cigarette.

In their quantitation (via their 4-nitrophenylhydrazone derivatives) of several aldehydes and ketones in the MSS from cigarettes made from flue-cured laminae and from flue-cured midribs, Sakuma et al. (3396) reported no significant differences between the MSS yields of the compounds listed in Table 3.5. However, many were much reduced when the cigarette was tipped with a charcoal filter.

TABLE 3.5
Aldehydes and Ketones in MSS from All-Lamina and All-Midrib Cigarettes

	In MSS from Flue-Cured Tobacco, µg/cig	
Carbonyl Compound	**Lamina**	**Midrib**
Formaldehyde	5	10
Acetaldehyde	685	779
Propanal	97	81
Propanal, 2-methyl-	103	57
Propenal (acrolein)	184	156
Butanal	36	21
2-Propanone (acetone)	217	220
2-Butanone	159	186

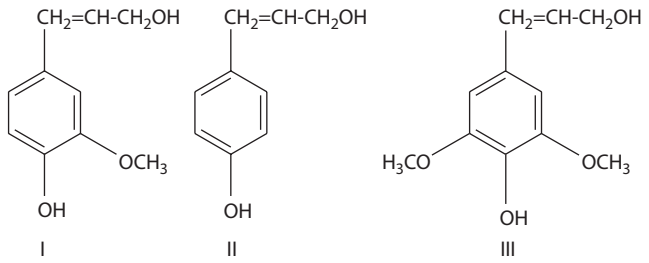


FIGURE 3.3 Phenolic alcohol components of lignin.

From their study of the pyrogenesis of acrolein (propenal) from glycerol, Doihara et al. (1964) and others deduced that a tobacco smoking product that contains glycerol as an humectant has an enhanced potential for the formation and release of acrolein (propenal) during smoking [see Wynder and Hoffmann (4337)].

In their study of the levels of acrolein, acetaldehyde, acetone, hydrogen cyanide, nitrogen oxides, nicotine, and total solids in pipe tobacco MSS, Harbin and Laurene (1497) reported that the acrolein delivery increased as the glycerol level was increased by addition but the acrolein delivery eventually leveled off when the glycerol addition exceeded 6%.

From an examination of the structure of lignin [cf. Ball (176a)], it is obvious why its pyrolysis products include a variety of phenolic aldehydes and acids, many of which have been identified in cigarette MSS. Lignin is composed of coniferyl alcohol {I}, *p*-coumaryl alcohol {II}, and sinapyl alcohol {III} in a variety of ratios that are dependent on the plant species (Figure 3.3).

3.1 ASSERTION OF ALDEHYDES AND KETONES AS CILIASTATIC TOBACCO SMOKE COMPONENTS

The reports by Wynder et al. (4306a, 4306c) in the early 1950s that cigarette smoke tar or CSC was tumorigenic to mouse skin prompted an intense search for the responsible component(s). Initially, the PAHs were selected for investigation because of the wealth of chemical and biological data generated on a great number of them following the synthesis of DB[*a,h*]A in 1929 (760, 1184), the isolation and identification of B[*a*]P from coal tar in 1932 (796a, 797), and the demonstration of the potent tumorigenicity of both of them to mouse skin by the Kennaway group (194, 796a, 797, 2078). Almost immediately after the report by Wynder et al. (4306a) of the mouse-skin-painting results with tobacco tar, the PAHs were proposed by some investigators to be the major tumor initiators in CSC. Because of its level in CSC and its potency in mouse-skin tumorigenesis, B[*a*]P was defined as the most significant of the PAHs in tobacco smoke.

However, it was soon recognized that neither the B[*a*]P content nor its tumorigenicity could explain the biological response observed in the mouse-skin-painting bioassay. Similarly, neither the total content of the PAHs tumorigenic to mouse skin nor their summed tumorigenicities could explain the observed biological response. In fact, it was pointed out many times over the next several decades that the levels of B[*a*]P and other tumorigenic PAHs in tobacco smoke condensate accounted for less than 3% of the observed tumorigenicity [Wynder and Wright (4353, 4354), Wynder and Hoffmann (1959b, 1959c, 1961a, 1963, 1964, 1967, 1968A), Druckrey (1056), Roe (3310, 3311), USPHS (3999, 4005, 4009, 4010), Lazar et al. (2320), Stedman (3767), Selikoff et al. (3584a), Coultson (830)].

As early as the mid-1950s, Wynder and Wright (4353) noted that the concentration of B[*a*]P in CSC was insufficient to account for its observed carcinogenicity to mouse epidermis: "The concentration in which benzo[a]pyrene seems to be in cigarette tar is insufficient to account for the observed carcinogenic activity to mouse epidermis."

At the 1957 Blatnik Committee hearings, Wynder reported Wright's opinion [Wright (4282a)] on the subject as well as his own [Wynder (4296)]. Wynder noted that much attention had been directed at the PAH B[*a*]P. So much in fact that, as Wynder stated, B[*a*]P had become an issue in itself because it was one of the known (tumorigenic) substances and everyone tried to blame everything on it alone. During his testimony, he also noted that his Sloan Kettering group had repeatedly stated that the amount of B[*a*]P in tobacco tar was insufficient to explain the animal results published by his group. He added that cigarette tar contained numerous other B[*a*]P-related compounds much more active than B[*a*]P and they most likely accounted for the majority of the activity, and it was more or less academic whether it was B[*a*]P or a dibenzopyrene or a dibenzanthracene or a substituted B[*a*]P because they were all formed in the same manner during the tobacco smoking process. That same year, Wynder and Wright (4354) wrote that, to that date, no carcinogens had been identified in large enough quantities in tobacco tar or its fractions to account for the observed activity in skin-painting studies:

> We have demonstrated experimentally…that 0.0001 per cent or even 0.0005 per cent benzopyrene in acetone will not produce any tumors in the present experimental mouse or rabbit groups. Thus, there is conclusive proof that the animal results cannot be solely due to the benzopyrene content of tobacco [sic].

> The benzpyrene content of the total tar as well as the active fractions is far too low to account alone for the positive results [in laboratory animal]. So far, no carcinogens have been identified in large enough quantity in tobacco tar or its fractions to account for the observed activity.

These Wynder–Wright 1957 results led to an intensive but unsuccessful 18-month search for a "supercarcinogenic" PAH. The absence of such a PAH was subsequently confirmed by the USDA group at Athens, GA, by their identification of over 500 PAHs in the PAH fraction from cigarette MSS, an identification procedure that completely accounted for the fraction in the cigarette smoke studied (3732, 3736, 3756–3759).

In 1959, unable to explain the bioassay (mouse-skin-painting) results with CSC on the basis of either its B[*a*]P content (less than 2% explainable) or its total PAH content (less than 3% explainable), Wynder and Hoffmann (4307) at the 1959 American Association for Cancer Research (AACR) meeting added the concept of promotion by low-molecular-weight phenols to the concept of tumor initiation by PAHs in an attempt (unsuccessful) to explain the bioassay results. They reiterated their view the following year at the *1960 AACR conference* (4309):

> The phenol fraction could be established as an important promoting portion of the tobacco smoke condensate.

A similar comment that the amount of tumorigenic PAHs found in CSC could not by themselves account for the total biological activity observed was included in a more detailed publication (4307) of their AACR presentation. They also stated (4308) that the higher PAHs played an important role in the carcinogenicity of CSC, but when the various known concentrations of the carcinogenic PAHs as estimated in CSC were summed, it was obvious that they could not account for the established carcinogenicity of the CSC nor of its isolated PAH fraction:

> Several carcinogenic higher aromatic polycyclic hydrocarbons [are] present in tobacco smoke condensate. They include benzo[*a*]pyrene…, benzo[*e*]pyrene…, chrysene…, benz[*a*] anthracene…, dibenz[*a,h*]anthracene…, and dibenzo[*a,i*] pyrene… From the amount in which these materials have been found in tobacco smoke condensate it was evident that these, by themselves, could not account for the total biological activity observed.

In 1960, Van Duuren et al. (4027) reported the identification of several aza-arenes (dibenz[*a,h*]acridine, dibenz[*a,j*] acridine, dibenzo[*c,g*]carbazole) not only structurally similar to some of the known tumorigenic PAHs in CSC but also reported under certain conditions to be tumorigenic to mouse skin. Adding this class of tumorigenic cigarette smoke components to the assessment of the tumorigenicity of CSC failed to account for more than a few percent of the observed response.

However, it should be noted that Candeli et al. (587) could not confirm the findings of Van Duuren et al. on the presence of these three aza-arenes in cigarette MSS. During the next three decades, other research groups in Germany, Japan, and the United States were also unable to confirm the presence in cigarette MSS of dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and dibenzo[*c,g*]carbazole [3260, 3414, Table 12-7 in (172)].

Wynder and Hoffmann (4311) wrote that the PAHs in CSC accounted for not more than 3% of the total biological activity observed in mouse-skin bioassays:

> The polynuclear aromatic hydrocarbons are mainly formed during the combustion of tobacco. The tobacco of our standard cigarettes contains only very minute quantities of benzo(a)pyrene (0.02 ppm). A bioassay indicates that these polycyclic hydrocarbons of the condensate by themselves, however, can account for not more than 3 per cent of the total biological activity.

Wynder and Hoffmann (4312) also wrote that the established carcinogenicity of CSC to mouse epidermis could to a great extent be accounted for on the basis of initiating carcinogens, largely PAHs, and promoting substances, a major group of which was the phenols. This statement was not true in 1961, nor is it true now.

In their lengthy 1964 review of tobacco carcinogenesis, Wynder and Hoffmann (4319) stated that no one could deny that tobacco products were tumorigenic even though no single component in tobacco smoke could by itself or jointly with other components account for the observed tumorigenic activity of such tobacco products to the skin of laboratory animals:

> It is furthermore true that none of the agents is carcinogenic in the concentrations in which they are present in tobacco products.

Wynder and Hoffmann (4332) expressed similar views on the tumorigenicity of tobacco smoke components in their 1967 book, but they continued to maintain that the PAHs in cigarette smoke were important as tumor initiators:

> While BaP and other carcinogenic PAH can by themselves account for only a small portion of the total tumorigenic activity of cigarette smoke condensate, probably less than 2%, they are, nevertheless, of obligatory importance as tumor initiators.

The next year, Wynder and Hoffmann (4342) wrote:

> Carcinogenic polynuclear hydrocarbons in the concentrations present in tobacco "tar" clearly do not, by themselves, account for the observed carcinogenicity.

On several occasions, the U.S. Surgeon General in his periodic reports on smoking and health discussed the relationship between the levels of PAHs in cigarette smoke, their tumorigenic potency to mouse skin, and the observed biological response with CSC in mouse-skin-painting bioassays:

> The results of a number of such assays [mouse skin-painting] present a puzzling anomaly: the total tar from cigarettes has about 40 times the carcinogenic potency of the benzo(a)pyrene present in the tar. The other carcinogens

known to be present in tobacco smoke are, with the exception of dibenzo(a,i)pyrene, much less potent than benzo(a) pyrene and they are present in smaller amounts. Apparently, therefore, the whole is greater than the sum of the known parts. (3999)

Unable to explain the observed tumorigenicity to mouse skin of CSC in terms of its content of known tumorigenic PAHs and/or tumorigenic aza-arenes, Wynder and Hoffmann (4307, 4309–4313) added the concept of promotion to their arsenal with particular emphasis on this property of the nontumorigenic PAH and low-molecular-weight phenolic components in the CSC. Inclusion of the concepts of initiation, promotion, and cocarcinogenesis by cigarette smoke components could only account for a small percentage of the number of tumor-bearing animals in the mouse skin-painting studies. This inability to explain the results observed in laboratory animals was a major creditability problem in the attempt to relate the laboratory animal data with CSC to human smoking experience.

In an attempt to offset their failure to explain the mouse skin-painting bioassay results with CSC on the basis of its content of tumorigenic PAHs and aza-arenes, promoting and/or cocarcinogenic phenols, and promoting and/or cocarcinogenic nontumorigenic PAHs, Wynder and Hoffmann (4314, 4315) added the concept of ciliastasis in an attempt (unsuccessful) to explain cigarette smoke tumorigenicity in smokers' lungs. It was proposed that impairment of ciliary action would result in prolonged exposure of the ciliated tissue to the inhaled particle and the tumorigens contained therein. Obviously, ciliastasis is not relevant to the initiation of tumors in the mouse skin-painting bioassay with CSC.

Cilia are small, hairlike entities covering the surface of certain portions of the upper respiratory tract,* and these beat rhythmically and synchronously to move a thin layer of mucus upward toward the mouth where it is swallowed or expectorated. Inhaled particle may be entrained in this mucus and thus removed from the respiratory tract by its cilia-induced movement. Impairment of ciliary activity results in a failure to clear particles from the respiratory tract. This impairment of ciliary activity, known as ciliastasis, may be produced by a variety of inhaled materials. [A detailed definition of cilia and description of their action appear in Rivera (3184a).] Many of the early laboratory investigations on ciliastasis produced by cigarette MSS and/or its components were studies involving ciliated tissue from clams, mussels, or extirpated lung tissue from rabbits, etc.

Usually, Hilding (1652a) is credited with initiating the interest in respiratory tract ciliastasis produced by cigarette MSS. In 1956 and 1957, he reported the results of his studies of the effect of cigarette smoke on ciliated tissue in the lungs of cows. However, numerous reports on studies of the ciliastatic action of cigarette MSS had appeared in the literature during the preceding two decades.

* Other anatomical sites in the mammalian body possess ciliated tissue, but these have no relevance to the discussion of tobacco smoke inhalation.

In the late 1930s, Mendenhall and Shreeve (2530a) and Proetz (2991a) described their studies on ciliastasis. Mendenhall and Shreeve (2530a) reported that nicotine in cigarette MSS did not appear to be a contributor to ciliastasis in extirpated bovine tracheal tissue exposed to cigarette MSS, but the difference they observed between the smokes from nonmentholated *vs.* mentholated cigarettes indicated that menthol had a ciliastatic effect. However, in 1952, Rakieten et al. (3072b) reported no difference between the MSSs from nonmentholated *vs.* mentholated cigarettes in the ciliastasis induced in ciliated tissue from humans, rabbits, or rats. Their findings conflicted with those reported by Mendenhall and Shreeve. Rakieten et al. (3072b) also reported that nicotine contributed only slightly to the observed ciliastatic effect of cigarette MSS.

Representative studies on ciliastasis produced by cigarette MSS include those of Dalhamn (891a), Falk et al. (1175), Kotin and Falk (2179), and Ballenger (178). In all these studies, cigarette MSS was reported to be ciliastatic in in vitro systems. Falk et al. reported that nicotine was involved in the ciliastasis induced by cigarette smoke. However, Guillerm et al. (1451a) reported that neither nicotine nor hydrogen cyanide was a contributor to the ciliastasis produced by cigarette MSS when tested individually at the concentrations determined in cigarette MSS. They reported that all the aldehydes and ketones tested at their concentrations in cigarette MSS were ciliastatic and acetaldehyde and acrolein appeared to act synergistically in the ciliastatic action.

In 1962, Wynder and Hoffmann (4314) combined the ciliastasis concept with the three tumorigenesis factors mentioned earlier: it was proposed that impairment of ciliary action would result in prolonged exposure of the ciliated tissue to the inhaled particle and the tumorigens contained therein. For the CSC, they reported low-molecular-weight phenols to be in vitro ciliastats and that cellulose acetate filters plasticized with triacetin substantially reduced the ciliastatic effect of phenols. The same year, Davis and George (911a) reported the effectiveness of triacetin-plasticized cellulose acetate in reducing the phenols level in cigarette MSS with the corresponding reduction of the observed ciliastasis.

Because of the assertion that low-molecular-weight phenols were promoters for tumorigenic PAHs and thus played a role in CSC tumorigenesis and possibly in cancer causation in smokers, research was under way to find methods to reduce their levels in cigarette MSS, e.g., the studies at Lorillard on selective phenols filtration by Spears (2399, 3765), at R.J. Reynolds Tobacco Co. (RJRT) by Laurene (2295) and Laurene et al. (2306), by Hoffmann and Wynder (1791), Mokhnachev et al. (2579), and Morie (2628, 2629, 2636); on phenol precursors by Rodgman et al. (3251, 3277, 3305, 3306); and on the precursors in tobacco of the low-molecular-weight phenols in tobacco smoke by Wynder and Hoffmann (4317). Obviously, the results of these studies were equally applicable to reducing levels of phenols because of their alleged ciliastatic action in the respiratory tract.

Wynder and Hoffmann (4317) and Wynder et al. (4350) reported the results of their study of the ciliastatic components

in CSC: Nicotine was not a factor in the ciliastasis of CSC; the phenolic fraction and the acidic fraction were significant ciliastats.

The same year, Kensler and Battista (2083, 2084) reported their findings on the ciliastatic activity of vapor-phase components of cigarette MSS and its reduction by activated carbon filters. Falk et al. (1173a, 1175) also described the effect of many of the same smoke components on mucus flow. Hydrogen cyanide, acrolein, formaldehyde, acetaldehyde, nitrogen oxides, ammonia, and phenol were considered important vapor-phase ciliastats.*

The Kensler–Battista research on the effectiveness of carbon in reducing vapor-phase ciliastats in cigarette MSS was reported within a few months of the publication of the *Reader's Digest* article on the effectiveness of carbon-containing filters in reducing ciliastats in cigarette MSS and the appearance in the marketplace of Liggett and Myers (L&M) Lark cigarette. Its filter included a chamber filled with a specially treated carbon based on a patent issued to Keith of L&M R&D. The Kensler–Battista study was performed at A.D. Little and was contracted by L&M (2083, 2084).

Because of these reports on vapor-phase components of cigarette MSS, emphasis at RJRT R&D was shifted from attempts to reduce the levels of the phenols reported to be promoters or cocarcinogens to attempts to reduce the levels of vapor-phase components reported to be ciliastatic. These vapor-phase components included the simpler, volatile phenols which equilibrate between MSS vapor phase and particulate phase. From 1963 to 1972, a great variety of filter-tip additives were examined with respect to their ability to remove specific MSS components reported to be ciliastatic in in vitro experiments.

After the Kensler–Battista publications, numerous publications appeared on the reduction of the delivery of ciliastatic components by filter tips (893a), on the ciliastatic action of nicotine (178), and on the ciliastatic activity of phenol (295).

In a preliminary study, Rodgman et al. (3306) examined the removal of water-soluble vapor-phase ciliastatic components from cigarette MSS by saliva and mucous secretions in the upper respiratory tract. They reported that the levels of representative ciliastats such as the aldehydes and ketones were substantially reduced in the oral cavity, resulting in a diminution of the levels reaching the ciliated tissue in the lower respiratory tract. Rodgman et al. also emphasized that such oral cavity absorption of water-soluble ciliastats did not substantially affect the levels of ciliastatic components in the particulate phase. External impetus for this investigation was provided by comments in the Advisory Committee's 1964 Report to the U.S. Surgeon General (3999) on the possible oral cavity removal of water-soluble ciliastats, by comments by Dalhamn and his colleagues (893a, 894b) on the ciliastatic activity of filtered and nonfiltered cigarette MSS, and by Wynder (4301).

In 1965, Wynder et al. (4304) wrote:

> The principle volatile ciliatoxic components appear to be water-soluble… Important considerations are the temperature of the respiratory tract…and the nature of the overlying mucous coat, the layer that all ciliastatic components penetrate to act upon cilia…

In their study, Rodgman et al. (3306) showed that passage of cigarette MSS over moistened filter paper strips substantially reduced the levels of the vapor-phase ciliastats but did not produce much effect on the "tar" delivery. Rodgman and Cook (3289) examined a variety of carbon-containing filter tips and found that the delivery of several vapor-phase ciliastats (the aldehydes and ketones) could be reduced substantially by some of them. In some instances, the ciliastatic components adsorbed on the carbon were eluted from the carbon as the fire cone approached the filter tip and the filter-tip temperature was increased. As a result, the levels of these components were inordinately increased in the last few puffs from the cigarette. RJRT was not the only U.S. tobacco company interested in the removal of water-soluble ciliastats from cigarette MSS.†

Industrial Bio-Test Laboratories (3A12), under contract to RJRT, conducted a series of studies on in vitro ciliastasis of cigarette MSS from 1964 through 1967. Major findings included the following: (1) The theory of reduction of the levels of ciliastats in the smoke stream by moist surfaces was confirmed. (2) The ciliastatic activity of the MSS particulate phase was essentially unchanged by passage over moist surfaces. (3) The ciliastatic activity of cigarette MSS was substantially reduced by passage of the MSS through a carbon-containing filter tip.

In 1966, Dalhamn (891a) and Dalhamn and Rylander (893c) reported on the effect of filtration on the delivery of ciliastatic compounds in MSS. They reported that in vitro ciliastats were present in both the vapor and particulate phases of MSS.

In their 1964 lengthy review and 1967 book, Wynder and Hoffmann (4319, 4332) commented on ciliastasis induced by cigarette MSS as follows:

> All studies reported to date have shown that cigarette smoke affects the metachronic activity of cilia, a motion that is necessary to propel the viscid mucoid mass. During inhalation, in the absence of effectively beating cilia, mucus flow slows down and perhaps stops. At that time, components in cigarette smoke may act upon the underlying cells, as can the entrapped particles.

* Because of its vapor pressure properties, phenol is present in both the particulate phase and the vapor phase of cigarette MSS aerosol. Thus, it is amenable to removal from the vapor phase by selective filtration and to reduction of its level in the particulate phase by all the technologies whereby MSS particulate phase or "tar" delivery is reduced, e.g., filtration efficiency, air dilution (increased paper porosity, filter-tip ventilation), inclusion of expanded tobacco in the blend.

† In 1965, American Tobacco marketed the Waterford cigarette whose filter contained encapsulated water. Prior to smoking the cigarette, the smoker would gently squeeze the filter tip, rupture the capsules to release the encapsulated water which would spread throughout the interstices between the filter-tip fibers. Water-soluble MSS vapor-phase components would be "scrubbed" from the smoke stream. The Waterford had a very short life in the market place.

In their mid-1960s publications, Wynder and Hoffmann commented several times on the fact that most of the known ciliastatic components of MSS demonstrated to be ciliastatic in various in vitro systems were water soluble and this property would markedly influence their fate and behavior during and after inhalation. Wynder and Hoffmann (4330) noted:

> As far as human smoking habits are concerned, it remains also to be estimated to which extent volatile smoke components reach the bronchial tree. Preliminary studies indicate that a significant proportion of the gaseous components is being retained within the oral cavity.

Later, Wynder and Hoffmann [see p. 542 in (4332)] wrote:

> Water-soluble volatile components, which are primarily responsible for the results of the acute in vitro short-term cilia toxicity tests, are, to a large extent, removed when cigarette smoke contacts the saliva in the mouth and the abundant secretions of the trachea and main bronchi.

They added [see p. 646 in (4332)]:

> In man's manner of smoking, however, volatile components are retained to a significant degree in the oral cavity and may, therefore, be far less important than when tested experimentally.

These words, perhaps prophetic, were shown to be true by Dalhamn et al. (892) who reported in 1968 that as much as 60% of the water-soluble (and ciliastatic) components of cigarette MSS were absorbed in the oral cavity of the human smoker, whereas the absorption of water-insoluble (and nonciliastatic) components such as isoprene was low (about 20%). They also reported that about 16% of the MSS particulate matter was retain in the mouth. Mouth absorption of acetaldehyde and acetone averaged about 57%. Earlier, Rodgman et al. (3306) had conducted a study similar to but much less elaborate than that of Dalhamn et al. (892). Rodgman et al. studied the mouth absorption of components of the MSS from five different brands: The total absorption of all vapor-phase aldehydes and ketones averaged 53%; the absorption of isoprene averaged less than 10%.

The more than a dozen cigarette brands tipped with carbon-containing filter tips were already losing market share by the time Dalhamn et al. reported the results of their study of the mouth absorption of water-soluble vapor-phase components (892). Their scientific communication, plus the consumer-unacceptable "carbon-filter" off-taste, not only produced a further reduction of sales but also diminished interest, both within and outside of the tobacco industry, in vapor-phase ciliastats as participants in respiratory problems attributed to cigarette MSS.

From 1968 through 1972, study continued not only at RJRT R&D but also throughout the tobacco industry on ways to reduce the levels of vapor-phase components, many of which were reported to be ciliastatic in in vitro systems. The major effort was aimed at reducing the level of hydrogen cyanide (a potent in vitro ciliastat) because of its level in cigarette MSS (about 200–400 μg from a cigarette delivering 15–25 mg of FTC "tar"), its toxicity (other than ciliastasis) when examined alone, and the fact that consumers would be more familiar with the toxic properties of hydrogen cyanide (also known as hydrocyanic acid or "cyanide") than with the toxic properties of MSS components such as acrolein or phenol. Most of the effort during this period dealt with filter-tip additives other than carbon.

Thus, in the late 1960s, it was known that in vitro ciliastatic components in the vapor phase of MSS were not reaching the ciliated areas of the respiratory tract in the concentrations first considered to be a problem and the levels of the ciliastatic components in the MSS particulate phase could be controlled by the filtration methods used to control "tar" delivery. Another technology to control the *per cigarette* deliveries of both vapor-phase and/or particulate-phase MSS components (whether they be ciliastatic or not) was air dilution via filter-tip ventilation. At RJRT R&D, basic research on this cigarette design technology, subsequently classified as significant in the generation of a "safer" or "less hazardous" cigarette, was pursued into the mid-1970s (3116a, 3119a, 3120).

Dalhamn (891c) stated with regard to a "less hazardous" cigarette:

> If…one were to venture a reply to the question of what a less hazardous cigarette would be like, I cannot for the moment find a better one than that given by Rylander and myself [to the 1968 Consumer Subcommittee of the U.S. Senate Committee on Commerce]:
>
> Our belief, based upon the scientific knowledge available at present, is that the only way to guarantee a reduction in the harmful effects of inhaled smoke is to decrease the overall exposure. This can be done by reducing the number of cigarettes smoked or by using filter cigarettes, provided the reduction brought about by the filter will equal in all respects and for all potentially hazardous compounds the reduction in dose obtained if the number of cigarettes is reduced. Due to the limited amount of data and the difficulty of extrapolating from laboratory findings to man, we believe that a reduction of only selected components of cigarette smoke cannot be accompanied by a statement guaranteeing a reduction in the harmful effects of inhaled smoke.

The topic dealing with ciliastasis and MSS ciliastats (from testing in in vitro systems) is of particular interest with respect to the ETS situation because of the data showing:

1. The major ciliastatic components in tobacco smoke are water soluble. These include formaldehyde, acetaldehyde, crotonaldehyde, ethyl carbamate, and hydrazine:* All are water-soluble tobacco smoke

* Other water-soluble tobacco smoke components categorized as ciliastats on the basis of in vitro test results include ammonia, hydrogen cyanide, acrolein, acetone, nitrogen dioxide, low-molecular-weight phenols. The phenols are distributed between the particulate and vapor phases of tobacco smoke.

components that appear as tumorigens on the various published lists of tumorigens in tobacco smoke (1727, 1740, 1741, 1743, 1744).
2. Dose reduction (effectively, dilution) of MSS or some of its "ciliastatic" components or ciliastatic fractions eventually results in a dose or concentration level at which no ciliastasis is produced in the in vitro systems used.
3. A large proportion of the inhaled MSS components categorized as ciliastats (and in some instances as tumorigens) does not reach the ciliated areas of the respiratory tract because of their removal from the smoke stream during passage over the moist tissues of the mouth and trachea [cf. Rodgman et al. (3306), Dalhamn et al. (892)].
4. Ciliastatic compounds inhaled nasally are removed from the inhaled gas stream by "resorption."

This raises the question as to how much formaldehyde or acetaldehyde or crotonaldehyde in ETS, an already extremely dilute system, will reach the lung whether inhaled orally or nasally! Are the levels of these tobacco smoke components in ETS sufficient for these compounds to be included on the Hoffmann and Hecht list (1727) or the Occupational Safety and Health Administration (OSHA) list (2825) or the Hoffmann and Hoffmann lists (1740, 1741, 1743) or the Hoffmann et al. list (1744)?

3.2 CILIASTASIS STUDIES WITH CIGARETTE SMOKE CONDENSATE FRACTIONS

Wynder and Hoffmann (4314) and Wynder et al. (4350) in their study with mussels of the ciliastatic activity of aqueous extracts of various fractions of CSC demonstrated that reduction of the applied dose of each of the fractions tested eventually changed the ciliastasis from "immediate and complete" to "none." Their findings are summarized in Table 3.6.

Calculation of the ratio Dc/Do, where Dc is the dose producing "immediate and complete" ciliastasis and Do is the dose producing "zero" ciliastasis, gives values ranging from 6 to 24, i.e., a 24-fold dilution of every mainstream CSC fraction tested in this study resulted in or would result in a nonciliastatic situation.

The data in Table 3.6 originally presented at the annual AACR meeting by Wynder and Hoffmann (4314) were subsequently published, but in less detail, by Wynder et al. (4350).

3.3 CILIASTASIS STUDIES WITH INDIVIDUAL CIGARETTE MAINSTREAM SMOKE COMPONENTS

Examination of the in vitro ciliastasis produced by a variety of MSS components reveals that for all components studied, there is a level below which no ciliastasis is observed. Guillerm et al. (1451a) reported the results of their study on the effect of various MSS components in the in vitro system, ciliated rat trachea. Concentrations less than those shown in Table 3.7 produced no ciliastasis in ciliated rat trachea. All of the compounds listed in Table 3.7 are primarily vapor-phase components of MSS.

Wynder et al. (4350) in their study of the phenolic components of cigarette smoke also reported that reduction of the concentrations of solutions of the simple phenols (phenol, *o*-cresol, *m*-cresol, *p*-cresol, *o*-ethylphenol, 2,4-dimethylphenol) from 1.0% to 0.05% (a 20:1 dilution) reduced the ciliary activity of each solution in an in vitro system (ciliated mussel tissue) to zero.

At the highest concentration (1.0%), the phenol derivatives demonstrated greater ciliastatic effects than did phenol itself. At the lowest concentrations tested (0.05%), none of the phenols induced ciliastasis.

TABLE 3.6
In Vitro Ciliary Activity, Cigarette Smoke Fractions, and Dose Level

Smoke Fraction from Which Aqueous Extract Was Obtained	% of Smoke[a]	Immediate and Complete Ciliastasis at Dc[b]	Complete Ciliastasis in 10–40 min at D10	No Apparent Ciliastasis at Do	Dc/Do
Phenolic fraction	9.3 (16.0)[c]	0.03	0.015	0.002	15
Acidic fraction[d]	2.2 (11.0)	0.04	0.02	0.007	6
Neutral fraction	47.2 (0.9)	—	0.27	0.034	8[e]
"Insoluble" fraction	14.0 (20.0)	1.1	0.55	0.055	20
Basic fraction	8.7 (65.0)	1.95	0.98	0.08	24

[a] The unit for Dc, D10, and Do is g/100 mL.
[b] The values for each fraction as a percentage of total smoke condensate were previously described by Wynder and Hoffmann (4311, 4312).
[c] Number in parentheses is percentage of smoke fraction that is soluble in water.
[d] Phenol-free.
[e] Value for D10/Do.

TABLE 3.7
Lowest Concentrations in Ringer Solution Leading to Ciliastasis in Ciliated Rat Trachea

Compound	Concentration, µg/L
Propenal	90
Formaldehyde[a]	200
Acetaldehyde[a]	3,000
Propanal	3,500
Propanal, 2-methyl-	4,500
2-Furaldehyde	7,500
2-Butanone	80,000
2-Propanone	100,000

[a] On various lists of tobacco smoke tumorigens (1727, 1740, 2825).

3.4 NOSE INHALATION OF ENVIRONMENTAL TOBACCO SMOKE *VS*. MOUTH INHALATION OF MAINSTREAM SMOKE

On several occasions, Rodgman (3255, 3255a, 3257) discussed the effect of water solubility of tobacco smoke components reported to be ciliastatic in in vitro systems on the ultimate exposure of the smoker's lungs to MSS or the nonsmoker's lungs to ETS.

Early in the study of the effect of MSS components on ciliary activity in in vitro systems, it was realized that all of the MSS components (formaldehyde, acetaldehyde, acrolein, hydrogen cyanide, formic acid, acetic acid, etc.) that produced ciliastasis in the in vitro systems were water soluble. This observation led to proposals by Dalhamn and Sjoholm (894b), Dalhamn and Rylander (893a), Rodgman et al. (3306), Wynder (4301), USPHS (3999), Wynder et al. (4304, 4305), and Wynder and Hoffmann (4332, 4342) that this water solubility would result in removal of substantial amounts of the in vitro ciliastatic components from the MSS by their solution in the aqueous fluids coating the surfaces of the oral cavity and trachea during the time that the MSS was held in and/or traversed these portions of the respiratory tract. The levels of ciliastats reaching the ciliated areas in the smoker's lower respiratory tract would produce insignificant ciliastasis, if any at all. This "scrubbing" of ciliastatic components from the inspired MSS stream was demonstrated in smokers by Rodgman et al. (3306) and Dalhamn et al. (892, 893). Nasally inhaled components are removed in the nasal cavity by "resorption," a process similar to the "scrubbing" of water-soluble components from gas streams such as MSS vapor phase.

Dalhamn, in his 1961 study of ciliastatic activity demonstrated that sulfur dioxide was a powerful ciliastat in vitro at or below 100 ppm but did not produce ciliastasis in vivo at or below 100 ppm because much of the sulfur dioxide was removed in the nasal cavity (891a). Sulfur dioxide was subsequently identified as a minor tobacco smoke vapor-phase component (3882). Dalhamn (891a) found that in rabbits exposed to 300, 200, and 100 ppm of sulfur dioxide, the percentage showing cessation of ciliary activity within 45 min was 90, 60, and 0, respectively. Removal of inhaled components in the nasal cavity, termed "resorption," is similar to the "scrubbing" of water-soluble components from gas streams, e.g., MSS vapor phase. This nasal resorption is an important process not only from a ciliastasis–MSS component point of view but also from an ETS point of view since ETS, in contrast to MSS which is primarily inhaled via the mouth, is inhaled primarily through the nose. ETS vapor-phase components that would be removed through resorption in the nasal cavity include formaldehyde, acetaldehyde, crotonaldehyde, hydrazine, and possibly ethyl carbamate, five MSS components listed by Hoffmann and Hecht (1727) as "tumorigens" in MSS. Thus, very little, if any, of these water-soluble components, already highly diluted in ETS, would reach the lungs and the ciliated tissue to be involved in lung cancer causation attributed to ETS by some authors. As noted by Aviado (126a), data from inhalation studies in animals indicate it is unlikely that either formaldehyde or hydrazine contribute to pulmonary carcinogenesis.

In 1965, Dalhamn and Rylander (893b) commented on the possible differences in the effects produced by mouth inhalation *vs*. nose inhalation of tobacco smoke:

> The most important point is probably that the smoke is administered through the mouth. If smoke is administered through the nose quite different absorption conditions are present, and it is likely that the smoke which enters the lungs differs considerably from that inhaled through the mouth. This could also be one of the factors which explains why in animal experiments no tumor-producing effects have been found by tobacco smoke in inhalation studies where the smoke was administered through the nose.

In 1968, Dalhamn et al. published the results of their studies with humans on the mouth absorption (892) and lung retention (893) of various components of cigarette smoke. As noted earlier, the findings that a substantial percentage of the levels of MSS water-soluble components demonstrated to be ciliastatic in vitro is absorbed in the oral cavity lessened the interest in ciliastasis produced by MSS components. The data generated by Dalhamn et al. also served a second useful purpose in that they demonstrated (1) the remarkable difference, albeit with respect to only a few MSS smoke components, between the compositions of inhaled and exhaled MSS and (2) all of the few components measured in the inhaled MSS were found in the exhaled MSS, i.e., none was 100% retained in the lungs, etc., nor 100% absorbed in the oral cavity.

These data are summarized in Tables 3.8 and 3.9. It is obvious that mouth absorptions of such water-soluble ciliastats as acetaldehyde (60%) and acetone (56%) are substantial (Table 3.8); whereas, the mouth absorptions of the relatively water-insoluble components isoprene (20%), toluene (28%), and CO (3%) are much less.

The data in Table 3.9 are derived from those of Dalhamn et al. (892, 893). The change in the composition of the MSS delivered by the cigarette to the composition of the MSS exhaled by the smoker is readily seen from the ratios, e.g., acetaldehyde is inhaled by the smoker at a ratio of 31.3 µg/mg TPM but is

TABLE 3.8
Lung Retention and Mouth Absorption of Several Cigarette MSS Components

		Per Cigarette MSS					
		Inhalation into Lungs			Held in Mouth for 2 s		
Smoke Component	Delivery	Retention	%	Exhaled	Absorbed in Mouth[a]	%	Exhaled
Acetaldehyde, µg	940	930	99	10	560	60	380
Acetone, µg	570	490	86	80	320	56	250
Acetonitrile, µg	320	282	91	28	230	74	80
Isoprene, µg	560	554	99	6	110	20	450
Toluene, µg	250	232	93	18	70	28	180
CO, mg	30.0[b]	16.2	54	13.8	0.9	3	29.1
TPM, mg	30.0	28.8	96	1.2	4.8	16	25.2

[a] No inhalation.
[b] Per cigarette CO yield assumed to be the same as per cigarette TPM yield.

TABLE 3.9
Difference between Composition of Inhaled and Exhaled MSS and between Mouth-Held and Exhaled MSS

		Per Cigarette Ratios, µg/g TPM or µg/g TPM	
Smoke Component	Delivery Ratio	Inhalation into Lungs and Exhaled, Exhaled MSS Ratio	Held in Mouth for 2 s[a] and Exhaled, Exhaled MSS Ratio
Acetaldehyde, µg	31.3	8.3	15.1
Acetone, µg	19.0	66.7	9.9
Acetonitrile, µg	10.3	23.3	3.2
Isoprene, µg	18.7	5.0	17.9
Toluene, µg	8.3	15.0	3.2
CO, mg	1.0[b]	11.5	1.15
TPM, mg	1.0	1.0	1.0

[a] No inhalation.
[b] Per cigarette CO yield assumed to be the same as per cigarette TPM yield.

exhaled at a ratio of 8.3 µg/mg TPM; acetone is inhaled at a ratio of 19.0 µg/mg TPM but exhaled at a ratio of 66.7 µg/mg TPM. Similarly, the MSS composition is altered by holding the smoke in the mouth without inhalation. Since these exhaled smokes—whether originally inhaled, held in the mouth with no or minimal inhalation, or some blend of both (inhalation and mouth retention)—ultimately contribute to ETS, it is obvious that the contribution is not equivalent quantitatively to the MSS originally generated by the cigarette.

The data presented by Dalhamn et al. (892, 893) on lung retention of MSS components were similar to data reported earlier by Laskowski (2267) and to data on lung retention and mouth absorption of ciliastats by Rodgman et al. (3306). The various sets of data are summarized in Table 3.10. Each set of data indicates that exhaled MSS is substantially different quantitatively from the inhaled MSS.

If cigarette MSS is mouth inhaled and held for any length of time (a few seconds) in the mouth prior to being drawn into the lungs, some of the MSS water-soluble vapor-phase components are "scrubbed" from the smoke stream and reach the ciliated areas at much reduced concentrations. This is also true to a lesser degree for water-soluble components of the particulate phase (see Tables 3.8 through 3.10). The exposure of the lungs to "resorbed" entities alleged to be tumorigenic will be much less than some authors claim. Similarly, in nose inhalation of ETS, some of its water-soluble components (formaldehyde, acetaldehyde, crotonaldehyde, ethyl carbamate, hydrazine)—alleged to be tumorigenic at the levels in MSS—will be "resorbed" in the nasal cavity and reach ciliated areas at concentrations reduced not only by the "resorption" mechanism but also by the dilution inherent in ETS generation from exhaled MSS and SSS produced during inter- and intrapuff smoldering. The exposure of the lungs to these "tumorigens" will obviously be substantially less than some writers claim.

Thus, these mechanisms—"scrubbing" and "resorption"—effective in substantially diminishing the amounts of

TABLE 3.10
Lung Retention and Mouth Absorption Data

	% Retention or Absorption					
	Laskowski (2267)		Rodgman et al. (3306)		Dalhamn et al. (892, 893)	
Smoke Component	**LR**	**MA**	**LR**	**MA**	**LR**	**MA**
Aldehydes and ketones[a]	99	—	80–90	40–67	—	—
Acetaldehyde	—[b]	—	—	—	99	60
Acetone	—	—	—	—	86	56
Acetonitrile	—	—	—	—	91	74
Isoprene	—	—	80–92	5–10	99	20
Toluene	—	—	—	—	93	28
TPM	—	—	80–90	10–15	96	16
Nicotine	67	—	—	—	—	—
Pyridine	98	—	—	—	—	—
Ammonia	98	56	—	—	—	—
Phenols	57	—	—	—	—	—
Carboxylic acids	44	—	—	—	—	—
CO	—	—	—	—	54	3

LR, percentage retained in lungs; MA, percentage absorbed in mouth.

[a] About 70%–75% of the volatile aldehydes and ketones in MSS is acetaldehyde plus acetone. For cigarettes in the 1950s and 1960s, the acetaldehyde–acetone ratio approximated 2:1.

[b] —, Not determined.

MSS water-soluble in vitro ciliastats that reach the lung during active smoking will be operative during ETS inhalation, whether oral or nasal, and diminish the amounts of the same and similar ETS components that reach the lung. This diminution in amounts will be particularly pertinent in the case of the smoke components formaldehyde, acetaldehyde, crotonaldehyde, ethyl carbamate, and hydrazine on the Hoffmann and Hoffmann "List of 60" (1740).

The following paragraphs include comments about two of the much researched smoke components formaldehyde and acetaldehyde:

Formaldehyde yields in cigarette range from 3.4 μg for filtered cigarettes to 283 μg in unfiltered cigarettes (2564, 3427). This compound is usually found in the vapor phase. The suggested formation mechanism for formaldehyde is destructive distillation and pyrolysis of celluloses, starch, pectins, lignin, and sugars [Burton (535), Chortyk and Schlotzhauer (722), Gager et al. (1264, 1265), Green (1351), Johnson et al. (1960), Stedman (3797)].

In both indoor and outdoor air in the United States, formaldehyde is usually present at the generally nonirritating level of approximately 0.06 ppm (1145a). In May 1992, OSHA ruled the exposure limit to formaldehyde be reduced from 3 to 0.75 ppm (2683a). Although most significant exposure to formaldehyde is generally industrial, it also naturally occurs in food, e.g., fruits and vegetables (2111b). Levels of formaldehyde in fruits and vegetables range from 3.3 μg/g in spinach to 17.3 μg/g in apples (3986a).

Formaldehyde is tumorigenic and mutagenic only at doses many-fold higher than that seen in cigarette MSS. Whether formaldehyde is mutagenic at noncytotoxic doses remains controversial due to the small number of studies and the variability of results (1873a). Formaldehyde has been reportedly found to induce aneuploidy (2363a, 2868a). In addition, results from some studies have suggested that humans routinely exposed to formaldehyde display increases in chromosomal aberrations and sister chromatid exchanges in peripheral lymphocytes. However, rodents treated with formaldehyde in vivo gave negative results for chromosomal aberrations and assays for lethal mutations. Additional rodent studies on DNA damage showed unconvincing results as well (1873a).

The overall tumorigenicity of formaldehyde was tested in two strains of rats and one strain of mice. Significant increases in squamous-cell carcinomas of the nasal cavity were observed in both rat strains after inhaling highly cytotoxic doses of formaldehyde. However, no carcinomas were observed in any of the mice inhaling the same dose (2086a). In other studies to evaluate formaldehyde tumorigenicity, mice and hamsters were exposed via inhalation, rats via subcutaneous injection, and rabbits via exposure in oral tanks. At the time, the results from these studies were considered inadequate to evaluate the tumorigenic risk to humans. Although formaldehyde was tumorigenic in rats when administered at very high dose levels (2610a, 3789b), the evidence of its tumorigenicity in humans was considered by the International Agency for Research on Cancer (IARC) to be inadequate, until 2005 (3A03). Recently, IARC reevaluated the evidence on formaldehyde and reclassified it as a Group 1 human carcinogen (3A16).

As noted previously, the reported MSS yield of acetaldehyde ranged from 18 (1853a) to 2815 μg/cig (2564) for

TABLE 3.11
Tobacco and/or Tobacco Smoke Aldehydes and Ketones Used in Flavor Formulations

CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Smoke	Tobacco
Aldehydes				
100-52-7	Benzaldehyde	Benzaldehyde	+	+
10031-82-0	Benzaldehyde, 4-ethoxy-	*p*-Ethoxybenzaldehyde	–	–
90-02-8	Benzaldehyde, 2-hydroxy-	Salicylaldehyde	+	+
121-33-5	Benzaldehyde, 4-hydroxy-3-methoxy-	Vanillin	+	+
120-14-9	Benzaldehyde, 3,4-dimethoxy-;	Veratraldehyde	–	+
529-20-4	Benzaldehyde, 2-methyl-	*o*-Tolualdehyde	+	+
620-23-5	Benzaldehyde, 3-methyl-	*m*-Tolualdehyde	+	+
104-87-0	Benzaldehyde, 4-methyl-	*p*-Tolualdehyde	+	+
122-03-2	Benzaldehyde, 4-(1-methylethyl)-	Cuminaldehyde	+	+
122-78-1	Benzeneacetaldehyde	Phenylacetaldehyde	+	+
4411-89-6	Benzeneacetaldehyde, α-ethylidene-	2-Phenyl-2-butenal	+	+
120-57-0	1,3-Benzodioxole-5-carboxaldehyde	Piperonal	+	+
96-17-3	Butanal, 2-methyl-	2-Methylbutyraldehyde	+	–
590-86-3	Butanal, 3-methyl-	3-Methylbutyraldehyde	+	+
25152-84-5	2,4-Decadienal	*trans, trans*-2,4-Decadienal	+	+
112-31-2	Decanal- {capraldehyde}	Decanal	–	+
66-25-1	Hexanal- {caproic aldehyde}	Hexanal	+	+
6728-26-3	2-Hexenal, (*E*)	2-Hexenal	+	+
110-62-3	Pentanal	Valeraldehyde	+	+
78-84-2	Propanal, 2-methyl-	Isobutyraldehyde	+	+
104-55-2	2-Propenal, 3-phenyl-	Cinnamaldehyde	+	+
13679-70-4	2-Thiophenecarboxaldehyde, 5-methyl-	5-Methyl-2-thiophenecarboxaldehyde	+	+
7774-82-5	2-Tridecenal	2-Tridecenal	–	+
Ketones				
107-88-0	1,3-Butanediol	1,3-Butanediol	+	+
431-03-8	2,3-Butanedione {diacetyl}	2,3-Butanedione	+	+
78-93-3	2-Butanone	2-Butanone	+	+
513-86-0	2-Butanone, 3-hydroxy-	Acetoin	+	+
5471-51-2	2-Butanone, 4-(4-hydroxyphenyl)-	4-(p-Hydroxyphenyl)-2-butanone	+	–
23696-85-7	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- {β-damascenone}	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-but-2-en-4-one	+	+
35044-68-9 23726-92-3	2-Buten-1-one, 1-(2,6,6-trimethylcyclohex-1-enyl)- {β-damascone}	4-(2,6,6-Trimethylcyclohex-2-enyl)-but-2-en-4-one	+	+
623-15-4	3-Buten-2-one, 4-(2-furanyl)-	4-(2-Furyl)-3-buten-2-one	+	+
122-57-6	3-Buten-2-one, 4-phenyl-	4-Phenyl-3-buten-2-one	+	+
127-41-3	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	α-Ionone	+	+
14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	β-Ionone	+	+
89-80-5	Cyclohexanone, 5-methyl-2-(1-methylethyl)-	l-Menthone	+	+
1125-21-9	2-Cyclohexene-1,4-dione, 2,6,6-trimethyl-	2,6,6-Trimethylcyclohex-2-ene-1,4-dione	+	+
13215-88-8	2-Cyclohexen-1-one,4-(2—(2-butenylidene)-3,5,5-trimethyl-	4-(2-Butylidene-3,5,5-trimethyl)-2-cyclohexen-1-one	+	+
99-49-0	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)-	*l*-Carvone	+	+
89-81-6	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-	*d*-Piperitone	–	+
6091-50-5				
13494-06-9	1,2-Cyclopentanedione, 3,4-dimethyl-	3,4-Dimethyl-1,2-cyclopentanedione	+	–
13494-07-0	1,2-Cyclopentanedione, 3,5-dimethyl-	3,5-Dimethyl-1,2-cyclopentanedione	+	–
80-71-7	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	Methylcyclopentenolone	+	+
100-06-1	Ethanone, 1-(4-methoxyphenyl)-	Acetanisole	+	+
98-86-2	Ethanone, 1-phenyl-	Acetophenone	+	+
32974-92-8	Ethanone, 1-(5-ethylpyrazintl)-	2-Acetyl-3-ethylpyrazine	+	–
1193-79-9	Ethanone, 1-(2-furanyl 5-methyl)-	2-Acetyl-5-methylfuran	+	+
122-00-9	Ethanone, 1-(4-methylphenyl)-	4-Methylacetophenone	+	+
1333-52-4	Ethanone, 1-(naphthalenyl)-	Methyl naphthyl ketone	+	–

TABLE 3.11 (continued)
Tobacco and/or Tobacco Smoke Aldehydes and Ketones Used in Flavor Formulations

CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Smoke	Tobacco
22047-25-2	Ethanone, 1-pyrazinyl-	Acetylpyrazine	–	+
1122-62-9	Ethanone, 1-(2-pyridinyl)-	2-Acetylpyridine	+	+
350-03-8	Ethanone, 1-(3-pyridinyl)-	3-Acetylpyridine	+	+
1072-83-9	Ethanone, 1-(1*H*-pyrrol-2-yl)-	Methyl 2-pyrrolyl ketone	+	+
24295-03-2	Ethanone, 1-(2-thiazolyl)-;	2-Acetylthiazole	+	–
110-43-0	2-Heptanone	2-Heptanone	+	+
5166-53-0	3-Hexen-2-one, 5-methyl-	5-Methyl-3-hexen-2-one	+	+
119-61-9	Methanone, diphenyl-	Benzophenone	+	–
1937-54-8	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-	Solanone	+	+
821-55-6	2-Nonanone	2-Nonanone	+	+
600-14-6	2,3-Pentanedione	2,3-Pentanedione	+	–
123-76-2	Pentanoic acid, 4-oxo-	Levulinic acid	+	+
107-87-9	2-Pentanone	2-Pentanone	+	+
141-79-7	3-Penten-2-one, 4-methyl- {mesityl oxide}	4-Methyl-3-penten-2-one	+	+
127-17-3	Propanoic acid, 2-oxo-	Pyruvic acid	+	+
4940-11-8	4*H*-Pyran-4-one, 3-hydroxy-2-ethyl-	Ethylmaltol	+	–
118-71-8	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-	Maltol	+	+
593-08-8	2-Tridecanone	2-Tridecanone	–	+
3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl- {geranylacetone}	6,10-Dimethyl-5,9-undecadien-2-one	–	+
112-12-9	2-Undecanone	2-Undecanone	+	+

nonfiltered cigarettes. However, a substantial difference exists between the analytically derived yields of acetaldehyde and other water-soluble vapor-phase components reported to be ciliastatic and the smoker's exposure to them. Dalhamn et al. (892) described how a substantial percentage of water-soluble components such as acetaldehyde are removed from the vapor phase of the smoke stream by solution in the aqueous fluids coating the oral cavity, thus never reaching the upper or lower respiratory tract. The proposed mechanisms of formation for acetaldehyde are destructive distillation and pyrolysis, and its major precursors are reported to be the celluloses, pectins, starch, lignin, and sugars [Burton (535), Chortyk and Schlotzhauer (722), Gager et al. (1264, 1265), Green (1351), Johnson et al. (1960), Stedman (3797)].

Additional complexities exist regarding the predictability of biological activity. For example, a significant amount of vapor-phase water-soluble components such as formaldehyde and acetaldehyde are "scrubbed" from the smoke stream into solution by the fluids coating the oral cavity and upper respiratory tract; thus, they reach the lung at a diminished level (892, 893). Similarly, only a modest percentage of a water-insoluble component such as isoprene is retained by the smoker because a significant portion of it is exhaled. In light of these phenomena and the fragmentary nature of the data on actual exposure and retention, the possible physiological effect of formaldehyde, acetaldehyde, and isoprene at the cited cigarette MSS delivery ranges cannot be extrapolated. Very few studies have been performed in which a smoking machine or system was modified to approximate the effect of oral cavity fluids on the retention of specific MSS components. It has been known since the early 1950s and confirmed in the 1960s that different classes of smoke components are retained to different degrees by the smoker (892, 2267, 3255, 3257, 3306). Thus, the composition of the cigarette MSS retained by the smoker is significantly different from that exhaled by the smoker. Also, both the biologically retained and exhaled smokes are obviously different compositionally from the cigarette MSS retained and analyzed by the smoking machine-collection system.

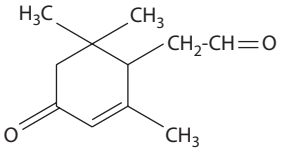
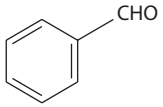
While much emphasis was placed on the aldehyde and ketone components in the vapor phase of cigarette MSS because of their in vitro ciliastatic activity, much research was also conducted after the mid-1950s to identify aldehyde and ketone components in the particulate phase of cigarette MSS primarily because many were found to contribute consumer-acceptable flavor and aroma properties to the MSS. As noted by Rodgman (3266), many of the aldehydes and ketones used by the tobacco industry in its flavor formulations [see listing by Doull et al. (1053)] are known components of untreated tobacco and/or its smoke. Thus, such additives are not strangers to the tobacco and/or its smoke, but their addition increases the consumer-acceptable flavorants. Table 3.11 lists some of the tobacco and/or tobacco smoke components that have been or are used in flavor formulations.

Tables 3.12 and 3.13 list the aldehydes and ketones, respectively, reported as tobacco and/or tobacco smoke components. The aldehydes number 297 with 187 identified in tobacco smoke, 217 in tobacco, and 107 in both. The ketones number 1253 of which 736 have been identified in tobacco smoke, 799 in tobacco, and 282 in both. Tables 3.12 and 3.13 are followed by Table 3.14 which depicts the chronology of many of the studies on aldehydes and ketones in tobacco and tobacco smoke.

TABLE 3.12
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	75-07-0	Acetaldehyde CH_3-CH═O	37, 38, 69, 73, 83, 85, 126a, 126b, 156, 167, 172, 173a, 174a, 174b, 174c, 174e, 199, 213, 239, 270, 299, 314, 329, 337, 348, 376, 402, 405, 407, 408, 480, 491, 500, 544–546, 564, 568b, 603, 605, 639, 643, 645, 688, 722, 762, 764a, 778, 804, 830a, 892, 893, 916, 929, 966, 988a, 1023, 1039, 1050, 1051, 1063–1075, 1140, 1148, 1153, 1154, 1167, 1168, 1217, 1237–1239, 1283, 1284, 1329, 1330, 1332–1334, 1348–1352, 1354, 1360, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1418, 1422, 1426, 1427, 1437, 1445, 1449, 1487, 1489, 1492, 1495–1497, 1586, 1589, 1590, 1634, 1637, 1668, 1673, 1674, 1693, 1709, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1803, 1808, 1822, 1829, 1835b, 1840, 1842, 1870, 1871, 1875, 1884, 1963, 1971, 2002, 2003, 2063, 2070, 2079, 2081–2086, 2089, 2091, 2131, 2134a, 2144, 2159, 2170, 2252, 2270, 2293, 2296, 2298, 2301, 2302, 2304, 2305, 2313a, 2337, 2411, 2444, 2452, 2483, 2506, 2507, 2519, 2520, 2525, 2537, 2543, 2545, 2558, 2570, 2573–2575, 2582, 2591, 2601b, 2634, 2644, 2683, 2690–2695, 2702, 2761, 2762, 2765, 2767, 2775, 2777, 2781, 2782, 2799a, 2800, 2804, 2822, 2825, 2857, 2858, 2866, 2868, 2887, 2927, 2936, 2939, 2942, 2948, 3007, 3059, 3088, 3105, 3116, 3131, 3132, 3135, 3136, 3140, 3169, 3187, 3190, 3251, 3254, 3255, 3257, 3260, 3264, 3265, 3289, 3300, 3302, 3306, 3308, 3370, 3373, 3396, 3418, 3431, 3436, 3438, 3479, 3482, 3493, 3508, 3530, 3551, 3557, 3559, 3577, 3579, 3581–3584, 3692, 3713, 3714, 3794, 3797, 3817, 3844, 3871, 3876, 3880, 3882, 3883, 3897, 3901, 3904, 3935, 3939, 3952, 3973, 3976, 3984, 3992, 4005–4007, 4009–4011, 4052, 4056, 4062, 4078, 4104, 4109, 4155, 4159, 4162, 4249, 4254–4258, 4288, 4290, 4301, 4304, 4319, 4330, 4332, 4342, 4365, 4394,	120, 212, 568b, 984, 1550, 1590, 1893b, 2079, 2270, 2293, 2337, 2702, 2702a, 2860a, 2914, 2939, 3194, 3350, 3626, 3797, 3973, 3974a, 3974b, 4223, 4225, 5053, 5079, 5165, 5811b, 5896	1228, 1330, 1332, 1354, 1360, 1375a, 1377, 1378, 2244, 2506, 2507, 3401, 4052, 4056

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Acetaldehyde (cont.)	4418, 5006, 5034, 5049, 5065, 5069, 5079, 5135, 5136, 5508, 5512, 5531, 5547, 5679, 5692, 5770, 5811b, 5835, 5836, 5869a, 3A12, 4A02		
2.	5371-49-3	Acetaldehyde (acetyloxy)- CH_3-COO-CH_2-CH═O	568b, 3553, 3653, 4249, 5811b	568b, 2336, 2337a, 4249	
3.	6542-88-7	Acetaldehyde, amino- H_2N-CH_2-CH═O	568b, 3410, 4249		
4.	141-46-8	Acetaldehyde, hydroxy- {glycolaldehyde} HO-CH_2-CH═O	568b, 2939, 3553, 3559, 3797, 4249, 5811b	568b, 3973, 3974a, 4079, 4249, 5811b	3401, 3402, 3405
5.	10312-83-1	Acetaldehyde, methoxy- CH_3O-CH_2-CH═O	1039		
6.	298-12-4	Acetic acid, oxo- {glyoxylic acid} O═CH-COOH	1310, 2939, 3059, 3302	120, 1310, 1312, 2939, 3797, 3973, 3974a, 5651, 5811b	
7.	16825-04-0	Acetaldehyde, (2,6,6-trimethyl- 4-oxo- 2-cyclohexen-1-ylidene)- 		943, 2389, 2544, 3543, 3547, 5811b	
8.	4471-47-0	Acetonitrile, oxo- O═CH-CN	314, 568b, 1367, 2545, 4249		
9.	87-72-9 5328-37-0	*L*-Arabinose HO-CH_2-$(CHOH)_3$-CH═O	1351, 2145, 2939, 3302, 4249, 5811	120, 158, 344a, 830a, 1263, 1351, 2070, 2270, 2338, 3059, 3075, 3797, 3973, 3974a, 4249, 5811, 5811b	
10.	147-81-9	*DL*-Arabinose	5580, 5811b	5079, 5785, 5811b	
11.	98530-09-7	Arabogalactan		1971, 5777	
12.	100-52-7	Benzaldehyde 	156, 157, 239, 299, 568b, 591, 830a, 966, 1168, 1215, 1238, 1313, 1360, 1364, 1365, 1368, 1371, 1375a, 1377, 1426, 1427, 1437, 1884, 1949, 1971, 2079, 2088, 2089, 2170, 2270, 2337, 2387, 2506, 2507, 2543, 2545, 2702, 2731, 2735, 2761, 2762, 2765, 2766, 2773–2775, 2799a, 2912, 2939, 3255, 3266, 3302, 3308, 3410, 3555, 3648, 3797, 3876, 4155, 4159, 4249, 4304, 4570a, 5034, 5079, 5811b	120, 404, 568b, 937, 984, 1053, 1063–1066, 1068–1074, 1189, 1368, 1379, 1550, 1590a, 1615, 1854, 1949, 2282, 2337, 2339a, 2386, 2389, 2544, 2611, 2702, 2860a, 2862, 2917a, 2939, 3188, 3194, 3205, 3217, 3219, 3266, 3354, 3539, 3543, 3547, 3550, 3555, 3560, 3561, 3648, 3797, 3905, 3973, 3974a, 4098a, 4249, 5811b	1360, 1375a, 1377, 2387, 2506, 2507, 3401, 3402, 3404

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

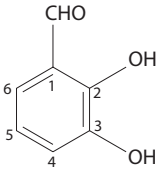
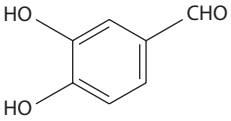
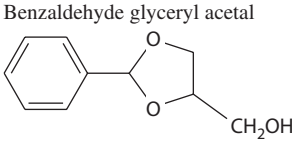
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
13.	1620-980	Benzaldehyde, 3,5-di(1,1-dimethylethyl)-4-hydroxy-		2917a	
14.	579-66-8	Benzenamine, 2,6-diethyl-	5811	5811	
15.	33774-71-9	Benzaldehyde, dihydroxy-	4249	3748	
16.	24677-78-9	Benzaldehyde, 2,3-dihydroxy- 	2939, 3302, 3712, 4249	3797	
17.	95-01-2	Benzaldehyde, 2,4-dihydroxy-	4249		3395, 4249
18.	1194-98-5	Benzaldehyde, 2,5-dihydroxy-	3395, 3712, 4249		3395
19.	139-85-5	Benzaldehyde, 3,4-dihydroxy- {protocatechualdehyde} 	1626, 1884, 2092, 2939, 3712, 3741, 3743, 3797, 4249, 4378, 4379	2092, 3748, 3749, 3751, 3797, 3973, 3974a, 4249	3395
20.	86-51-1	Benzaldehyde, 2,3-dimethoxy-	568b, 4249	568b, 4249	
21.	613-45-6	Benzaldehyde, 2,4-dimethoxy-		3219, 4249	
22.	93-02-7	Benzaldehyde, 2,5-dimethoxy-	5811	5811	
23.	4925-88-6	Benzaldehyde, 2,5-dimethoxy-4-methyl-	2601a		
24.	3392-97-0	Benzaldehyde, 2,6-dimethoxy-	2767, 3266, 3557, 4249	938, 1256, 3219, 3266, 4249	
25.	120-14-9	Benzaldehyde, 3,4-dimethoxy- {veratraldehyde}	568b, 1238, 4249	172a, 174b, 568b, 938, 1053, 1254, 1256, 3266, 3370, 3767a, 4249	
26.	7311-34-4	Benzaldehyde, 3.5-dimethoxy-	568b, 4249	568b, 4249	
27.	134-96-3	Benzaldehyde, 3,5-dimethoxy-4-hydroxy- {syringaldehyde}	568b, 1238, 1884, 2042, 2043, 2046, 3302, 3308, 3712, 3797, 4163, 4249, 4379	404, 568b, 3797, 3974a, 4249	3395
28.	708-76-9	Benzaldehyde, 4,6-dimethoxy-2-hydroxy-	568b, 4249	568b, 4249	
29.	15764-16-6	Benzaldehyde, 2,4-dimethyl-	3387, 4249, 5811b		
30.	5779-94-2	Benzaldehyde, 2,5-dimethyl-			3402a, 4249
31.	100-10-7	Benzaldehyde, 4-(dimethylamino)-	568b, 4249		
32.	121-32-4	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}	568b, 2731, 2735, 3266, 3712, 4050, 4249, 4566	568b, 633, 1053, 2281, 2282, 2478, 2699, 3266, 3643, 3894, 4050, 4249	
33.	10031-82-0	Benzaldehyde, 4-ethoxy-		172a, 174b, 1053, 3266	
34.	2539-53-9	Benzaldehyde, 4-ethoxy-3-hydroxy-		5811b	
35.	53951-50-1	Benzaldehyde, ethyl-		3186, 3188, 4249	
36.	4748-78-1	Benzaldehyde, 4-ethyl-	1371, 3266, 3410, 4249	172a, 174b, 1053, 3266	
37.	1319-88-6	Benzaldehyde glyceryl acetal 		172a, 174b, 1053, 3266	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
38.		Benzaldehyde, hydroxy-	5034		
39.	90-02-8	Benzaldehyde, 2-hydroxy- {salicylaldehyde}	414, 568b, 1238, 1378, 1586, 1626, 1789, 1884, 1906, 2088, 2327c, 2939, 3059, 3266, 3302, 3308, 3557, 3559, 3712, 3797, 4249, 4313, 4317, 4319, 4332, 5811b	120, 172a, 174b, 568b, 937, 1053, 2339a, 2862, 2939, 3059, 3266, 3370, 3973, 3974a, 4249, 5811b	1378, 3395, 3401, 3402, 3404
40.	106799-60-4	Benzaldehyde, hydroxymethoxy-		2339, 5811b	
41.	148-53-8	Benzaldehyde, 2-hydroxy-3-methoxy-	5034	3430, 5811b	
42.	698-27-1	Benzaldehyde, 2-hydroxy-4-methyl-		172a, 174b, 1053, 3266	
43.	100-83-4	Benzaldehyde, 3-hydroxy-	568b, 1238, 1364, 1884, 2327c, 2545, 2767, 3302, 3308, 3557, 3712, 3797, 4163, 4249, 4379, 5811b	568b, 3797, 3973, 3974a, 4249	3404
44.	123-08-0	Benzaldehyde, 4-hydroxy-	568b, 1238, 2042, 2043, 3302, 3308, 3559, 3712, 3797, 4163, 4249, 4379, 5811b	568b, 3797, 3973, 3974a, 4249, 5811b	3395, 3404
45.	121-33-5	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}	568b, 1105, 1238, 1352, 1358, 1360, 1361, 1364, 1375, 1375a, 1375b, 1586, 2042–2044, 2327c, 2339, 2570, 2601a, 2640, 2762, 2765, 2767, 3224, 3266, 3302, 3308, 3553, 3557, 3712, 3745, 3797, 4050, 4249, 4379, 5034, 5811b	172a, 174b, 404, 568b, 633, 935, 1053, 1063–1066, 1068–1074, 1105, 1352, 1379, 1590a, 1825, 2281, 2338, 2339, 2339a, 2478, 2389, 2544, 2611, 2699, 2917a, 3159, 3215, 3219, 3266, 3370, 3550, 3643, 3767a, 3797, 3973, 3974a, 4050, 4249, 5811b	1360, 1375a, 3395
46.		Benzaldehyde, 4-hydroxy-3-methoxy-, labeled with ^{14}C {vanillin-^{14}C}	1105	1105	
47.		Benzaldehyde, hydroxymethyl-	1275, 2767, 4249		
48.	97122-27-5	Benzaldehyde, hydroxy-3-methyl-	3557		
49.	57295-30-4	Benzaldehyde, 3-hydroxy-4-methyl-	1375, 1375b, 4249		
50.	15174-69-3	Benzaldehyde, 4-hydroxy-3-methyl-	1375, 1375b		
51.		Benzaldehyde, methoxy-	3893, 4249, 5034		
52.	135-02-4	Benzaldehyde, 2-methoxy-	5811a		
53.	591-31-1	Benzaldehyde, 3-methoxy-	568b, 4249		
54.	123-11-5	Benzaldehyde, 4-methoxy-{*p*-anisaldehyde}	278, 568b, 1884, 3266, 4036, 4249, 5811b	45, 120, 172a, 174b, 568b, 1053, 1379, 2862, 2917a, 2939, 3059, 3266, 3370, 3797, 3905, 3973, 3974a, 4249, 5811b	
55.	1334-78-7	Benzaldehyde, methyl-	2543, 2731, 2735, 2773, 3410, 4249	2094, 4249	

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

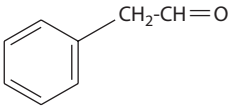
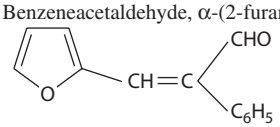
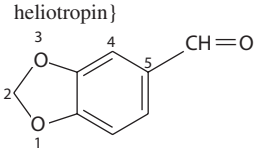
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
56.	529-20-4	Benzaldehyde, 2-methyl-{*o*-tolualdehyde}	299, 568b, 937, 3266, 3404, 3797, 4249, 5811b	937, 172a, 174b, 568b, 1053, 3266, 3370, 3797, 4249, 5811b	3402, 3404
57.	620-23-5	Benzaldehyde, 3-methyl-{*m*-tolualdehyde}	568b, 1884, 3266, 3302, 3794, 4249, 5811b	120, 172a, 174b, 524, 568b, 1053, 2389, 2544, 2722, 2862, 2939, 3266, 3370, 3547, 3797, 3974a, 4249, 5811b	3402, 3404
58.	104-87-0	Benzaldehyde, 4-methyl-{*p*-tolualdehyde}	299, 568b, 1526, 1427, 3266, 4249, 5811b	172a, 174b, 404, 568b, 1053, 2917a, 3266, 3370, 3547, 3905, 4249	3402, 3404
59.	122-03-2	Benzaldehyde, 4-(1-methylethyl)-{cuminaldehyde}	568b, 1238, 3266, 4249	172a, 174b, 568b, 937, 1053, 1156, 3266, 4090, 4249	
60.	29344-95-4	Benzaldehyde, 2,3,4,5-tetramethyl-		2917a	
61.	487-68-3	Benzaldehyde, 2,4,6-trimethyl-	5811, 5811a, 5811b		
62.	122-78-1	Benzeneacetaldehyde {phenylacetaldehyde} 	299, 568b, 1238, 1949, 2769, 3266, 4159, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1063–1066, 1068–1074, 1590a, 1662, 1949, 2282, 2286, 2337, 2389, 2544, 2917a, 3266, 3370, 3543, 3547, 3549, 3550, 3560, 3561, 4249, 5811b	
63.	4411-89-6	Benzeneacetaldehyde, α-ethylidene-{2-phenyl-2-butenal}	568b, 1587, 3266, 4249, 5811b	174b, 568b, 943, 1053, 2389, 2544, 3266, 3547, 3561, 4249, 5811b	
64.	57568-60-2	Benzeneacetaldehyde, α-(2-furanylmethylene)- 		943, 1587, 3547, 4249	
65.	65545-81-5	Benzeneacetaldehyde,α-(2-furanylmethylene)-,(*E*)-		5811	
66.	5031-83-4	Benzeneacetaldehyde, α-(2-phenylethylidene)-	5811b	3561	
67.	104-09-6	Benzeneacetaldehyde, 4-methyl-		1053, 3266	
68.	104-53-0	Benzenepropanal	5811b	172a, 174b, 1053, 3266	
69.	103-95-7	Benzenepropanal, α-methyl-4-(1-methylethyl)-{cyclamen aldehyde}		172a, 174b, 1053, 3266	
70.	80638-48-8	Benzenepropanal, 4-hydroxy-3-methoxy-	3712	5811b	
71.	120-57-0	1,3-Benzodioxole-5-carboxaldehyde {piperonal; heliotropin} 	1238, 2478, 3266, 3894, 4249	172a, 174b, 1053, 1254, 1256, 1590a, 1662, 2478, 3266, 3370, 3643, 3894, 4249	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
72.	4265-16-1	2-Benzofurancarboxaldehyde	568b, 4249		
73.	4250-90-2	Benzo[*g*]pteridine-10(2*H*)-acetaldehyde, 3,4-dihydro-7,8-dimethyl-2,4-dioxo-		4249	
74.	61892-65-7	[2,3′-Bipyridine]-1(2*H*)-carboxaldehyde, 3,6-dihydro-, (S)-{*N*′-formylanatabine}	568b, 3739, 3740, 4249, 5811b	64, 568b, 3550, 3973, 4236, 4249, 5811b	
75.	123-72-8	Butanal {butyraldehyde} $H_3C\text{-}(CH_2)_2\text{-}CH{=}O$	174a, 174b, 174c, 174e, 299, 314, 564, 568b, 605, 688, 764a, 1038, 1039, 1140, 1238, 1365, 1374, 1375, 1375b, 1386, 1412–1414, 1416, 1419, 1634, 1853b, 2079, 2089, 2170, 2270, 2310, 2313a, 2337, 2519, 2520, 2545, 2591, 2702, 2767, 2782, 2804, 2822, 2887, 2939, 3007, 3059, 3105, 3135, 3136, 3254, 3300, 3302, 3308, 3396, 3436, 3557, 3794, 3901, 3935, 4078, 4249, 4304, 4319, 4570a, 5034, 5049, 5079, 5135, 5136, 5770, 5811b, 5835, 5836	568b, 1550, 1893b, 2337, 2914, 3350, 3626, 3797, 3973, 3974a, 5811b	2244
76.	4390-05-0	Butanal, 4-amino- $H_2N\text{-}(CH_2)_3\text{-}CH{=}O$		555b, 3973	
77.	34764-22-2	Butanal, 3,4-dihydroxy- $HOCH_2\text{-}CHOH\text{-}CH_2\text{-}CH{=}O$	3553, 4249		
78.	2109-98-0	Butanal, 2,3-dimethyl-	4570a		
79.	97-96-1	Butanal, 2-ethyl-{diethylacetaldehyde} $(C_2H_5)_2{=}CH\text{-}CH{=}O$	568b, 1238, 4249	568b, 3186, 3188, 4249	
80.	107-89-1	Butanal, 3-hydroxy-{aldol} $H_3C\text{-}CHOH\text{-}CH_2\text{-}CH{=}O$	568b, 2170, 2702, 2939, 3302, 3876, 4249, 5079		
81.		Butanal, 3-hydroxy-2-oxo-{methylreductone} $H_3C\text{-}CHOH\text{-}CO\text{-}CH{=}O$		3797, 4249	
82.	25714-71-0	Butanal, 4-hydroxy- $HO\text{-}(CH_2)_3\text{-}CH{=}O$	3553, 4249		
83.		Butanal, 4-(2-hydroxyethoxy)- $HO\text{-}CH_2CH_2\text{-}O\text{-}(CH_2)_3\text{-}CH{=}O$	3553, 4249		
84.	96-17-3	Butanal, 2-methyl-{2-methylbutyraldehyde} $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH{=}O$	299, 314, 568b, 1221, 1063–1066, 1068–1074, 1221, 1360, 1375a, 1418, 1419, 1999, 2337, 2545, 2767, 3219, 3266, 3308, 3508, 4249, 4570a, 5770, 5811b	172a, 174b, 568b, 1053, 1550, 2337, 2339a, 2917a, 3186, 3188, 3266, 4249, 5811b	1360, 1375a
85.	590-86-3	Butanal, 3-methyl-{3-methylbutyraldehyde; isovaleraldehyde} $(H_3C)_2{=}CH\text{-}CH_2\text{-}CH{=}O$	173a, 299, 314, 405, 407, 408, 568b, 605, 1039, 1063–1066, 1068–1074, 1140, 1238, 1348–1350, 1354, 1360, 1365, 1375, 1375a, 1375b, 1412–1414, 1416, 1418, 1419, 1884, 2003, 2293, 2337, 2573–2375, 2767, 2782, 2804, 2927, 3254, 3266, 3302, 3308, 3413, 3508, 3557, 3794, 3817, 4052, 4056, 4162, 4249, 4319, 4570, 5034, 5770, 5811b	172a, 174b, 568b, 647, 909, 937, 1053, 1157, 1550, 1615, 2337, 2339a, 2914, 2917a, 2939, 3188, 3266, 3350, 3370, 3626, 3797, 3974a, 4223, 4225, 4249, 5811b	1354, 1360, 1375a, 4052, 4056
86.	7729-27-3	Butanal, 4-(methylamino)- $H_3C\text{-}NH\text{-}(CH_2)_3\text{-}CHO$		4249, 4707	

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

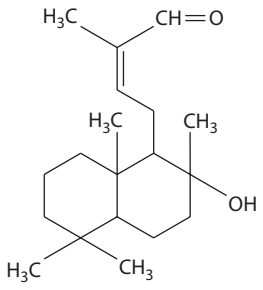
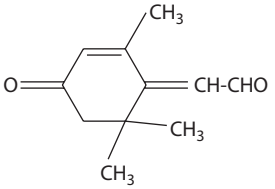
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
87.	64091-90-3	Butanal, 4-(methylnitrosamino)-4-3-(pyridyl)-	See 3-Pyridinebutanal, γ-(methylnitrosoamino)-		
88.	40654-82-8	Butanal, 2-methyl-4-phenyl- C_5H_6-$(CH_2)_2$-CH(CH_3)-CH═O		1053, 3266	
89.	4417-81-6	Butanal, 2-oxo-{ethylglyoxal} H_3C-CH_2-CO-CH═O	1238, 3902, 4249		
90.	1758-51-6	Butanal, 2,3,4-trihydroxy-, (R*,R*)- $HOCH_2$-$(CHOH)_2$-CH═O		3797, 4249, 5811b	
91.	638-37-9	Butanedial {succinaldehyde} O═CH-$(CH_2)_2$-CH═O	1361, 3405, 4249, 5811b		3401, 3402, 3405
92.	2338-03-6	Butanoic acid, 2-amino-4-oxo-, (S)- O═CH-CH_2-CH(NH_2)-COOH		4249	
93.	4170-30-3	2-Butenal {crotonaldehyde} H_3C-CH═CH-CH═O	112, 126a, 174b, 174c, 239, 270, 299, 329, 405, 407, 408, 480, 564, 568b, 591, 605, 689, 764a, 830a, 1063–1074, 1140, 1148, 1153, 1217, 1348–1351, 1354, 1375a, 1378, 1386, 1412–1414, 1416, 1418, 1419, 1586, 1589, 1634, 1727, 1741, 1773, 1842, 2002, 2079, 2088, 2089, 2313a, 2337, 2387, 2506, 2507, 2520, 2543, 2545, 2570, 2591, 2761, 2762, 2765, 2767, 2777, 2782, 2804, 2857, 2887, 2927, 2939, 3007, 3029, 3133, 3135, 3136, 3140, 3187, 3255, 3257, 3265, 3300, 3302, 3308, 3441a, 3482, 3530, 3557, 4005–4007, 4052, 4056, 4078, 4079, 4162, 4249, 4257, 4290, 4304, 4319, 5006, 5022, 5034, 5049, 5065, 5069, 5070, 5508, 5770, 5811b, 5836	120, 568b, 984, 2337, 2862a, 2917a, 2939, 3797, 3974a, 3974b, 4249, 5053, 5065, 5811b	1354, 1375a, 1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404, 4052, 4056
94.	123-73-9	2-Butenal (*E*)	5811, 5811a	5811, 5811a	
95.	15798-64-8	2-Butenal (*Z*)	5811a	5811a	
96.	1115-11-3	2-Butenal, 2-methyl- H_3C-CH═C(CH_3)-CH═O	299, 314, 568b, 1063–1066, 1068–1074, 1365, 2761, 2765, 2766, 2769, 3555, 3559, 4249, 5770	404, 568b, 3186, 3188, 4249	
97.	497-03-0	2-Butenal, 2-methyl-, (*E*)-{tiglic aldehyde}	5811, 5811a, 5811b		
98.	107-86-8	2-Butenal, 3-methyl-{senecialdehyde} H_3C-C(CH_3)═CH-CH═O	299, 568b, 1371, 3559, 4249		
99.	83841-47-8	2-Butenal, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-2-methyl-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		4249, 4950, 5811b	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

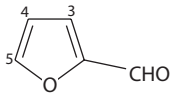
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
100.	7319-38-2	3-Butenal $H_2C{=}CH\text{-}CH_2\text{-}CH{=}O$	314, 1367, 2545, 4249		
101.	1119-19-3	2-Butynal $H_3C\text{-}C{\equiv}C\text{-}CH{=}O$	2506, 4249		
102.	116-26-7	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-{safranal}	5811b	404, 568b, 1149, 1149a, 2095, 2338, 2339a, 2339b, 2917a, 3186, 3188, 3218, 3547, 4249, 5811b	
103.	2043-61-0	Cyclohexanecarboxaldehyde		4249	
104.	1321-16-0	Cyclohexenecarboxaldehyde	5811, 5811a, 5811b		
105.	1192-88-7	1-Cyclohexene-1-carboxaldehyde	2731, 2735, 4249, 5811b		
106.	18378-66-0	1-Cyclohexene-1-carboxaldehyde, 3-oxo-2,6,6-trimethyl-		5811, 5811b	
107.	432-25-7 52844-21-0	1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- {β-cyclocitral}	5811b	404, 568b, 937, 2339a, 2389, 2544, 2917a, 3218, 3547, 4249, 5811, 5811a, 5811b	
108.	60026-16-6	Cyclohexenylideneacetaldehyde, 4-oxo-2,6,6-trimethyl- 		5811, 5811b	
109.	33320-27-3	1,3-Cyclopentadiene-1-carboxaldehyde	2767, 4249		
110.	20497-93-2	Cyclopentanecarboxaldehyde, 2-hydroxy-1-methyl-{two isomers}		568b, 3547, 4249	
111.	2363-88-4	2,4-Decadienal	2388, 4249	3186, 4249	
112.	25152-84-5	2,4-Decadienal, (*E,E*)-	568b, 3266, 3553, 4249	568b, 1053, 3186, 3188, 3266, 4249	
113.	112-31-2	Decanal {capraldehyde}	60, 568b, 1238, 3302, 4249, 5811b	172a, 174b, 404, 568b, 937, 1053, 2337, 2389, 2544, 2913a, 3266, 3370, 4249, 5811b	
114.	2497-25-8	2-Decenal, (*Z*)- $H_3C\text{-}(CH_2)_6\text{-}CH{=}CH\text{-}CH{=}O$		3266	
115.	3913-71-1	2-Decenal, (*E*)-		4249	
116.	58474-80-9	3-Decenal $H_3C\text{-}(CH_2)_5\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}O$		1053, 3266	
117.	30390-50-2	4-Decenal		5811	
118.	21662-09-9	4-Decenal, (*Z*)-		5811	
119.	112-54-9	Dodecanal $H_3C\text{-}(CH_2)_{10}\text{-}CH{=}O$	5811b	568b, 1053, 3266, 4249	
120.	2400-66-0	Eicosanal $H_3C\text{-}(CH_2)_{18}\text{-}CHO$		1248, 4249, 5811b	

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
121.	107-22-2	Ethanedial {glyoxal} O═CH-CH═O	552, 1238, 1239, 1375, 1375a, 1375b, 1377, 1378, 1491, 2469, 2939, 3251, 3254, 3302, 3341, 4249, 5680, 5811b, 5835	2939, 3797, 3974a, 4249, 5811b, 17B59	1228, 1375a, 1377, 1378
122.	50-00-0	Formaldehyde H-CH═O	69, 73, 126, 126a, 126b, 126d, 172, 172c, 174a, 174b, 174c, 174e, 213, 237, 239, 243, 270, 376, 402, 405, 407, 408, 486, 544–546, 564, 591, 603, 688, 722, 748, 764a, 778, 872, 929, 1023, 1039, 1049, 1051, 1063–1074, 1099, 1140, 1148, 1217, 1218, 1238, 1283, 1284, 1292, 1329, 1330, 1332–1334, 1336, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1437, 1442, 1443, 1445, 1487, 1492, 1589,1668–1670, 1673, 1674, 1695, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1835c, 1840, 1842, 1870, 1871, 2022, 2079, 2083–2085, 2086b, 2089, 2133, 2134a, 2170, 2180, 2195, 2200, 2252, 2270, 2293, 2310, 2313a, 2343, 2354, 2452, 2456, 2524, 2529, 2537, 2543, 2545, 2558, 2570, 2591, 2601b, 2683, 2690–2695, 2702, 2702a, 2706, 2761, 2762, 2775, 2777, 2782, 2799a, 2804, 2822, 2825, 2887, 2927, 2939, 3007, 3059, 3116, 3133, 3135, 3136, 3149, 3169, 3187, 3190, 3251, 3254, 3255, 3257, 3260, 3264, 3265, 3300, 3302, 3308, 3335, 3370, 3396, 3427, 3431, 3436, 3438, 3493, 3557, 3713, 3776, 3789b, 3791, 3844, 3871, 3872, 3880, 3882, 3897, 3912, 3924, 3952, 3963, 3992, 4010, 4011, 4078, 4159, 4249, 4259, 4288, 4301, 4304, 4305, 4319, 4342, 4360, 4689, 4743, 4816, 5006, 5065, 5069, 5079, 5124, 5423, 5508, 5512, 5529, 5531, 5679, 5692, 5811b, 5835, 5836, 5869a, 3A01, 3A02, 3A03, 3A05, 3A06, 3A07, 3A10, 3A11, 3A12, 3A16, 3A20, 3A21, 3A23, 3A24, 3A25	2703, 2939, 3335, 3626, 3797, 3973, 3974a, 3974b, 4249, 5053, 5079, 5811b	1228, 1330, 1332, 1354, 1375a, 1377, 1378
123.	39276-09-0	Furancarboxaldehyde	3865b, 4249, 4553		

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
124.	98-01-1	2-Furancarboxaldehyde {furfural; 2-furaldehyde} 	157, 172, 174a, 239, 270, 299, 314, 375, 376, 402, 564, 568b, 722, 775, 916, 924, 1039, 1099, 1140, 1215, 1238, 1239, 1338, 1339, 1348–1350, 1354, 1361, 1364, 1371, 1375, 1375a, 1375b, 1377, 1378, 1416, 1418, 1419, 1427, 1437, 1586, 1589, 1590, 1634, 1649, 1666, 1949, 1958, 1960, 1971, 2079, 2088, 2089, 2170, 2200, 2270, 2337, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2573–2375, 2591, 2604, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 2887, 2939, 3106, 3127, 3187, 3190, 3255, 3257, 3300, 3302, 3308, 3324, 3397, 3410, 3462, 3530, 3553, 3555, 3557, 3559, 3648, 3653, 3795, 3822, 3826, 3913, 3992, 4079, 4159, 4202, 4259, 4319, 4378, 4407, 5034, 5073, 5079 5099, 5100, 5124, 5140, 5359, 5420, 5770, 5811b, 5835	120, 404, 524, 568b, 965, 984, 1063–1066, 1068–1074, 1550, 1590, 1590a, 1949, 2079, 2337, 2339a, 2386, 2389, 2544, 2860a, 2917a, 2939, 3188, 3194, 3547, 3555, 3626, 3648, 3873, 3973, 3974a, 4202, 4249, 5073, 5079, 5132, 5234, 5303, 5811b	1228, 1354, 1375a, 1377, 1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404
125.		2-Furancarboxaldehyde, hydroxy-	1375a, 1377		1375a, 1377
126.	25376-49-2	2-Furancarboxaldehyde, (hydroxymethyl)-		924, 2939, 4249	
127.	26895-04-5	2-Furancarboxaldehyde, methyl-	297, 2506, 2507, 2767, 4249, 5034, 5811b		2506 (0), 2507 (0), 3402, 3404
128.	33342-48-2	2-Furancarboxaldehyde, 3-methyl-	568b, 1357, 4249		
129.	32529-53-6	2-Furancarboxaldehyde, 5-acetyl-	568b, 1140, 2570, 4249	568b, 2389, 2544, 3547, 4249, 5811b	
130.	10551-58-3	2-Furancarboxaldehyde, 5-[(acetyloxy)methyl]-	5811b	404, 3557, 4249	
131.	23074-10-4	2-Furancarboxaldehyde, 5-ethyl-	5811, 5811a, 5811b		
132.	67-47-0	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	341, 568b, 722, 723, 924, 1063–1066, 1068–1074, 1350, 1354, 1360, 1364, 1365, 1371, 1375a, 1377, 1882, 1958, 1960, 2337, 2387, 2493, 2543, 2545, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 2939, 3302, 3308, 3397, 3410, 3462, 3530, 3553, 3557, 3559, 4159, 4163, 4249, 4378, 4379, 4407, 5034, 5811b	120, 568b, 965, 984, 2337, 2389, 2544, 2722, 2860a, 2930, 2917a, 2939, 3194, 3430, 3547, 3549, 3797, 3973, 3974a, 4249, 5811b	1354, 1375a, 1360, 1375a, 1377, 2387, 3393, 3401, 3402, 3404, 3405
133.	21300-07-2	2-Furancarboxaldehyde, 5-methoxy-		3823, 4249	
134.		2-Furancarboxaldehyde, 5-methoxy-?-methyl-		833, 4249	3402, 3404
135.	1917-64-2	2-Furancarboxaldehyde, 5-(methoxymethyl)-	3404, 4249		

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

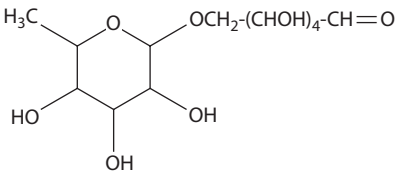
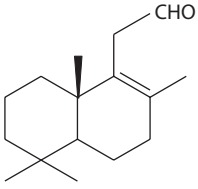
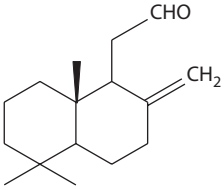
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
136.	620-02-0	2-Furancarboxaldehyde, 5-methyl-	156, 157, 299, 568b, 722, 775, 1099, 1140, 1215, 1364, 1365, 1337, 1339, 1360, 1371, 1375, 1375a, 1375b, 1378, 1427, 1590, 1949, 1971, 2337, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2628, 2629, 2636, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 3302, 3397, 3410, 3530, 3553, 3555, 3557, 3648, 3795, 3797, 3826, 4104, 4159, 4249, 4407, 5073, 5811b	120, 404, 524, 568b, 965, 984, 1063–1066, 1068–1074, 1590, 1590a, 1949, 2337, 2386, 2389, 2544, 2860a, 2917a, 2939, 3188, 3430, 3543, 3547, 3555, 3560, 3561, 3648, 3797, 3974a, 4249, 5073, 5811b	1360, 1375a, 1378, 2387, 2506, 2507, 3401, 3402, 3404
137.		2-Furancarboxaldehyde, 5-(2-phenylethenyl)-	568b, 4249	568b, 4249	
138.	498-60-2	3-Furancarboxaldehyde	299, 568b, 1063–1066, 1068–1074, 2506, 2507, 2545, 2731, 2735, 3255, 3559, 4249, 5811b	404, 568b, 4249, 5811b	2244, 2506, 2507, 3401, 3402, 3404
139.	823-82-5	2,5-Furandicarboxaldehyde	568b, 1364, 3553, 4249	568b, 3547, 4249	3401
140.	90-74-4	*D*-Glucose, 6-*O*-(6-deoxy-α-*L*-mannopyranosyl)- {rutinose} 		1971, 5777, 5811	
141.	56797-42-3	8,11-Heptadecadienal, (*Z,Z*)-		4249, 4609	
142.	629-90-3	Heptadecanal $H_3C\text{-}(CH_2)_{15}\text{-}CH{=}O$		2094, 4249	
143.	56797-44-5	8,11,14-Heptadecatrienal, (*Z,Z,Z*)-		4249, 4609	
144.	4313-03-5 5910-85-0	2,4-Heptadienal $O{=}CH\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}O$		172a, 174b, 404, 568b, 937, 1053, 1854, 2389, 2544, 2917a, 3266, 3370, 3547, 4249, 5811b	
145.	111-71-7	Heptanal $H_3C\text{-}(CH_2)_5\text{-}CH{=}O$	568b, 1238, 4249, 4434		
146.	2363-85-1	Heptanal, 2-oxo- $H_3C\text{-}(CH_2)_4\text{-}CO\text{-}CH{=}O$	568b, 4249		
147.	2463-63-0	2-Heptenal $H_3C\text{-}(CH_2)_3\text{-}CH{=}CH\text{-}CH{=}O$		404, 1053, 3266	4249, 4856
148.	30567-26-1	2-Heptenal, 2-methyl- $H_3C\text{-}(CH_2)_3\text{-}CH{=}C(CH_3)\text{-}CH{=}O$	642, 4249		
149.	6728-31-0	4-Heptenal $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}(CH_2)_2\text{-}CH{=}O$		172a, 174b, 1053, 3266, 4249	
150.	629-80-1	Hexadecanal $H_3C\text{-}(CH_2)_{14}\text{-}CH{=}O$		2094, 4249	
151.	80466-34-8	2,4-Hexadienal	4570a, 5811b	1157, 2041a, 4249, 5811b	
152.	142-83-6	2,4-Hexadienal, (*E,E*)-	568b, 3559, 4249	321a, 568b, 4249	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
153.	66-25-1	Hexanal {caproic aldehyde} H_3C-$(CH_2)_4$-CH═O	568b, 1140, 1238, 1416, 1418, 1419, 2270, 2337, 2939, 3266, 3302, 3308, 3452, 3797, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 1053, 1550, 1615, 1893b, 2337, 2339b, 3186, 3188, 3266, 3370, 3973, 4249	
154.	15303-46-5	Hexanal, 2-(1-methylethyl)-5-oxo-		568b, 2917a, 3547, 4249	
155.	2363-84-0	Hexanal, 2-oxo- H_3C-$(CH_2)_3$-CO-CH═O	3902, 4249		
156.	25346-59-2	Hexanal, 4-oxo- H_3C-CH_2-CO-$(CH_2)_2$-CH═O		1980	
157.	1335-39-3	Hexenal		1824a, 2339a, 5811b	
158.	505-57-7	2-Hexenal H_3C-$(CH_2)_2$-CH═CH-CH═O	568b, 2444, 3266, 3559, 4249, 5811b	174b, 404, 568b, 1590a, 2339b, 2917a, 3188, 3266, 4249	
159.	6728-26-3	2-Hexenal, (*E*)-	568b, 2444, 3266, 4249	172a, 568b, 1053, 1157, 3266, 3370, 4249, 5811b	
160.	16635-54-4	2-Hexenal, (*Z*)-	2444, 3559, 4249	1157, 3266, 4249	
161.		2-Hexenal, 2,5-dimethyl-	4570a		
162.	28467-88-1	2-Hexenal, 2-methyl- H_3C-$(CH_2)_2$-CH═C(CH_3)-CH═O	1374, 4249, 4570a		
163.		2-Hexenal, 5-methyl-	4570a		
164.	21834-92-4	2-Hexenal, 5-methyl-2-phenyl-		1053, 3266, 3370	
165.	10111-08-7	1*H*-Imidazole-2-carboxaldehyde	568b, 4249		
166.	37414-44-1	1*H*-Indene-2-carboxaldehyde, 2,3-dihydro-	2769, 4249		
167.	30084-91-4	1*H*-Indene-5-carboxaldehyde, 2,3-dihydro-	568b, 2767, 4249		
168.	487-89-8	1*H*-Indole-3-carboxaldehyde		568b, 3879a, 4249, 4468	
169.	68985-11-5	1-Naphthaleneacetaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-,(4aS-*trans*)- 		947, 1156, 4090, 4249	
170.	3243-36-5	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-methylene-,[1S-(1α,4aβ,8aα)]- 		947, 1156, 2338, 4090, 4249	
171.	68982-27-4	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-oxo-, [1R-(1α,4aβ,8aα)]-		4249	

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

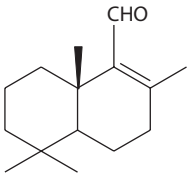
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
172.	68985-10-4	1-Naphthalenecarboxaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)- 		947, 1156, 4090, 4249	
173.	6750-03-4 5910-87-2	2,4-Nonadienal, (*E,E*)-	568b, 1144, 4249	568b, 3547, 4249, 5811b	
174.		2,4-Nonadienal, 6-methyl-		568b, 3547, 4249	
175.		2,4-Nonadienal, 8-methyl-		3547, 4249	
176.	26370-28-5	2,6-Nonadienal {leaf aldehyde violet}		404, 568b, 3547, 4249	
177.	557-48-2	2,6-Nonadienal, (*E,Z*)-		1053, 2336, 3266, 3370, 3547, 4249, 5811b	
178.	129777-21-5	2,6-Nonadienal, 2-methyl-5-(1-methylethyl)-8-oxo-, (*E,E*)-(+)-		4249, 5811b	
179.	124-19-6	Nonanal {pelargonaldehyde} $H_3C\text{-}(CH_2)_7\text{-}CH{=}O$	568b, 1238, 4249, 5811b	172a, 174b, 568b, 1053, 2282, 3153, 3266, 3370, 3547, 4249, 5811b	
180.	2463-53-8	2-Nonenal $H_3C\text{-}(CH_2)_5\text{-}CH{=}CH\text{-}CH{=}O$	568b, 3255, 4249	404, 568b, 1053, 2336, 3153, 3266, 3547, 3550, 3850, 4249	
181.	18829-56-6	2-Nonenal, (*E*)-		404, 1053, 2336, 3153, 3205, 3266, 4249, 4332, 5811b	
182.		2-Nonenal, 2,3-dimethyl-8-oxo-		2917a	
183.	2277-19-2	6-Nonenal, (*Z*)-		4249, 5811b	
184.	56554-87-1	16-Octadecenal		404	
185.	141-27-5 5392-40-5	2,6-Octadienal, 3,7-dimethyl-{citral}	278, 568b, 3266, 4249, 5811	172a, 174b, 568b, 1053, 3266, 3370, 5811	
186.	106-26-3	2,6-Octadienal, 3,7-dimethyl-, (*Z*)-	568b, 4249		
187.	124-13-0	Octanal $H_3C\text{-}(CH_2)_6\text{-}CH{=}O$	568b, 1238, 4249, 5770, 5811b	172a, 174b, 404, 568b, 1053, 3266, 3370	
188.		Octanal, 2,7-dimethyl-7-hydroxy-		568b, 4249	
189.	107-75-5	Octanal, 3,7-dimethyl-7-hydroxy-{hydroxycitronellal}		172a, 174b, 568b, 1053, 3266, 4249	
190.	2548-87-0	2-Octenal		1053, 3266	
191.	73757-28-5	2-Octenal, 2-propyl-		568b, 4249	
192.		2-Octenal, 4-(1-methylethyl)-		3547, 4249	
193.	106-23-0	6-Octenal, 3,7-dimethyl-{citronellal} $(H_3C)_2{=}C{=}CH\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH{=}O$	568b, 1238, 3193, 3266, 3302, 4249	174b, 568b, 1156, 2917a, 3266, 4090	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
194.	102673-27-8	4,9-Pentadecadienal, 6-(acetyloxy)-8-hydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4E,6R*,8R*,9E,11S*)]-		4249	
195.	95360-16-0	4,9-Pentadecadienal, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4E,6R*,8S*,9E,11S*)]-		4249	
196.	2765-11-9	Pentadecanal $H_3C\text{-}(CH_2)_{13}\text{-}CH{=}O$		568b, 937, 2095, 3547, 4249	
197.	68982-28-5	Pentadecanal, 2-ethylidene-6,10,14-trimethyl- H-$[CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_2]_3\text{-}CH_2\text{-}CH(=CH\text{-}CH_3)\text{-}CH{=}O$		947, 1156, 4090, 4249	
198.	764-40-9	2,4-Pentadienal $H_2C{=}CH\text{-}CH{=}CH\text{-}CH{=}O$	1140, 1419, 2767, 4249, 5811b	5811b	
199.	110-62-3	Pentanal {valeraldehyde} $CH_3\text{-}(CH_2)_3\text{-}CH{=}O$	568b, 605, 1039, 1140, 1238, 1365, 1374, 1375, 1375b, 1412–1414, 1416, 1418, 1419, 1615, 2002, 2337, 2573–2575, 2782, 2804, 2887, 3254, 3266, 3302, 3308, 3413, 3557, 3797, 3817, 4249, 4319, 4570a, 5811b, 5896	172a, 174b, 404, 568b, 1053, 1550, 1615, 1893b, 2337, 2914, 3186, 3188, 3266, 3370, 3547, 3626, 3797, 3973, 3974a, 4223, 4225, 4249, 5811b, 5896	
200.		Pentanal, methyl-	2782, 2804		
201.	123-15-9	Pentanal, 2-methyl- $CH_3\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}CH{=}O$	568b, 1140, 2337, 2543, 2773, 2782, 3219, 3302, 3308, 3797, 4249, 4570a		
202.	15877-57-3	Pentanal, 3-methyl-	4570a, 5811b		
203.	1119-16-0	Pentanal, 4-methyl- $CH_3\text{-}CH(CH_3)\text{-}(CH_2)_2\text{-}CH{=}O$	2575, 4249, 4570a		
204.	7332-93-6	Pentanal, 2-oxo- $CH_3\text{-}(CH_2)_2\text{-}CO\text{-}CH{=}O$	1238, 3902, 4249		
205.	626-96-0	Pentanal, 4-oxo- $CH_3\text{-}CO\text{-}(CH_2)_2\text{-}CH{=}O$	3988a, 5811b		3402, 3404, 3405, 4249
206.	31424-04-1	Pentenal	642, 4249		
207.	764-39-6	2-Pentenal	4249	429b, 5811b	
208.	1576-87-0	2-Pentenal, (*E*)-	568b, 4249		
209.		2-Pentenal, 2,3-dimethyl-	4570a		
210.		2-Pentenal, 2,4-dimethyl-	4570a		
211.		2-Pentenal, methyl-	5034, 5770		
212.	623-36-9	2-Pentenal, 2-methyl-	568b, 1075, 2506, 2507, 3797, 4249, 4570a, 5770, 5811b		2506 (0), 2507 (0)
213.	5362-56-1	2-Pentenal, 4-methyl-	4570a	2917a	
214.	5604-55-7	3-Pentenal		4092, 4249	
215.	53448-06-9	3-Pentenal, (*Z*)-		568b, 4249	
216.	5187-71-3	4-Pentenal, 2-methyl-	568b, 1140, 1419, 4249		
217.	3973-43-1	4-Pentenal, 4-methyl-		3797, 4249	
218.	71635-28-4	1-Piperidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)-		568b, 1156, 2497, 2566, 2567, 4090, 4249, 5811b	

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
219.	123-38-6	Propanal {propionaldehyde} $H_3C\text{-}CH_2\text{-}CH{=}O$	172, 174a, 174b, 174c, 174e, 299, 314, 405, 407, 408, 480, 564, 568b, 591, 605, 639, 688, 722, 764a, 778, 830a, 929, 1050, 1063–1074, 1140, 1167, 1168, 1238, 1239, 1284, 1348–1351, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1415, 1418, 1419, 1445, 1449, 1495, 1586, 1589, 1668, 1853b, 1875, 1966, 2003, 2079, 2089, 2091, 2134a, 2144, 2270, 2310, 2313a, 2337, 2506, 2507, 2519, 2520, 2525, 2543, 2545, 2570, 2573–2575, 2591, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2887, 2927, 2939, 3007, 3105, 3132, 3135, 3136, 3190, 3254, 3257, 3300, 3302, 3308, 3396, 3431, 3436, 3438, 3482, 3530, 3557, 3583, 3584, 3817, 3901, 3940, 3992, 4052, 4056, 4078, 4104, 4135, 4162, 4249, 4290, 4304, 4319, 4570a, 5006, 5028, 5065, 5069, 5811b, 5835, 5836, 5869a	568b, 1550, 1893b, 2337, 2914, 2939, 3350, 3626, 3797, 3829e, 3973, 3974a, 4223, 4249, 5811b, 5896	1228, 1354, 1375a, 1377, 1378, 2244, 2506, 2507, 4052, 4056
220.	630-19-3	Propanal, 2,2-dimethyl- {pivalaldehyde} $(H_3C)_3{\equiv}C\text{-}CH{=}O$	568b, 1140, 1413, 1414, 1416, 1418, 1419, 1422, 2767, 2782, 2804, 3255, 3308, 3436, 4249, 4319, 5811b		
221.	367-47-5	Propanal, 2,3-dihydroxy- {glyceraldehyde} $HOCH_2\text{-}CH_2OH\text{-}CH{=}O$	1238, 5811b	3973, 5811b	
222.	142-10-9	Propanal, 2,3-dihydroxy-, 3-phosphate		555b	
223.	78-84-2	Propanal, 2-methyl-{isobutyraldehyde} $(H_3C)_2{=}CH\text{-}CH{=}O$	111, 299, 314, 605, 1038, 1039, 1063–1066, 1068–1074, 1140, 1238, 1284, 1338, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1412–1414, 1415, 1418, 1419, 1495, 1586, 1589, 1634, 1875, 2002, 2003, 2270, 2293, 2301, 2310, 2313a, 2337, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 2782, 2804, 2939, 3105, 3132, 3254, 3257, 3266, 3302, 3308, 3396, 3413, 3557, 3793, 3817, 3901, 3935, 4052, 4056, 4104, 4162, 4249, 4290, 4319, 4570a, 5770, 5811b	120, 172a, 174b, 984, 1053, 1157, 1550, 2282, 2293, 2337, 2339a, 2860a, 2914, 2939, 3186, 3188, 3194, 3266, 3350, 3370, 3626, 3797, 3935, 3974a, 4223, 4225, 4249, 5811b, 5896	1354, 1375a, 1377, 1378, 2244, 2506, 2507, 4052, 4056
224.	1646-87-3	Propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb Sulfoxide}		1280, 2650a, 4249, 4271a, 5811b	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

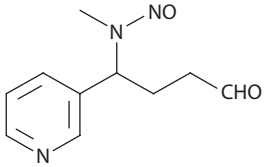
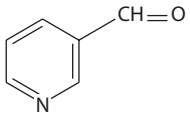
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
225.	78-98-8	Propanal, 2-oxo-{pyruvaldehyde; methylglyoxal} H_3C-CO-CH═O	568b, 1238, 1239, 1491, 2270, 2337, 2939, 3251, 3266, 3302, 3341, 3515, 3553, 4079, 4249, 5680, 5811b	120, 568b, 826a, 2153b, 2337, 2939, 3266, 3797, 3974a, 4079 4249, 5079, 5811b	1228, 4249
226.		Propanal, 2-oxo-3-hydroxy-{reductone} $HOCH_2$-CO-CH═O		3797	
227.	2134-29-4	Propanal, 3-hydroxy-	5034		
228.	3268-49-3	Propanal, 3-(methylthio)-{methional}	568b, 1365, 3255, 3266, 3854, 4249, 5770	174b, 568b, 1053, 3266, 4249	
229.	85502-23-4	Propanal, 3-(nitrosomethylamino)- CH_3-N(NO)-$(CH_2)_2$-CHO		2791	
230.	542-78-9	Propanedial H_2C═$(CHO)_2$	1256a, 4249, 4732, 4968, 5811b		
231.	4464-20-4	Propanedial, dihydroxy- $(HO)_2$═C═$(CH$═$O)_2$		4249, 4946	
232.	497-16-5	Propanedial, oxo- O═C═$(CHO)_2$		120, 2939, 3797, 4249	1377, 4249
233.	107-02-8	2-Propenal {acrolein} H_2C═CH-CH═O	83, 111, 112, 126a, 126b, 126d, 172, 173a, 174a, 174b, 174c, 174e, 203, 213, 237, 239, 270, 280, 314, 299, 329, 337, 376, 402, 405, 407, 408, 480, 491, 494, 495, 568b, 591, 603, 639, 645, 688, 722, 748, 764a, 778, 830a, 860, 915, 929, 1023, 1039, 1048, 1050, 1051, 1063–1074, 1099, 1140, 1148, 1153, 1167, 1168, 1217, 1238, 1283, 1284, 1329–1334, 1336, 1338, 1348–1351, 1354, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412, 1413, 1416, 1418, 1419, 1437, 1442, 1449, 1487, 1489, 1492, 1495–1497, 1586, 1589, 1634, 1637, 1638, 1673, 1674, 1709, 1727, 1741, 1744, 1760, 1773, 1781, 1803, 1807a, 1829, 1840, 1842, 1870, 1871, 1875, 1947, 1956, 2063, 2070, 2079, 2083–2085, 2091, 2131, 2133, 2134a, 2170, 2252, 2270, 2296, 2301, 2302, 2304, 2305, 2313a, 2337, 2411, 2452, 2506, 2507, 2520, 2524, 2537, 2543, 2545, 2558, 2570, 2591, 2601b, 2634, 2644, 2683, 2761, 2762, 2765, 2767, 2775, 2777, 2781, 2782, 2800, 2804, 2822, 2857, 2927, 2939, 3007, 3087, 3088, 3116, 3126, 3131, 3132, 3135, 3136, 3145, 3169, 3187, 3190, 3251,	568b, 2337, 3974a, 4249, 5053, 5811b	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 2244, 2506, 2507, 3401, 4052, 4056

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		2-Propenal {acrolein} (cont.)	3254, 3255, 3257, 3264, 3265, 3300, 3302, 3308, 3370, 3396, 3441a, 3482, 3493, 3530, 3551, 3557, 3577, 3692, 3844, 3871, 3880, 3882, 3883, 3885, 3897, 3901, 3976, 3984, 3992, 4005–4007, 4010, 4011, 4052, 4056, 4078, 4104, 4159, 4162, 4249, 4257, 4259, 4288, 4290, 4301, 4319, 4330, 4360, 4418, 5006, 5022, 5028, 5034, 5065, 5070, 5079, 5490, 5512, 5531, 5547, 5554, 5556, 5583, 5811b, 5836, 5869a, 3A08, 3A17, 3A25		
234.	636-38-4	2-Propenal, 2,3-dihydroxy-		3797, 4249	
235.	78-85-3	2-Propenal, 2-methyl-{methacrolein} $H_2C{=}C(CH_3)$-CH=O	173a, 299, 314, 405, 407, 408, 605, 1063–1066, 1068–1074, 1140, 1238, 1365, 1374, 1412–1414, 1416, 1418, 1419, 2545, 2559, 2559a, 2767, 2782, 2804, 2927, 3255, 3302, 3308, 3557, 3559, 3973, 4005–4007, 4249, 4319, 5034, 5811b	984, 1550	2244, 3401
236.	31704-79-7	2-Propenal, 2-methyl-3-(5-methyl-2-furanyl)-	568b, 1587, 4249, 5811b		
237.	101-39-3	2-Propenal, 2-methyl-3-phenyl-		1053, 3266	
238.	79407-66-2	2-Propenal, 3-(2,4-dihydroxyphenyl)-		3748, 3749, 3751, 4249	
239.	874-66-8	2-Propenal, 3-(2-furanyl)-2-methyl-	1587, 4249, 5811b		
240.	1504-74-1	2-Propenal, 3-(2-methoxyphenyl)-		568b, 4249	
241.	104-55-2	2-Propenal, 3-phenyl-{cinnamaldehyde}	568b, 1039, 1238, 3193, 3266, 3302, 4249	568b, 1053, 2389, 2544, 2611, 3193, 3266, 3370, 3975, 4249	
242.	14371-10-9	2-Propenal, 3-phenyl-, (*E*)-{*trans*-cinnamaldehyde}		429b	
243.	122-40-7	2-Propenal, 3-phenyl-, α-pentyl-		172a, 174b, 1053, 3266	
244.	100-73-2	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro-{acrolein dimer}	568b, 1587, 3169, 4249, 5811b	404, 568b, 4249	
245.	70898-35-0	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro-6-hydroxy-3-oxo-	1378	2939, 3797, 4249	1378
246.	5780-66-5	Pyrazinecarboxaldehyde	1062, 4249		
247.		Pyrazinecarboxaldehyde, 5-(2-furanyl)-3-methyl-		568b, 3547, 4249	
248.	1121-60-4	2-Pyridinecarboxaldehyde	568b, 4249, 5811b		
249.	42545-63-1	3-Pyridineacetaldehyde	568b, 1371, 4249		
250.	70898-37-2	3-Pyridinebutanal, γ-(methylamino)-		553, 2226, 4249	
251.	64091-90-3	3-Pyridinebutanal, γ-(methylnitrosoamino)-{NNA}	772, 1568, 1584, 4249	554, 772, 1565, 1584, 3973, 3974b, 5577, 5811b	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
252.	64142-45-6	3-Pyridinebutanal, γ-(methylnitrosoamino)-, (*Z*)- 	1012, 1563–1566, 1567a, 1569, 1702, 1751, 3256, 3491, 4249	466, 992, 1012, 1563–1565, 1567a, 1569, 1576, 1577, 1567a, 1702, 3491, 4249	
253.	76014-80-7	3-Pyridinebutanal, γ-oxo-		4249	
254.	500-22-1	3-Pyridinecarboxaldehyde {nicotinaldehyde; 3-formylpyridine} 	568b, 1078, 1364, 1371, 2228, 2545, 2724, 2775, 2939, 3302, 3308, 3491, 3499, 3505, 3967, 4249, 5034, 5811b	568b, 937, 2359, 2389, 2544, 2917a, 3491, 4249, 5811b, 17B07, 17B08, 17B33, 17B34, 17B37, 17B48	
255.	89145-04-0	1*H*-Pyrrolecarboxaldehyde		3905, 4249	
256.	78249-88-4	1*H*-Pyrrole-1-carboxaldehyde, 1-methyl-	5811, 5811a, 5811b		
257.		1*H*-Pyrrole-2-acetaldehyde, α-hydroxy-	1587, 4249		
258.	72693-01-7	1*H*-Pyrrole-2-acetaldehyde, α-oxo-	568b, 1587, 4249, 5811b		
259.	1003-29-8	1*H*-Pyrrole-2-carboxaldehyde	568b, 1075, 1360, 1371, 1375a, 1586, 1587a, 1590, 2337, 2387, 2545, 2570, 2761, 2765–2767, 2773, 2775, 2777, 3255, 3410, 3491, 3553, 3557, 3650, 4249, 5811b	404, 568b, 937, 965, 1590, 2282, 2337, 2386, 2389, 2544, 2917a, 3198, 3219, 3491, 3547, 3549, 3550, 3905, 3974a, 4249	1360, 1375a, 2387
260.	13788-32-4	1*H*-Pyrrole-2-carboxaldehyde, 1-(2-furanylmethyl)-		404, 568b, 3547, 3555, 4249	
261.	13678-79-0	1*H*-Pyrrole-2-carboxaldehyde, 1-(3-methylbutyl)-		568b, 937, 3491, 4249, 5811b	
262.		1*H*-Pyrrole-2-carboxaldehyde, ethyl-	1364, 1371		
263.	2167-14-8	1*H*-Pyrrole-2-carboxaldehyde, 1-ethyl-	568b, 2767, 3410, 4249		
264.		1*H*-Pyrrole-2-carboxaldehyde, methyl-	1370, 4249	2386, 4249	
265.	1192-58-1	1*H*-Pyrrole-2-carboxaldehyde, 1-methyl-	568b, 1587, 1587a, 1590, 2337, 2767, 3555, 4159	568b, 937, 965, 2337, 2339a, 2386, 2389, 2544, 3203, 3205, 3219, 3491, 3547, 3555, 3905	
266.	29813-44-3	1*H*-Pyrrole-2-carboxaldehyde, 5-(hydroxymethyl)-1-methyl-	568b, 1587, 4249, 5811b	404, 568b, 4249	
267.	52115-69-2	1*H*-Pyrrole-2-carboxaldehyde,5-[(acetyloxy)methyl]-		4249	
268.	1192-79-6	1*H*-Pyrrole-2-carboxaldehyde, 5-methyl-	568b, 1375, 1375b, 1586, 1587a, 2337, 2387, 2543, 2545, 2767, 2773, 3553, 3555, 3557, 4159, 4249	404, 568b, 2337, 2389, 2544, 3203, 3205, 3219, 3491, 3543, 3547, 3555, 3560, 3561, 4249	2387
269.	17619-39-5	1*H*-Pyrrole-3-carboxaldehyde, 2-methyl-	568b, 1371, 1586, 2543, 2767, 2773, 3410, 3553, 4249, 5811b	568b, 2544, 3549, 3550, 4249, 5811b	
270.	103002-58-0	1*H*-Pyrrole-3-carboxaldehyde,4,5-dihydro-2-methyl-		4159b, 4249	
271.	78210-62-5	1*H*-Pyrrole-3-carboxaldehyde, 5-ethyl-	568b, 1587, 4249, 5811b		
272.	3760-54-1	1-Pyrrolidinecarboxaldehyde	568b, 1371, 2543, 2773, 2775, 3410, 3553, 4249, 5811b	404, 568b, 2389, 2544, 3491, 4249, 5811b	

(*continued*)

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

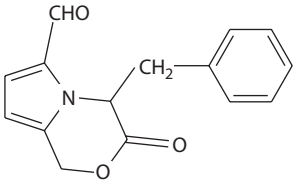
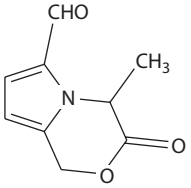
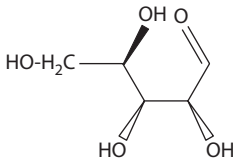
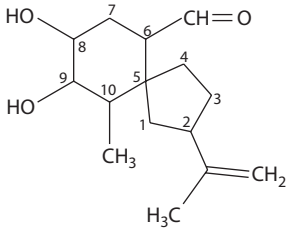
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
273.	78914-62-2	1-Pyrrolidinecarboxaldehyde, 2-methyl-, (R)-	568b, 3553, 4249	568b, 2544, 4249	
274.	38840-03-8 3000-81-5	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-,(S)-{*N*′-formylnornicotine}	568b, 830a, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 1586, 2601a, 2761, 2762, 2765–2767, 2777, 3255, 3410, 3553, 3739–3742, 4249, 4407, 5811b	64, 568b, 689, 994, 2359, 2952, 3491, 3549, 3550, 3742, 3973, 4133, 4249	1360, 1375a
275.	61480-98-6	2-Pyrrolidinecarboxaldehyde		568b, 4249, 4249	
276.	60026-15-5	3-Pyrrolidinecarboxaldehyde, 2-methyl-		2389, 2544, 3491, 4249	
277.	60026-28-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-3-oxo-4-(phenylmethyl)- 		965, 2337, 2389, 2544, 3491, 4249	
278.	35674-33-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-4-methyl-3-oxo- 		965, 2544, 3491, 4249, 5811b	
279.	2739-16-4	1(2*H*)-Quinolinecarboxaldehyde, 3,4-dihydro-		2917a	
280.	4363-93-3	4-Quinolinecarboxaldehyde		2917a	
281.	3615-55-2	Ribose, 5-(dihydrogen phosphate)		429b, 4249, 4670	
282.	50-69-1	*D*-Ribose 	5580	120, 344a, 2939, 3075, 3254, 3797, 3973, 3974a, 4249, 5811b	
283.	24259-59-4	*L*-Ribose		3075	
284.	55784-90-2	Spiro[4.5]decane-6-carboxaldehyde, 8,9-dihydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,9α,10β]]- 		1156, 4090, 4249, 4608	

TABLE 3.12 (continued)
Aldehydes in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

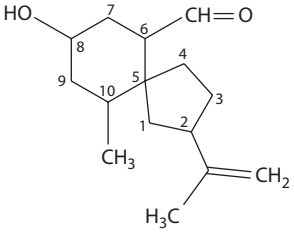
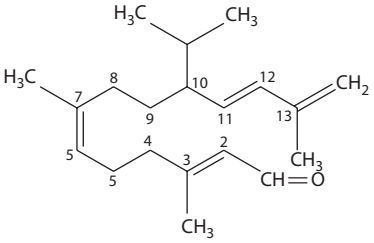
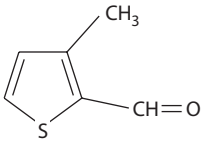
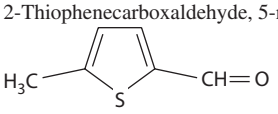
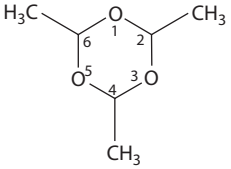
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
285.	35951-50-9	Spiro[4.5]decane-6-carboxaldehyde, 8-hydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,10β]]- 		1156, 4090, 4249, 4637	
286.	124-25-4	Tetradecanal {myristaldehyde} H_3C-$(CH_2)_{12}$-CHO	568b, 1366, 3266, 4249	404, 568b, 1053, 2093, 2094, 3266, 4249, 5811b	
287.	15371-32-1	2,6,11,13-Tetradecatetraenal, 3,7,13-trimethyl-10-(1-methylethyl)-, [S-(*E,E,E*)]- 		841, 943, 4089, 4249	
288.	125572-76-1	2,6,11,13-Tetradecatetraenal, 3,7,13-trimethyl-10-(1-methylethyl)-	4249, 5811b	9	
289.	98-03-3	2-Thiophenecarboxaldehyde	568b, 1360, 1375a, 2761, 4249	568b, 1590, 3547, 4249	1360, 1375a
290.	5834-16-2	2-Thiophenecarboxaldehyde, 3-methyl- 	568b, 2761, 2765, 2766, 3553, 4249, 5811b	568b, 937, 2389, 2544, 4249, 5811b	
291.	13679-70-4	2-Thiophenecarboxaldehyde, 5-methyl- 	568b, 1590, 2761, 2762, 2765, 2766, 2777, 3266, 4249, 4570a	568b, 937, 1053, 1590, 3266, 4249	
292.	10486-19-8	Tridecanal H_3C-$(CH_2)_{11}$-CH═O		568b, 2094, 4249	
293.	7774-82-5	2-Tridecenal		1053, 3266	
294.	123-63-7	1,3,5-Trioxane, 2,4,6-trimethyl- {paraldehyde; acetaldehyde trimer} 	156, 157, 568b, 4249		
295.	129970-88-3	5,9-Undecadienal, 6,10-dimethyl-2-methylene-		4249, 5811b	
296.	112-44-7	Undecanal	5811b	568b, 1053, 3266	
297.	112-45-8	10-Undecenal		1053, 3266	

TABLE 3.13
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

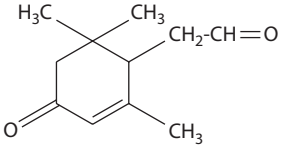
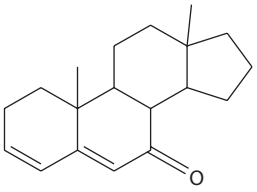
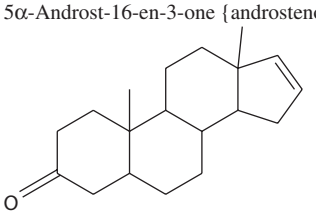
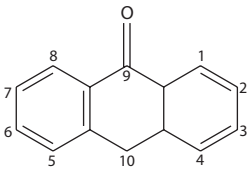
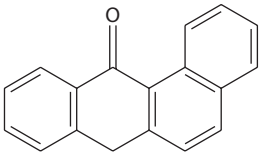
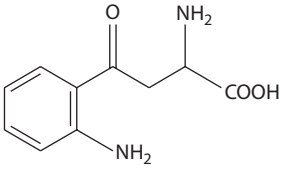
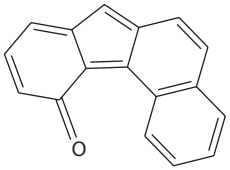
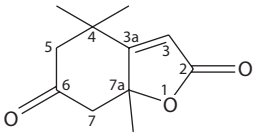
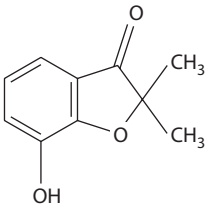
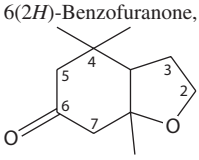
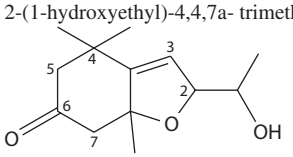
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	16825-04-0	Acetaldehyde,(2,6,6-trimethyl-4-oxo-2-cyclohexen-1-ylidene)- 		943, 2389, 2544, 3543, 3547, 5811b	
2.	7737-16-8	Acetamide, *N*-(2-oxopropyl)- CH_3-CO-NH-CH_2-CO-CH_3	568b, 3553, 4249, 5811b		
3.	32222-21-2	Androsta-3,5-dien-7-one 		2917a	
4.	18339-16-7	5α-Androst-16-en-3-one {androstenone} 		5811	
5.	90-44-8	9(10*H*)-Anthracenone (anthrone) 	278		
6.		Benz[*a*]anthrone 	1767a		
7.	343-65-7	Benzenebutanoic acid, α,2-diamino-γ-oxo-{kynurenine} 		4249	
8.	479-79-8	11*H*-Benzo[*a*]fluoren-11-one 	39		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
9.		1,3-Benzofurandione, 5-(1,1-dimethylheptyl)-	2601a		
10.	31297-30-0	2,3-Benzofurandione, 2,3-dihydro-4,7-dimethyl-	2601a		
11.	19355-58-9	2,6-Benzofurandione, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl- 		234, 1156, 1254, 1256, 3991, 4090, 4249, 5811b	
12.	124052-02-4	3(2*H*)-Benzofuranone, 2-(3,4-dihydroxyphenyl)-2,4,6-trihydroxy-		4249	
13.	17781-16-7	3(2*H*)-Benzofuranone, 7-hydroxy-2,2-dimethyl- 		5811, 5811b	
14.	117769-21-8	5(4*H*)-Benzofuranone, 2,7a-dihydro-2-(1-hydroxyethyl)-4,4-dimethyl-		4249, 5811b	
15.	39815-70-8	6(2*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl- 		037, 943, 1149, 1149a, 1156, 1254, 1256, 3206, 3210, 3218, 3219, 3550, 4090, 4249, 5811b	
16.	70875-03-5	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a- trimethyl- 		234, 1156, 1254, 1256 3206, 3210, 3218, 3549, 3991, 4090, 4249, 5811b	
17.	39815-73-1	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-		2544, 3219, 3549, 4249, 5811b	
18.	6136-68-1	Benzonitrile, 3-acetyl-	2767, 4249		
19.	124052-01-3	2*H*-1-Benzopyran-3,4-dione, 2-(3,4-dihydroxyphenyl)-2,5,7-trihydroxy-		4249	
20.	124052-00-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,3,5,7-tetrahydroxy-		4249	
21.	21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		120, 1626, 1837a, 1971, 2023, 2270, 2939, 3059, 3194, 3555, 3667, 3794, 3797, 3973, 3974a, 4249, 5079, 5255, 5256, 5724, 5747, 5811b, 5888	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

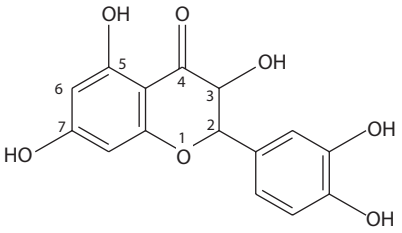
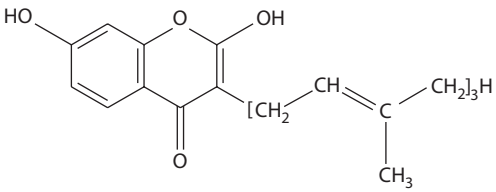
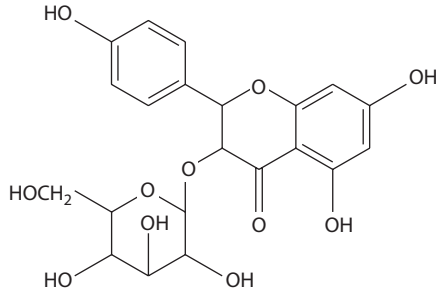
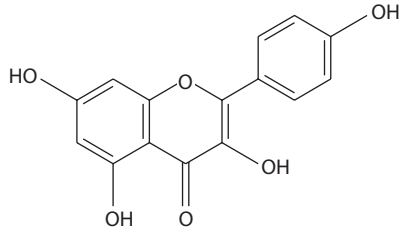
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
22.	117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin, 3,3a,4a, 5,7-pentahydroxyflavone 	3096, 3555	72, 120, 970, 1077b, 1837a, 2270, 2379, 2704a, 2939, 3059, 3462, 3555, 3685, 3794, 3797, 3974a, 4036, 4403, 4999, 5079, 5255, 5641, 5652, 5750, 5758, 5811b, 5904	
23.	7215-44-3 20188-84-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-O-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-{quercetin 3,3′-diglucoside}		4249, 5724, 5747, 5811, 5811b, 5888	
24.	1486-70-0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-methoxy-		3797, 3974a, 4249	
25.	2068-02-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5-hydroxy-3,7-dimethoxy-		3797, 3974a, 4249	
26.	491-50-9	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}		3797, 3974a, 4249	
27.	124051-99-6	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-[[2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,6-dihydroxy-3-oxo-4-benzofuranyl]oxy]-2,3-dihydro-3,5-dihydroxy-		4249	
28.	480-41-1	4*H*-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)- {naringenin}		970, 3797, 3974a, 4249	
29.	643-57-2	4*H*-1-Benzopyran-4-one, 2,7-dihydroxy-3-(3,7,11-trimethyldodeca-2,6,10-trienyl- {ammoresinol} 		3763, 5079	
30.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3,4-dihydroxyphenyl)- {3a,4a,5,7-tetrahydroxy-3-methylflavone}		4147, 5776, 5888	
31.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3-methyl-4-hydroxyphenyl)- {4a,5,7-trihydroxy-3,3a-dimethylflavone}		4147, 5888	
32.		4*H*-1-Benzopyran-4-one, 3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone}		5776	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
33.	480-10-4	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glucoside; 3,4a,5,7-tetrahydroxyflavone glucoside} 		120, 641, 830a, 835, 838, 840, 966, 970, 1626, 1971, 2023, 2270, 2939, 3059, 3161, 3555, 3646, 3738, 3797, 3974a, 4072a, 4249, 5079, 5724, 5753, 5758	
34.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5,7-tetrahydroxyflavone, 3-glucoside}		1625, 4147, 5353, 5724, 5834, 5888	
35.	57523-93-0	4*H*-1-Benzopyran-4-one, octahydro-2,5,5,7a-tetramethyl-		5811, 5811b	
36.	529-44-2	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(3,4,5- trihydroxyphenyl)- {myricetin}		5811, 5811b	
37.	520-18-3	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(4-hydroxyphenyl)- {kaempferol; 3,4a,5,7-tetrahydroxyflavone} 	2767, 3095a, 3555, 4249	1626, 1971, 2939, 3059, 3555, 3794, 4249, 5652, 5758	
38.	55136-76-0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
39.	142235-82-3	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2090b	
40.	19895-95-5	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
41.	522-12-3	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {quercetrin}	970	4036, 4249, 4573	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

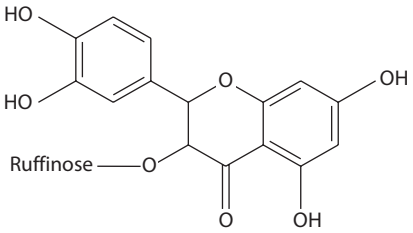
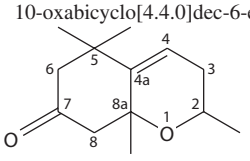
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
42.	55696-57-6	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-		4249	
43.	55804-74-5	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
44.	153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} 		69, 72, 120, 248, 385, 598, 828b, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1063–1066, 1068–1074, 1309, 1329, 1333, 1485, 1626, 1971, 2014, 2079, 2153a, 2270, 2313a, 2338, 2361, 2379, 2395, 2514, 2529, 2531, 2557a, 2704a, 2810–2812, 2939, 3059, 3096, 3161, 3367a, 3400, 3462, 3551, 3555, 3628, 3629, 3631, 3641, 3646, 3700, 3705, 3738, 3767, 3794, 3974a, 3974b, 3984, 3999, 4005–4007, 4036, 4156, 4157, 4249, 4403, 4999, 5079, 5110, 5156, 5157, 5189, 5204, 5217, 5304, 5305, 5310, 5576, 5591, 5596, 5641, 5652, 5661, 5681, 5697, 5698, 5724, 5747, 5750, 5780, 5788, 5808, 5809, 5831, 5834, 5888, 5889	
45.	17650-84-9	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		1309, 4249	
46.	30311-61-6	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-		2023, 5888	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
47.	34336-18-0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-L-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
48.	29859-91-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
49.	27554-19-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxy phenyl)-		1309, 4249	
50.	58934-57-9	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl) glucosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy- 2-(4-hydroxyphenyl)-		4249	
51.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-glucoside}		4147, 5888	
52.		4*H*-1-Benzopyran-4-one, 7-(β-*D*-rhamnoglucopyranosyloxy)-3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone, 7-rhamnoglucoside}		4147, 5888	
53.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-rhamnoglucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-rhamnoglucoside}		3095a, 4372, 5888	
54.	828-82-0	4*H*-1-Benzopyran-4-one, 3-ethyl-	568b, 4249		
55.	520-34-3	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-{diosmetin}		120, 4249, 4959	
56.	4382-17-6	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-methoxy-		3797, 4249	
57.		4*H*-1-Benzopyran-4-one, hydroxy-	1586, 2767, 4249		
58.	38445-24-8	4*H*-1-Benzopyran-4-one, 6-hydroxy-	1586, 2767		
59.	10236-47-2	4*H*-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}		970, 1305b, 3797, 3974a, 4249	
60.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,5′, 7-pentahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2023, 4249	
61.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,7-tetrahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		4249	
62.		5*H*-1-Benzopyran-7-one, 2,3,6,7,8,8a-hexahydro-2,5,5,8a-tetramethyl-		568b, 4249	
63.		7*H*-1-Benzopyran-7-one, 2,4a,5,6,8,8a-hexahydro-2,5,5,8a-tetramethyl-		404, 3547, 4249	
64.	20194-67-6	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-2,5,5,8a-tetramethyl- {1,5,5,9-tetramethyl-10-oxabicyclo[4.4.0]dec-6-en-3-one} 	297, 568b, 2767, 2769, 3557, 4249	568b, 937, 943, 1063–1066, 1068–1074, 1149, 1156, 1254, 1256, 1590a, 2338, 2339b, 2386, 2389, 2544, 2611, 3218, 3543, 3545, 3546, 3550, 3560, 3561, 4048, 4090, 4098a, 4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

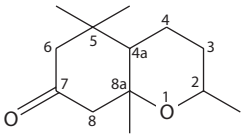
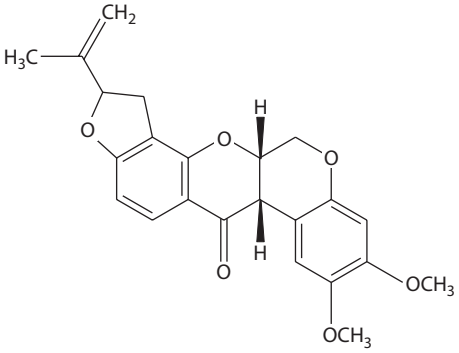
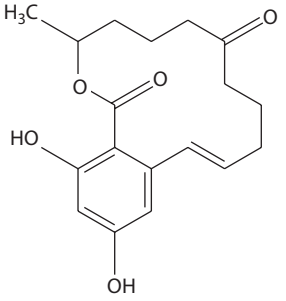
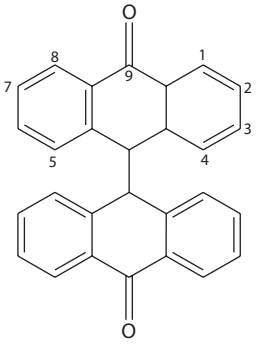
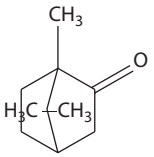
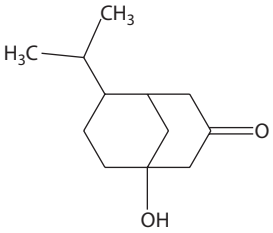
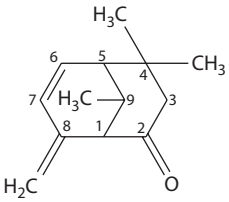
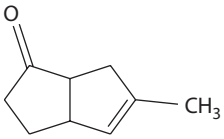
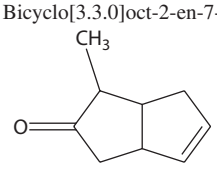
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
65.	52811-22-0	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-5,5,8a-trimethyl-	5811, 5811a, 5811b	5811, 5811a, 5811b	
66.	5835-18-7	7*H*-1-Benzopyran-7-one, octahydro-2,5,5,8a-tetramethyl- {7-chromanone, hexahydro-2,5,5,8a-tetramethyl-} 	568b, 1586, 2570, 2767, 2769	568b, 943, 1063–1066, 1068–1074, 1149, 1156, 1254, 1256, 1590a, 2282, 2338, 2339b, 2386, 2917a, 3205, 3218, 3223, 3545, 3550, 4090, 4098a	
67.	83-79-4	Benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6a*H*)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, [2R-(2α,6aα,12aα)]- {Rotenone®} 		3633, 3634, 21A14, 21A49	
68.	17924-92-4	1*H*-2-Benzoxacyclotetradecin-1,7(8*H*)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, [S-(*E*)]- 		4249	
69.	434-85-5	[9,9′-Bianthracene]-10,10′(9*H*,9′*H*)-dione {bianthrone; dianthraquinone} 	278, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
70.	1195-79-5	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-		3555	
71.	4695-62-9	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl- {*d*-fenchone}		1053, 3266	
72.	76-22-2	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- {camphor} 		568b, 1156, 1254, 1256, 2095, 2389, 2544, 4090, 4249, 5811b	
73.		Bicyclo[2.2.1]hept-2-ene, 5-acetyl- {ethanone, 1-bicyclo[2.2.1]hept-5-en-2-yl-}	5770		
74.	124749-69-5	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy- 6-(1-methylethyl)-, *endo*- 	4249		
75.	123695-64-7	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy- 6-(1-methylethyl)-, *exo*-	4249		
76.	61185-25-9	Bicyclo[3.3.1]non-6-en-2-one, 4,4,9-trimethyl- 8-methylene-, *anti*- 		945, 4249	
77.		Bicyclo[3.3.1]non-6-en-2-one, 4,9,9-trimethyl- 8-methylene-		945, 4249	
78.		Bicyclo[3.3.0]oct-2-en-6-one, 3-methyl- 	5770		
79.		Bicyclo[3.3.0]oct-2-en-7-one, 6-methyl- 	5770		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

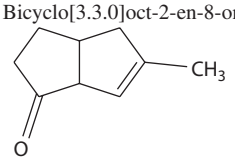
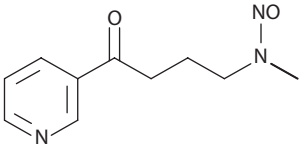
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
80.		Bicyclo[3.3.0]oct-2-en-8-one, 3-methyl- 	5770		
81.	70898-21-4	[2,3′-Bipyridin]-6′(1′*H*)-one, 3,4,5,6-tetrahydro-		4249	
82.		Butanal, 3-hydroxy-2-oxo- {methylreductone} H_3C-CHOH-CO-CH═O		3797, 4249	
83.	4417-81-6	Butanal, 2-oxo- {ethylglyoxal} H_3C-CH_2-CO-CH═O	1238, 3902, 4249		
84.	328-42-7	Butanedioic acid, oxo- {oxalacetic acid} HOOC-CO-CH_2-COOH		120, 3797, 3973	
85.	1438-90-0	1,2-Butanedione, 1-(2-furanyl)-	568b, 4249		
86.	431-03-8 29350-67-2	2,3-Butanedione {diacetyl; biacetyl} H_3C-CO-CO-CH_3	111, 112, 314, 480, 568b, 605, 966, 1140, 1067, 1153, 1231, 1232, 1238, 1239, 1348–1352, 1354, 1374, 1375, 1375a, 1375b, 1377, 1378, 1416, 1418, 1419, 1491, 1586, 1587, 1589, 1637, 1884, 1947, 1966, 2063, 2079, 2091, 2170, 2220, 2270, 2293, 2310, 2337, 2469, 2506, 2507, 2543, 2545, 2559, 2559a, 2570, 2704, 2765, 2767, 2775, 2777, 2782, 2804, 2822, 2857, 2866, 2939, 3059, 3105, 3254, 3255, 3266, 3300, 3302, 3308, 3341, 3413, 3475, 3557, 3794, 3876, 3897, 4005–4007, 4052, 4056, 4249, 4257, 4259, 4319, 4360, 4570a, 4732, 5034, 5079, 5680, 5811b, 5835	120, 174b, 568b, 1053, 1550, 2283, 2293, 2337, 2339a, 2704, 3186, 3188, 3266, 3561, 4249, 5079, 5371, 5372, 5811b	1354, 1375a, 1377, 1378, 2244, 2506, 2507, 3401, 3404, 4052, 4056
87.	597-04-6	Butanoic acid, 2,2-dimethyl-3-oxo-		568b, 4249	
88.	600-18-0	Butanoic acid, 2-oxo- H_3C-CH_2-CO-COOH	3302, 4249	1312	
89.		Butanoic acid, 3-methyl-, 4-oxopentyl ester	568b, 4279		
90.	541-50-4	Butanoic acid, 3-oxo- {acetoacetic acid} H_3C-CO-CH_2-COOH	3302, 4249	1312	
91.	141-97-9	Butanoic acid, 3-oxo-, ethyl ester		172a, 174b, 1053, 3266	
92.	105-45-3	Butanoic acid, 3-oxo-, methyl ester		568b, 4249	
93.	583-92-6	Butanoic acid, 4-(methylthio)-2-oxo- H_3C-S-$(CH_2)_2$-CO-COOH		429b, 4249, 4699	
94.	35734-62-4	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-	1364	2032, 4249, 5811b	
95.	51769-21-2	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (±)-		4249, 4495	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

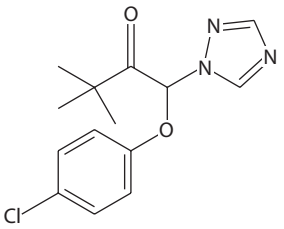
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
96.	495-40-9	1-Butanone, 1-phenyl-	2767, 2769, 4249, 5811b		
97.	61892-81-7	1-Butanone, 1-pyrazinyl-	568b, 3553, 4249		
98.		1-Butanone, 1-(methyl-2-pyridinyl)-	4570a		
99.		1-Butanone, 1-(3-methyl-2-pyridinyl)-	4570a		
100.		1-Butanone, 1-(4-methyl-2-pyridinyl)-	4570a		
101.	22971-32-0	1-Butanone, 1-(2-pyridinyl)-	4570a, 5811		
102.	1701-70-8	1-Butanone, 1-(3-pyridinyl)- {propyl pyridyl ketone}	568b, 1587, 2724, 2939, 3054, 3056, 3302, 3491, 4249, 5811b	120, 568b, 1225, 1226, 2359, 2724, 2939, 3056, 3444, 3491, 3974a, 4249, 4766	
103.	28384-26-1	1-Butanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-		4249, 4802	
104.	78210-70-5	1-Butanone, 2-methyl-1-(3-pyridinyl)-	568b, 1587, 4249, 5811b		
105.	68697-66-5	1-Butanone, 3-(methylthio)-1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-		3215, 4249, 4967	
106.		1-Butanone, 3-(methylthio)-1-(2,6,6-trimethylcyclohexenyl)-		3215, 4249, 4967	
107.	71278-11-0	1-Butanone, 4-amino-1-(3-pyridinyl)- {poikiline}	3302, 3742, 4207, 4213, 4248	120, 2270, 4207, 4249, 5079	
108.	59578-62-0	1-Butanone, 4-hydroxy-1-(3-pyridinyl)-	5087, 5508	4249, 5508	
109.		1-Butanone, 4-(methylamino)-1-(2,6-dihydroxy-3-pyridinyl)-		1101	
110.		1-Butanone, 4-(methylamino)-1-(6-hydroxy-pyridinyl)-		1101	
111.	2055-23-4	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)- {pseudooxynicotine}		553, 2221, 3974, 4236, 4249, 5079, 5222	
112.	64091-91-4 110053-55-9 121268-99-3 126165-82-0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}  {1-Butanone, 4-[(nitrosomethyl)amino]-1-(3-pyridinyl)-}	7, 23–26, 28–31, 34, 59, 70, 75, 97–99, 126, 126a, 126b, 172, 174b, 174c, 237, 239, 402, 458–460, 463, 478, 483, 484, 486, 501, 502, 508, 514, 568b, 572, 573, 595, 603, 688, 728, 772, 895, 998, 1001, 1002, 1004, 1006a, 1011, 1013–1016, 1016a, 1051, 1058, 1099, 1148, 1191–1200, 1373, 1386, 1445, 1557, 1564, 1566, 1567, 1567a, 1569–1571, 1571a, 1572, 1573a, 1580, 1584, 1674, 1679, 1685, 1692, 1696, 1702, 1710, 1725, 1727, 1728, 1730, 1731, 1736, 1741, 1746, 1750, 1751, 1768, 1769, 1781, 1842, 1870–1872, 1987, 1988, 2133, 2134a, 2142, 2168, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2879, 2949,	29, 33, 34, 64, 70, 97–99, 174c, 201, 324–326, 458, 463, 465, 468, 478, 483, 484, 486, 498, 501, 505, 508, 510, 548–550, 553, 554, 557, 568b, 595, 655, 720, 772, 895, 998, 1002, 1004, 1010, 1014, 1015, 1051, 1156, 1191–1200, 1385, 1564, 1566, 1567, 1567a, 1569–1571, 1573a, 1576, 1577, 1584, 1679, 1685, 1696, 1702, 1712, 1722, 1725, 1728, 1730, 1731, 1746, 1750, 1768, 1771, 1870–1872, 1988, 2050–2052, 2169,	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK} (cont.)	2991, 2992, 2993, 3007, 3094, 3178, 3179, 3180, 3181, 3182, 3184, 3190, 3255–3257, 3265, 3300, 3342, 3343, 3365, 3370, 3376, 3378, 3844, 3952, 3973, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5070, 5087, 5494, 5531, 5546, 5556, 5569, 5679, 5692, 5811, 5811a, 5811b, 5836	2235, 2326c, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2638, 2674, 2700, 2914–2917, 2949, 2992, 2996,2997, 3144a, 3176a, 3177, 3183, 3441a, 3491, 3773, 3774, 3816, 3943b, 3947, 3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4090, 4128, 4161, 4236, 4247, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5531, 5579, 5584, 5589, 5811, 5811a, 5811b	
113.	76014-82-9	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-, *N*-oxide		4249	
114.	78-93-3	2-Butanone {methyl ethyl ketone} $H_3C\text{-}CO\text{-}CH_2\text{-}CH_3$	37, 38, 111, 112, 172, 173a, 174b, 174c, 299, 314, 480, 544–546, 564, 568b, 605, 643, 645, 688, 764a, 778, 966, 1038, 1050, 1063–1074, 1140, 1153, 1154, 1215, 1238, 1284, 1348–1352, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1416, 1418, 1419, 1427, 1495, 1586, 1589, 1590, 1637, 1668, 1875, 1947, 1966, 2002, 2003, 2063, 2079, 2089, 2091, 2270, 2293, 2310, 2337, 2387, 2483, 2506, 2507, 2520, 2543, 2545, 2559, 2559a, 2570, 2591, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2858, 2866, 2939, 2942, 3007, 3059, 3105, 3132, 3135, 3136, 3254, 3255, 3266, 3300, 3308, 3396, 3413, 3431, 3436, 3438, 3482, 3493, 3530, 3551, 3555, 3557, 3692,	404, 568b, 647, 984, 1053, 1590, 2337, 2339a, 2914, 2939, 3266, 3555, 3626, 3797, 3974a, 4223, 4225, 4249, 5811b	1354, 1375a, 1377, 1378, 2244, 2387, 2506, 2507, 3401, 4052, 4056

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		2-Butanone {methyl ethyl ketone} (cont.)	3794, 3797, 3817, 3876, 3897, 3901, 3939, 4005–4007, 4052, 4056, 4078, 4104, 4162, 4249, 4257, 4290, 4319, 4360, 4570a, 5034, 5049, 5770, 5811b, 5836		
115.	1575-57-1	2-Butanone, 1-(acetyloxy)- $H_3C\text{-}CH_2\text{-}CO\text{-}CH_2\text{-}OOC\text{-}CH_3$	1238, 2570, 2731, 2735, 2767, 3553, 3557, 4249, 5811b		3401, 3402, 3404
116.	43121-43-3	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)- {Triadimefon®} 		3633	
117.	5077-67-8	2-Butanone, 1-hydroxy- $H_3C\text{-}CH_2\text{-}CO\text{-}CH_2OH$	568b, 1063–1066, 1068–1074, 1215, 2777, 4249, 5811b	568b, 2386, 3555, 4249, 5811b	3401, 3402, 3404, 3405, 4249
118.	1007-32-5	2-Butanone, 1-phenyl- $C_6H_5\text{-}CH_2\text{-}CO\text{-}CH_2\text{-}CH_3$	2767, 2769, 3557, 4249, 5811b		
119.	75-97-8	2-Butanone, 3,3-dimethyl- $H_3C\text{-}CO\text{-}C{\equiv}(CH_3)_3$	1238, 2387, 4249		2387
120.	38895-88-4	2-Butanone, 3,3-dimethyl-4-hydroxy-	568b, 4249		
121.	57011-15-1	2-Butanone, 3,4-dihydroxy- $H_3C\text{-}CO\text{-}CHOH\text{-}CH_2OH$	3553, 4249, 5811b		
122.	513-86-0	2-Butanone, 3-hydroxy- {acetoin} $H_3C\text{-}CO\text{-}CHOH\text{-}CH_3$	568b, 1063–1066, 1068–1074, 1426, 1427, 1882, 2337, 2761, 2762, 2765, 2766, 2777, 3266, 3410, 3555, 3559, 4249, 5811b	174b, 404, 568b, 1053, 2339a, 2339b, 2386, 2917a, 3266, 3549, 4249, 5811b	2244, 3401, 3402, 3404, 4249
123.	563-80-4	2-Butanone, 3-methyl- $H_3C\text{-}CO\text{-}CH{=}(CH_3)_2$	112, 568b, 605, 1039, 1140, 1238, 1365, 1412–1414, 1416, 1418, 1419, 1422, 1637, 2002, 2506, 2507, 2545, 2767, 2782, 2804, 3302, 3308, 3530, 3797, 3973, 4249, 5034, 5811b	568b, 2339a, 2722, 4249	2244, 2506, 2507
124.	53872-97-2	2-Butanone, 3-methyl-1-(3-pyridinyl)-	4249		
125.	10150-87-5	2-Butanone, 4-(acetyloxy)- $H_3C\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}OOC\text{-}CH_3$	568b, 1586, 2387, 2570, 2767, 3553, 3556, 4249, 5811b		2387

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

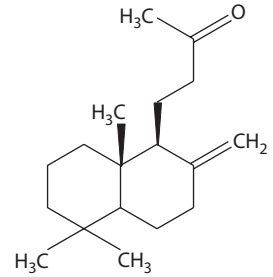
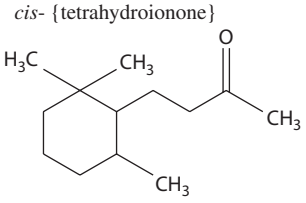
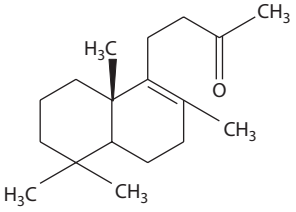
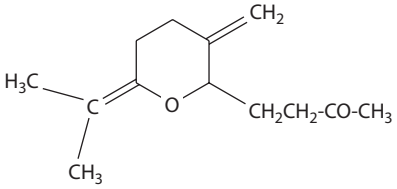
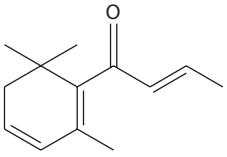
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
126.	10266-75-8	2-Butanone, 4-(decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl)-, [1S-(1α,4aβ,8aα)]- 		947, 1156, 4090	
127.	590-90-9	2-Butanone, 4-hydroxy- H_3C-CO-CH_2-CH_2OH	568b, 3553, 3555, 4249, 5811b	404, 568b, 4249, 5811b	
128.	1823-90-1	2-Butanone, 4-hydroxy-3,3-dimethyl- H_3C-CO-$C(CH_3)_2$-CH_2OH	3553, 4249, 5811b		
129.	5471-51-2	2-Butanone, 4-(4-hydroxyphenyl)-	374, 568b, 3266, 3712, 4249	172a, 174b, 568b, 1053, 3266, 3370	
130.	104-20-1	2-Butanone, 4-(4-methoxyphenyl)-		172a, 174b, 1053, 3266	
131.	34047-39-7	2-Butanone, 4-(methylthio)-	3410, 4570a, 4249, 4570a	937, 938, 1248, 2386, 4249	
132.	2550-26-7	2-Butanone, 4-phenyl-	1586, 2570, 2767, 2769, 3557, 4249, 5811b	2386, 4249	
133.	50767-77-6	2-Butanone, 4-(2-ethenyl-2,6,6-trimethylcyclohexyl)-		2, 13, 1662, 4249, 4780	
134.	133007-80-4	2-Butanone, 4-(6-ethenyl-2,2,6-trimethylcyclohexyl)-		5811, 5811b	
135.	699-17-2	2-Butanone, 4-(2-furanyl)-	5811, 5811a, 5811b	5811b	
136.	6138-85-8	2-Butanone, 4-(2,2,6-trimethylcyclohexyl)-		568b, 4249	
137.	60761-23-1	2-Butanone, 4-(2,2,6-trimethylcyclohexyl)-, *cis*- {tetrahydroionone} 		1156, 1662, 4090, 4249	
138.	52690-42-3	2-Butanone, 4-[2,2,6-trimethyl-6-(methylethylene)cyclohexyl]-		5811, 5811b	
139.	58720-40-4	2-Butanone, 4-(2,3,6-trimethylphenyl)-		4249, 4772, 5811b	
140.	20483-36-7	2-Butanone, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-		2339a, 2917a	
141.	14506-65-1	2-Butanone, 4-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, (4aS-*trans*)- 		947, 1156, 4090, 4249	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
142.	158815-72-6	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)-		4249, 5811b	
143.	158815-73-7	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)-		4249, 5811b	
144.	160115-51-5	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)- (+)-		4249	
145.	160115-52-6	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)- (−)-		4249	
146.		2-Butanone, 4-[5,6-dihydro-3-methyl-6-(1-methylethyl)-pyran-2-yl]		3547, 4249	
147.	5471-51-2	2-Butanone, 4-(4-hydroxyphenyl)-{4-(*p*-hydroxyphenyl)-2-butanone}	3266, 3712, 4249	172a, 174b, 1053, 3266, 3370	
148.	13679-56-6	2-Butanone, 4-(5-methyl-2-furanyl)-	2570, 4249	3547, 4249	
149.		2-Butanone, 4-(2-methyl-5-(1-methylethyl)-2-furanyl)-		3545	
150.		2-Butanone, 4-(2-methyl-6-(1-methylethyl)-2-tetrahydropyranyl)-		404, 3547, 4249	
151.		2-Butanone, 4-(4,5-dihydro-3-methylene-6-dimethylmethylene-2-pyranyl)- 		3545	
152.	54345-38-9	2-Buten-1-one, 1-(2,3,6-trimethylphenyl)-, (*E*)-		947, 4249	
153.	23726-93-4 23696-85-7	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)- {β-damascenone} 	568b, 775, 1371, 1663, 1949, 2765, 2766, 2773, 3266, 3410, 4249, 4570a	172a, 174b, 404, 543a, 568b, 936, 937, 1053, 1063–1066, 1068–1074, 1156, 1254, 1256, 1590a, 1949, 2338, 2339a, 2339b, 2386, 2389, 2544, 2611, 2917a, 3218, 3266, 3370, 3547, 3549, 4090, 4098a, 4159, 4249, 5811b	
154.		2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-{β-damascenone isomer}		404, 1156, 4090	
155.	80111-68-8 23770-92-3 35044-68-9	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)-{damascone}	568b, 1075, 2545, 4249	172a, 174b, 568b, 911, 937, 1053, 1063–1066, 1068–1074, 1156, 1254, 1256, 1590a, 2339a, 2339b, 2386, 2389, 2544, 3218, 3266, 3370, 3547, 3549, 4090, 4098a, 4249, 5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

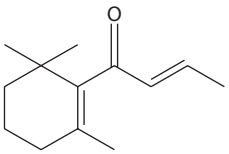
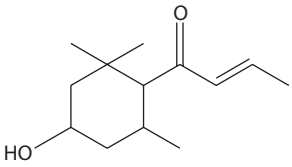
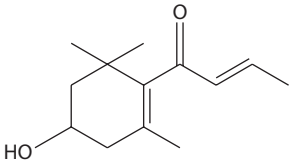
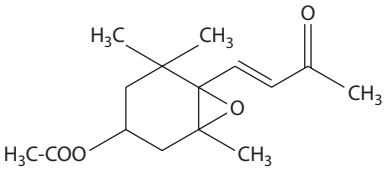
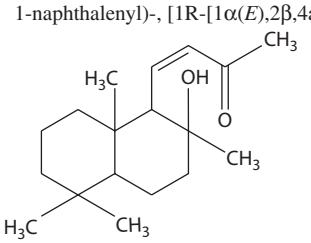
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
156.	23726-91-2	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-	4249	2339a, 3392, 4249, 5811b	
157.	23726-92-3 85949-43-5	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)- {β-damascone} 	1949, 2545, 3266	404, 908, 936, 937, 1156, 1256, 1949, 2389, 2544, 2611, 2917a, 3188, 3266, 3549, 4090, 4159	
158.	43052-87-5	2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-damascone}		5811, 5811b	
159.	102488-09-5	2-Buten-1-one, 1-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {3-hydroxy-β-damascone}	568b, 2601a, 4249	568b, 2338, 2917a, 4098a, 4249, 4495, 5811b	
160.	80508-24-3	2-Buten-1-one, 1-(3-pyridinyl)-	4249		
161.	53398-17-7	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethycyclohexanyl)- {4-hydroxydihydro-β-damascone} 		233, 2032, 5811, 5811b	
162.	56915-02-7	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-damascone} 	568b, 1063–1066, 1068–1074, 1360, 1361, 1365, 1371, 1375, 1375a, 1375b, 2543, 2545, 2761, 2762, 2767, 3410, 3553, 3557, 4249, 5811b	404, 568b, 1063–1066, 1068–1074, 1156, 1254, 1256, 1587a, 1590a, 2032, 2338, 2339a, 2339b, 2386, 2389, 2544, 3218, 3543, 3546, 3549, 3550, 3560, 3561, 4090, 4159, 4249, 5811b	1360, 1375a
163.	35734-61-3	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-	2765, 2766, 2773, 2775	404, 5811b	
164.	160550-79-8	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, [R-(*E*)]-		4249	
165.	87562-12-7	2-Buten-1-one, 1-[3-(formyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, (*E*)-		4249	
166.	62512-25-8	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-		4249, 4715	
167.	160550-77-6	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		4249, 4715	
168.	495-45-4	2-Buten-1-one, 1,3-diphenyl-		2917a	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
169.	78-94-4	3-Buten-2-one {methyl vinyl ketone} $H_2C{=}CH\text{-}CO\text{-}CH_3$	111, 112, 239, 314, 480, 568b, 1063–1066, 1068–1074, 1140, 1348–1351, 1354, 1365, 1374, 1375a, 1413, 1414, 1416, 1418, 1419, 1437, 1586, 1589, 1634, 1637, 1947, 2506, 2507, 2543, 2545, 2559, 2559a, 2570, 2761, 2762, 2765–2767, 2777, 2782, 2799a, 2804, 2939, 3255, 3308, 3396, 3530, 3557, 4052, 4056, 4104, 4319, 4570a, 5034, 5770, 5811b, 5869a	568b, 984, 1550, 2544, 4249	1354, 1375a, 2244, 2506, 2507, 3401, 4052, 4056
170.	814-78-8	3-Buten-2-one, 3-methyl- $H_2C{=}C(CH_3)\text{-}CO\text{-}CH_3$	112, 299, 1063–1066, 1068–1074, 1140, 1154, 1348–1350, 1354, 1365, 1375a, 1414, 1416, 1418, 1419, 1422, 1586, 1589, 2543, 2545, 2570, 2765, 2767, 2777, 3302, 3308, 3530, 3797, 5034, 5811b	1157, 1248, 4092, 4249, 5811b	1354, 1375a, 3401
171.	127-51-5	3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-isomethylionone}		1053, 3266	
172.	73892-47-4	3-Buten-2-one, 4-[3-(acetyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		4249	
173.	50281-40-8	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1R-[1α(*E*),4β,6α]]- 		1, 4249, 4573	
174.	50281-41-9	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1S-[1α(*E*),4α,6α]]-		1	
175.	52811-61-7	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-	5811, 5811a, 5811b		
176.	42569-64-2	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		5, 1151, 1156, 1248, 3561, 4090, 4249, 4780, 5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

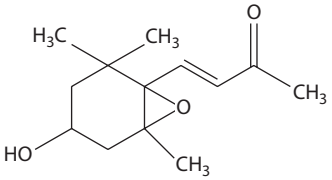
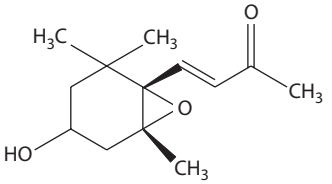
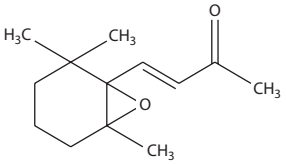
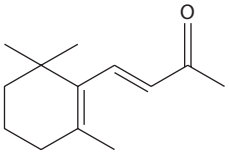
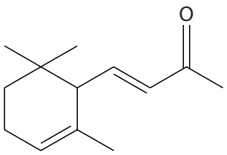
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
177.	54656-80-3	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1α(*E*),2α,4aβ,8aα]-(±)-		1151, 1156, 3561, 4090, 4249	
178.	36340-49-5	3-Buten-2-one, 4-(1,2-epoxy-2,6,6-trimethylcyclohexyl)-, (*E*)-		5811, 5811b	
179.	623-15-4	3-Buten-2-one, 4-(2-furanyl)-	568b, 1238, 1587, 3266, 4249, 5811b	568b, 1053, 3266, 3893, 4249	
180.	81540-27-4	3-Buten-2-one, 4-(2-furanyl)-3-methyl-	568b, 4249	568b, 4249	
181.	15356-75-9	3-Buten-2-one, 4(1-hydroxy-2,2-dimethyl-6-methylenecyclohexyl)-		568b, 4249, 5811, 5811b	
182.	15356-76-0	3-Buten-2-one, 4-(1-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)-		5811, 5811b	
183.	15401-34-0	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-		5811, 5811b	
184.	14398-34-6	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-		909, 1249, 1256, 4249	
185.	61892-82-8	3-Buten-2-one, 4-(4-hydroxy-1-cyclohexen-1-yl)-	568b, 2767, 3553, 4249, 5811b		
186.	31253-95-9	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)		5811, 5811b	
187.	50281-42-0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1S-[1α(*E*),4α,6α]]- 		1, 1156, 3547, 4090, 4249, 4780, 5811b	
188.	61116-99-2	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1R-[1α(*E*),4β,6α]]- 		1, 1156, 2338, 4090, 4249, 4780	
189.	72491-46-4	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-{4-hydroxy-β-ionone}		1156, 1249, 1254, 1256, 2386, 4090, 5811b	
190.	38963-41-6	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)-{4-hydroxy-α-ionone}	2767, 2769, 4249		
191.	23120-57-2	3-Buten-2-one, 4-(5-methyl-2-furanyl)-	568b, 1587, 4249, 5811b		
192.	66434-99-9	3-Buten-2-one, 4-(5-methyl-2-furanyl)-, (*E*)-		3547, 4249	
193.	98910-85-1	3-Buten-2-one, 4-(4-oxo-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-oxo-β-ionone}		568b, 4249	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
194.	122-57-6	3-Buten-2-one, 4-phenyl- C_6H_5-CH═CH-CO-CH_3	568b, 642, 2570, 3266, 4249	568b, 1053, 2389, 2544, 3266, 4249, 5811b	
195.	2433-57-0	3-Buten-2-one, 4-(1*H*-pyrrol-2-yl)-, (*E*)-	2775, 4249		
196.	79-69-6	3-Buten-2-one, 4-(2,5,6,6-tetramethyl-2-cyclohexen-1-yl)- {α-irone}		172a, 174b, 1053, 3266	
197.	23267-57-4	3-Buten-2-one, 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- 		937, 2339b, 2386, 2544, 2917a, 4249, 5811b	
198.	56681-06-2	3-Buten-2-one, 4-(2,3,6-trimethylphenyl)-		1156, 1254, 2389, 2544, 3547, 4090, 4249, 5811b	
199.	1203-08-3	3-Buten-2-one, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-{dehydro-β-ionone}	568b, 1360, 1375a, 2543, 2761, 2762, 4249	568b, 937, 943, 1063–1066, 1068–1074, 1590a, 2386, 2389, 2544, 2917a, 3547, 3549, 4249, 5811b	1360, 1375a
200.	14398-35-7	3-Buten-2-one,4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-,(*E*)-		1156, 3547, 4090, 5811b	
201.	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-{β-ionone} 	297, 568b, 1949, 3266, 4249	172a, 174b, 404, 543a, 568b, 908, 911, 937, 1053, 1156, 1254, 1854, 1949, 2338, 2339a, 2339b, 2386, 2389, 2544, 2611, 2917a, 3217, 3218, 3266, 3354, 3370, 3545, 3547, 3560, 3561, 3647, 4090, 4159, 4249, 5811b	
202.	79-77-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)-	5811b	1156, 4090, 5811b	
203.	127-41-3 8013-90-9	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- {α-ionone} 	3266, 4249, 5811b	172a, 174b, 404, 908, 1053, 1156, 1254, 1256, 2338, 2339a, 2339b, 2389, 2544, 2611, 2917a, 2939, 3218, 3266, 3370, 3560, 3561, 3647, 3973, 4090, 4249, 5811b	
204.	503-93-5	2,4-Cycloheptadien-1-one, 2,6,6-trimethyl- {eucarvone}		2339a	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

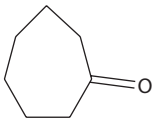
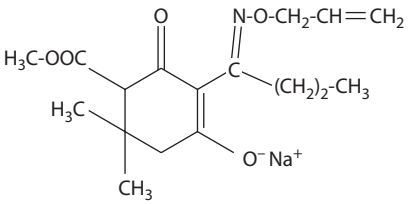
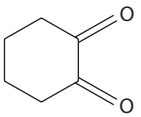
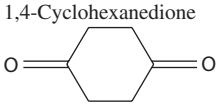
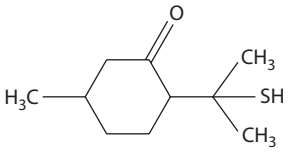
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
205.	502-42-1	Cycloheptanone {suberone} 	4249, 5811b	5811b	
206.	1121-66-0	2-Cyclohepten-1-one	5811, 5811a, 5811b		
207.	13487-30-4	2,4-Cyclohexadien-1-one, 2,6,6-trimethyl-	4570a		
208.		2,5-Cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)-4-hydoxy-4-methyl-		2917a	
209.	55635-13-7	Cyclohexanecarboxylic acid, 2,2-dimethyl-2,4-dioxo-3-(1-((2-propenyloxy)amino)butylidene)-, methyl ester, sodium salt {Alloxydim-sodium®} 		3633, 4271a	
210.	765-87-7	1,2-Cyclohexanedione 		2917a	
211.	18310-19-5	1,2-Cyclohexanedione, 4-methyl-	1375a, 1377		1375a, 1377
212.	3008-43-3	1,2-Cyclohexanedione, 6-methyl-		174b, 3266	
213.	126-81-8	1,3-Cyclohexanedione, 5,5-dimethyl-		568b, 4249	
214.	1919-64-8	1,3-Cyclohexanedione, 5,5-dimethyl-2-propyl-		2917a	
215.	1193-55-1	1,3-Cyclohexanedione, 2-methyl-	2570, 3553, 4249	2917a, 4249	
216.	637-88-7	1,4-Cyclohexanedione 	568b, 2570, 2767, 3553, 3557, 3559, 4249, 5811b	568b, 2389, 2544, 4249, 5811b	
217.	20547-99-3	1,4-Cyclohexanedione, 2,2,6-trimethyl- {4-ketodihydroisophorone}	568b, 3553, 3557, 4249, 5811b	404, 568b, 937, 1063–1066, 1068–1074, 1590a, 2282, 2337a, 2339a, 2339b, 2386, 2389, 2544, 2917a, 3205, 3218, 3219, 3545, 3547, 3560, 3561, 4249, 5811b	
218.	108-94-1	Cyclohexanone	112, 568b, 1140, 1238, 1371, 1419, 2543, 2570, 2773, 3410, 4249, 5811b	69, 568b, 4249, 4749	2244, 3402, 3404
219.	71607-84-6	Cyclohexanone, ethenylmethyl-	3497, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

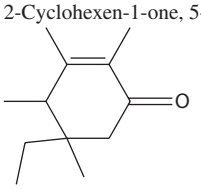
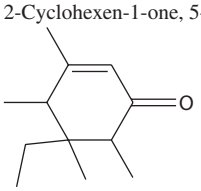
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
220.	50874-76-5	Cyclohexanone, trimethyl-		2389, 4249	
221.	2816-57-1	Cyclohexanone, 2,6-dimethyl-		2917a	
222.	7500-42-7	Cyclohexanone, 2-hydroxy-2,6,6-trimethyl-		404, 2389, 2544, 3547, 3550, 4249, 4780, 5811b	
223.	38462-22-5	Cyclohexanone, 2-(1-mercapto-1-methylethyl)-5-methyl- 		172a, 174b, 1053, 3266	
224.	583-60-8	Cyclohexanone, 2-methyl-		568b, 2339a. 4249	
225.	7764-50-3	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-	2601a		
226.	6909-25-7	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, (2S-*cis*)-		2339a	
227.	5948-04-9	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, *trans*-		2339a, 5811b	
228.	491-07-6	Cyclohexanone, 2-methyl-5-(1-methylethyl)-, (*E*)- {*dl*-isomenthone}		174b, 3266	
229.	499-70-7 59471-80-6	Cyclohexanone, 2-methyl-5-(1-methylethyl)- {carvomenthone}		568b, 4249	
230.		Cyclohexanone, 2-(1-methylethyl)- {two isomers}		404	
231.	15189-14-7	Cyclohexanone, 2,2,5,5-tetramethyl-		4249	
232.	2408-37-9	Cyclohexanone, 2,2,6-trimethyl- {2,6,6-trimethylcyclohexanone}	5811b	404, 1053, 2339a, 2389, 2544, 3218, 3266, 3547, 4249, 5811b	
233.		Cyclohexanone, 2,4,4-trimethyl-3-(1-oxobutyl)-		3547, 4249	
234.	591-24-2	Cyclohexanone, 3-methyl-	568b, 1238, 1348–1350, 3497, 4249, 5770		
235.	13368-65-5	Cyclohexanone, 3-methyl- (+)	5811, 5811b		
236.	60026-21-3	Cyclohexanone, 3,3,5-trimethyl-4-(3-oxo-1-butenyl)-		2338, 2339b, 2389, 2544, 3547, 4249, 5811b	
237.	123716-12-1	Cyclohexanone, 4-(1-methylethyl)-3-(2-oxopropyl)-	4249		
238.	72491-45-3	Cyclohexanone, 4-(2-butenylidene)-3,3,5-trimethyl-		568b, 4249, 5811b	
239.	20548-02-1	Cyclohexanone, 4-hydroxy-2,2,6-trimethyl-	568b, 937, 4249, 5811b	568b, 937, 943, 1254, 1256, 3206, 3218, 3219, 3543, 3550, 3561, 4249, 5811b	
240.	20548-03-2	Cyclohexanone, 4-hydroxy-3,3,5-trimethyl-	568b, 937, 4249	568b, 943, 1254, 1256, 3550, 4249, 5811b	
241.	589-92-4	Cyclohexanone, 4-methyl-	568b, 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
242.	529-00-0	Cyclohexanone, 5-methyl-2-(1-methylethenyl)- {isopulegone}		404, 3188, 4249, 4663	
243.	89-80-5 10458-16-7	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}	309, 568b, 1238, 1361, 1936, 3266, 4247, 4248	172a, 174b, 568b, 1053, 2339a, 2385a, 3266, 3370, 4249	
244.	14073-97-3	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, (L) {*L*-menthone}	5811, 5811a, 5811b		
245.	89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)- {pulegone}		2386, 2917a, 3188, 4249, 4750	
246.	133561-49-6	Cyclohexanone, 3,3,5-trimethyl-4-(3-oxobutyl)-		5811, 5811b	
247.	18378-66-0	1-Cyclohexene-1-carboxaldehyde, 3-oxo-2,6,6-trimethyl-		5811, 5811b	
248.		2-Cyclohexene, 1-(2-oxopropyl) 3,5,5-trimethyl-	2773, 4249	2544, 4249	
249.	35692-98-9	2-Cyclohexene-1,4-dione, 2-hydroxy-3,5,5-trimethyl-		404, 943, 2092, 3219, 3188, 4249	
250.	38770-37-5	2-Cyclohexene-1,4-dione, 2,5,5-trimethyl-	5811, 5811a, 5811b		
251.	1125-21-9	2-Cyclohexene-1,4-dione, 2,6,6-trimethyl- {4-ketoisophorone; 4-oxoisophorone}	568b, 1360, 1375a, 1949, 2543, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 3266, 4249, 5811b	404, 568b, 937, 1053, 1254, 1590a, 1949, 2338, 2386, 2389, 2544, 2917a, 3188, 3215, 3219, 3266, 3543, 3545, 3560, 3561, 3905, 4249	1360, 1375a
252.	930-68-7	2-Cyclohexen-1-one	299, 568b, 1371, 2506, 2507, 2543, 2545, 2601a, 2731, 2735, 2736, 2773, 2775, 3410, 3553, 3559, 4249, 4570a, 5811b	404, 568b, 3547, 3550, 4249, 5811b	2506, 2507
253.	133304-85-5	2-Cyclohexen-1-one, 3,4-dimethyl-2-hydroxy-	91c, 5811b		
254.	2748-09-6	2-Cyclohexen-1-one, 3,5-dimethyl-2-hydroxy-	91c, 5811b		
255.	2748-08-5	2-Cyclohexen-1-one, 3,6-dimethyl-2-hydroxy-	91c, 5811b		
256.	74051-80-2	2-Cyclohexen-1-one, 2-[1-(ethoximino)butyl]-5-[2-(ethylthio)-propyl]-3-hydroxy- {Sethoxydim®}		3633	
257.	41577-83-7	2-Cyclohexen-1-one, 3-ethyl-2-hydroxy-	91c, 5811b		
258.	10316-66-2	2-Cyclohexen-1-one, 2-hydroxy-	91c, 5811b		
259.	490-03-9 3400-78-0	2-Cyclohexen-1-one, 2-hydroxy-3-methyl- {diosphenol}	91c, 5811, 5811a, 5811b	2917a	
260.	55310-49-1	2-Cyclohexen-1-one, 2-hydroxy-3-propyl-	91c, 5811, 5811a, 5811b		
261.		2-Cyclohexen-1-one, 2-hydroxy-3,5,5-trimethyl-	91c		
262.	1121-18-2	2-Cyclohexen-1-one, 2-methyl-	1360, 1375a, 2543, 2761, 2773, 4249, 4570a		1360, 1375a

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
263.	99-49-0 6485-40-1	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*l*-carvone}	568b, 2570, 2769, 3266, 3557, 4249, 5811, 5811a, 5811b	172a, 174b, 568b, 1053, 1156, 1254, 1256, 2339a, 2389, 2544, 3188, 3266, 3370, 4090, 4249, 5811, 5811a, 5811b	
264.	2244-16-8	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*d*-carvone}	2570, 3557, 4249	174b, 1256, 2544, 3266, 4249	
265.	43205-82-9	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)- {dihydrocarvone}	568b, 4249		
266.		2-Cyclohexen-1-one, 2-propyl-3-methyl- {two isomers}	4570a		
267.		2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(1,3-butadienyl)-	4570a		
268.	27185-77-9	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-	1075, 4249	1256, 2338, 2339b, 3549, 4249, 5811b	
269.	29790-29-2	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-, (1*E*)-		5811b	
270.	20013-73-4	2-Cyclohexen-1-one, 2,6,6-trimethyl-		568b, 2339a, 4249, 4780	
271.	5220-49-5	2-Cyclohexen-1-one, 3-amino-	3553, 4249		
272.	67401-25-6	2-Cyclohexen-1-one, 3-(2-butenyl)-2,4,4-trimethyl-, (*Z*)-		948, 1254, 1256, 4249, 4690, 5811b	
273.	1193-18-6	2-Cyclohexen-1-one, 3-methyl-	2775, 4249, 4570a	404, 937, 2917a, 4249	
274.	89-81-6	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- {*D*-piperitone}	5811b	404, 568b, 1053, 1156, 2095, 2389, 2544, 3266, 3370, 3547, 4090, 4098a, 4249, 5811b	
275.		2-Cyclohexen-1-one, 3-methyl-2-(1,3-pentadienyl)-	4570a		
276.	17369-60-7	2-Cyclohexen-1-one, 5-ethyl-2,3,4,5-tetramethyl- 		1053, 3266	
277.		2-Cyclohexen-1-one, 5-ethyl-3,4,5,6-tetramethyl- 		1053, 3266	
278.	78-59-1	2-Cyclohexen-1-one, 3,5,5-trimethyl- {isophorone}	568b, 722, 1360, 1371, 1375a, 1949, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2777, 3410, 3557, 4249, 4570a, 5811b	404, 568b, 937, 943, 1254, 1949, 2338, 2339a, 2386, 2389, 2544, 2917a, 3188, 3205, 3217, 3219, 3543, 3547, 3560, 3561, 4249, 5811b	1360, 1375a

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

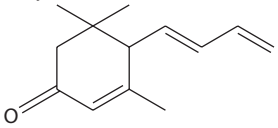
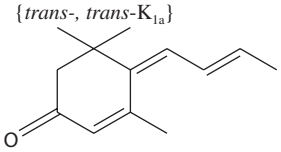
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
279.	51771-56-3	2-Cyclohexen-1-one, 3,5,5-trimethyl-2-(1-methylethenyl)-	2543, 2773, 4249	2389, 2544, 4249, 5811b	
280.	53398-09-7	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(1-oxo-2-butenyl)-		404, 3547, 4249	
281.	60026-25-7	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(1-propenyl)-	2543, 2773, 4249	2389, 2544, 4249, 5811b	
282.	33601-06-8	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-,(R)-(+)-		1149a, 2338, 2339b, 2389, 2544, 3218, 4249	
283.	20194-68-7	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-		568b, 4249, 5811b	
284.	79734-43-3	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-, (*E*)- {3-oxo-α-ionone}		5811, 5811b	
285.	20548-00-9	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-methylene- {methyleneisophorone}		937, 943, 1149, 1149a, 2389, 2544, 3206, 3210, 3218, 3219, 4249, 5811b	
286.		2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-triethyl-	4570a		
287.	5896-02-6	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-trimethyl- 	1586, 2767, 3553, 3557, 4249, 4570a, 5811b	943, 2386, 2389, 2544, 3200, 3219, 3547, 3550, 4249, 5811b	
288.	38818-55-2	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-trimethyl-, (*E*)-	2601a	5811b	
289.	102488-06-2	2-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-, (*E*)		5811, 5811b	
290.	77761-55-8	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)- 3,5,5-trimethyl-		3973, 4249, 4909	
291.	77842-24-1	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)- 3,5,5-trimethyl- {isomer}		4249, 4909	
292.		2-Cyclohexen-1-one, 4-(2-butenyl)-3,5,5-trimethyl-		4249, 4780	
293.	13215-88-8	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-	1075, 2570, 2777, 3266, 3288, 3302, 3410, 3553, 3557, 5811b	922b, 943a, 1053, 1063–1066, 1068–1074, 1254, 1256, 1590a, 1854, 2338, 2389, 2544, 3266, 3288, 3355, 3547, 4098a, 4249, 5811b	
294.	5164-78-3	2-Cyclohexen-1-one, 4-(2-butenylidene)- 3,5,5-trimethyl-, (*E,E*)- {megastigmatrienone} {*trans-, trans*-K_{1a}} 	568b, 775, 1063–1066, 1068–1074, 1352, 1364, 1365, 1371, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2766, 2767, 2773, 2775, 3251, 3288, 3302, 3308, 3397, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2282, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249, 5811b	2387

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
295.	5298-13-5	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*E,Z*)- {megastigmatrienone} {*trans-, cis*-K_{2a}}	568b, 775, 1063–1066, 1068–1074, 1352, 1360, 1364, 1365, 1371, 1375a, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 3251, 3288, 3302, 3308, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249, 5811b	1360, 1375a, 2387
296.	5492-79-5	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,E*)- {megastigmatrienone}{*cis-, trans*-K_{1b}}	568b, 775, 1063–1066, 1068–1074, 1352, 1360, 1364, 1365, 1371, 1375a, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3251, 3288, 3302, 3308, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249	1360, 1375a, 2387
297.	5164-79-4	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,Z*)- {megastigmatrienone} {*cis-, cis*-K_{2b}}	568b, 775, 1063–1066, 1068–1074, 1352, 1364, 1365, 1371, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3251, 3288, 3302, 3308, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249	2387
298.		2-Cyclohexen-1-one, 4-(3-butenylidene)-3,5,5-trimethyl-	2762, 4249	2386, 4249	
299.		2-Cyclohexen-1-one, 4-ethyl-		404	
300.	62512-22-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-		4249	
301.	77699-19-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-,[R-[R*,R*-(*E*)]]-		4249, 4715	
302.	159813-37-3	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-,[4R-[4R*(1*E*,3S*)]]-		4249, 4715	
303.	54835-70-0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-4-hydroxy-3,5,5-trimethyl-,[R-[R*,S*-(*E*)]]-		321c, 1361, 4249, 4713	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

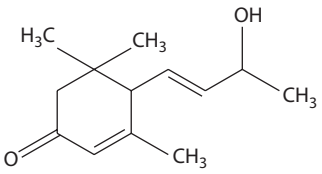
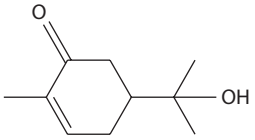
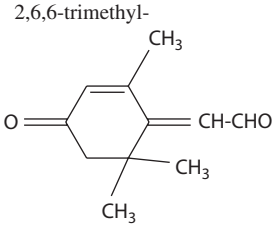
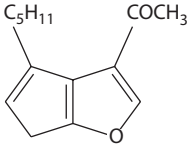
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
304.	62512-23-6	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butyl]-3,5,5-trimethyl-		4249, 4715	
305.	91048-13-4	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy) butylidene]-3,5,5-trimethyl-		4249, 4715	
306.	34318-21-3	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {4-keto-α-ionol} 	568b, 1361, 1371, 1375, 1375b, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3255, 3553, 3557, 4249, 4570a	404, 568b, 908, 1063–1066, 1068–1074, 1149, 1149a, 1156, 1254, 1256, 1587a, 1590a, 2338, 2339b, 2386, 2389, 2544, 3217, 3547, 3549, 3550, 4090, 4249	2387
307.	52210-15-8	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-	1371, 2601a, 3410	1149, 1149a, 1156, 1587a, 4090	
308.	68759-08-0	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [S-[R*,S*-(*E*)]]-	1371	1149, 1149a, 1156, 1587a, 4090	
309.	60047-19-0	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl-{4-ketodihydro-α-ionol}	1375, 1375b, 3553, 3557, 4249	52, 404, 937, 943, 1149a, 1254, 1256, 1590a, 2386, 2389, 2544, 3218, 3547, 3549, 4249, 5811b	
310.	36151-02-7	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl-, [R-(R*,R*)]-	568b, 2601a, 4249	568b, 1063–1066, 1068–1074, 2917a, 4249, 5811b	
311.	60026-24-6	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-	2570	1254, 1256, 2338, 2389, 2544, 4249, 4780, 5811b	
312.	102488-07-3	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-, (*E*)	5811, 5811b	5811, 5811b	
313.	19620-37-2	2-Cyclohexen-1-one, 4-hydroxy-2,6,6-trimethyl-		937, 943, 2389, 2544, 3218, 4249, 5811b	
314.	14203-59-9	2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-		568b, 937, 4249	
315.		2-Cyclohexen-1-one, 4-hydroxy 4-(3-methyl-1,3-dibutenyl)-3,5,5-trimethyl-	568b, 4249		
316.	7070-24-8	2-Cyclohexen-1-one, 4-hydroxy-4-(3-oxo-1-butenyl)-3,5,5-trimethyl-		5811, 5811b	
317.	23526-45-6	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-(+) {Blumenol A}		5811b	
318.	24427-77-8	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {vomifoliol}	568b, 1365, 1587, 4249	568b, 1587,1587a, 2338, 3549, 4249	
319.	23069-00-3	2-Cyclohexen-1-one, 4-hydroxymethyl-3,5,5-trimethyl-	568b, 4249	568b, 4249	
320.	500-02-7	2-Cyclohexen-1-one, 4-(1-methylethyl)-		404, 5811	
321.	51171-72-3	2-Cyclohexen-1-one, 4-phenyl-	2769, 4249		
322.	1073-13-8	2-Cyclohexen-1-one, 4,4-dimethyl-	4570a		
323.	5715-25-3	2-Cyclohexen-1-one, 4,5-dimethyl-		2917a	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
324.	7712-46-1	2-Cyclohexen-1-one, 5-(1-hydroxy-1-methylethyl)-2-methyl 		937, 1156, 4090, 4249	
325.	56691-69-1	2-Cyclohexen-1-one, 5-[1-(acetyloxy)-1-methylethyl]-2-methyl-, (R)-		937, 1156, 4090	
326.	499-74-1	2-Cyclohexen-1-one, 6-methyl-3-(1-methylethyl)-	568b, 2767, 2769, 3557, 4249, 5811b	568b, 1156, 2095, 4090, 4249	
327.	4096-34-8	3-Cyclohexen-1-one	568b, 1368, 3559, 4249		
328.		3-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-		3550, 4249, 4780	
329.	102488-08-4	3-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-, (*E*)		5811, 5811b	
330.	471-01-2	3-Cyclohexen-1-one, 3,5,5-trimethyl-	2444, 4249		
331.	69874-67-5	5-Cyclohexen-1-one, 2-acetyl-3,5,5-trimethyl-	568b, 4249		
332.	60026-16-6	Cyclohexenylideneacetaldehyde, 4-oxo-2,6,6-trimethyl- 		5811, 5811b	
333.	126458-49-9	4*H*-Cyclopenta[3′,4′]cycloocta[1′,2′:1,5]cyclopent[1,2-*b*]oxiren-4-one, 1,2,2a,5,6,8,9,10,10a,10b-decahydro-2,6,10a-trimethyl-8-(1-methylethyl)-, [2aS-(2aα,3aS*,6β,8β,10aβ,10bβ)]-		4249	
334.	86154-08-7	4*H*-Cyclopenta[3′,4′]cycloocta[1′,2′:1,5]cyclopent[1,2-*b*]oxiren-4-one, 1,2,2a,7,7a,8,9,10,10a,10b-decahydro-2a,6,10a-trimethyl-8-(1-methylethyl)-, (2aα,3aR*,7aβ,8β,10aβ,10bβ)-		4087, 4249	
335.	142750-40-1	4,10(1*H*,5*H*)-Cyclopentacycloundecenedione, 2,3,3a,6,7,11,12,12a-octahydro-1,3,12-trihydroxy-3,8,12-trimethyl-5-(1-methylethyl)-, (1R*,3S*,3aR*,5S*,8Z,12R*,12aR*)- (–)-		4249	
336.	541-91-3	Cyclopentadecanone, 3-methyl-		1053, 3266	
337.		2,4-Cyclopentadien-1-one, 2,3-dimethyl-4-hydroxy-	1586, 2767		
338.	94618-71-0	2,4-Cyclopentadien-1-one, 2-methyl-	1371, 3410		
339.		Cyclopenta[*b*]furan, 3-acetyl-4-pentyl- 	3553, 4249	404	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

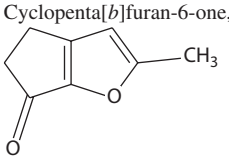
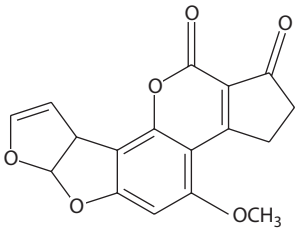
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
340.		Cyclopenta[*b*]furan-6-one, 4,5-dihydro-2-methyl- 	3553, 4249	404	
341.	1162-65-8	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-, (6aR-*cis*)-{aflatoxin B_1} 	158a, 2024, 2484, 3721, 3970, 3986 [added aflatoxin B_1 not transferred intact to smoke]	158a, 2024, 2484, 3721, 3970, 3975 [not found in tobacco]	
342.	7220-81-7	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,8,9,9a-hexahydro-4-methoxy-, (6aR-*cis*)-{aflatoxin B_2}		4039b, 4254, 4754	
343.	1211-29-6	Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester {methyl jasmonate}		5811, 5811b	
344.	28473-29-2	Cyclopentanedione{two isomers}	1378, 4249		1378
345.	3008-40-0	1,2-Cyclopentanedione	91, 2493, 3553, 4249, 5811b	2917a	3401, 3402, 3404, 3405
346.		1,2-Cyclopentanedione, 4-acetyl-		737, 4249	
347.		1,2-Cyclopentanedione, 3,4-diethyl-	91, 1352, 1586, 2767, 2773, 4249		
348.	54362-49-1	1,2-Cyclopentanedione, 3,5-diethyl-	91, 1352, 1582, 4249		
349.	72692-92-3	1,2-Cyclopentanedione, 3,3-dimethyl-	91, 568b, 1063–1066, 1068–1074, 1365, 1367, 3553, 4249	568b, 3547, 4249	
350.	13494-06-9	1,2-Cyclopentanedione, 3,4-dimethyl-	91, 568b, 1063–1066, 1068–1074, 1215, 1352, 1586, 2543, 2545, 2767, 3266, 3553, 3557, 4249, 4570a, 5811b	172a, 174b, 568b, 1053, 4266	
351.	13494-07-0	1,2-Cyclopentanedione, 3,5-dimethyl-	91, 568b, 1352, 1375, 1375b, 1378, 1586, 2327c, 2767, 3266, 3553, 3557, 4249, 5811b	568b, 1053, 3266	1378
352.	13494-08-1	1,2-Cyclopentanedione, 3-ethyl-	91, 568b, 1352, 1360, 1365, 1375, 1375a, 1375b, 1586, 2761, 2762, 2765–2767, 3553, 3557, 4249, 5811b		1360, 1375a, 3402

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
353.		1,2-Cyclopentanedione, 3-ethyl-3-methyl-	91, 1364, 1367, 4249		
354.		1,2-Cyclopentanedione, 3-ethyl-4-methyl-	91, 1378		1378, 4249
355.	71608-11-2	1,2-Cyclopentanedione, 3-ethyl-5-methyl- = 1,2-Cyclopentanedione, 5-ethyl-3-methyl-	91, 1063–1066, 1068–1074, 1352, 1364, 1375, 1375b, 1378, 4249		1378, 4249
356.		1,2-Cyclopentanedione, hydroxy-	1367, 4249		
357.	765-70-8	1,2-Cyclopentanedione, 3-methyl- {cyclotene}	91, 172, 775, 1063–1066, 1068–1074, 1352, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1744, 1842, 1882, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3266, 3394, 3397, 3410, 3553, 3557, 4249, 4570a, 5512	174b, 2386, 2389, 2544, 3266, 3905, 4249, 5811b	1360, 1375a, 1377, 1378, 2387, 3401, 3402, 3405
358.	60386-55-2	1,2-Cyclopentanedione, 3-(1-methylethyl)-	91, 568b, 1352, 1586, 2767, 3557, 4249		
359.	72693-09-5	1,2-Cyclopentanedione, 4-(1-methylethyl)-	91, 1587, 4249, 5811b		
360.	71608-12-3	1,2-Cyclopentanedione, 3-methyl-5-propyl-	91, 1352, 1582, 1586, 4249		
361.	69745-71-7	1,2-Cyclopentanedione, 3-phenyl-	568b, 1586, 2767, 3226, 3557, 4249		
362.	4542-64-7	1,2-Cyclopentanedione, 4-phenyl-	568b, 1586, 4249		
363.	23747-37-7	1,2-Cyclopentanedione, 3-propyl-	91, 568b, 1582, 1586, 2767, 3557, 4249		
364.	3859-41-4	1,3-Cyclopentanedione	568b, 4249, 5034, 5811b	568b, 2917a, 4249	
365.	34598-80-6	1,3-Cyclopentanedione, 2,4-dimethyl-	1352, 3553, 4249, 5811b		
366.	823-36-9	1,3-Cyclopentanedione, 2-ethyl-	568b, 1352, 3553, 4249, 5811b		
367.	765-69-5	1,3-Cyclopentanedione, 2-methyl-	568b, 1352, 3553, 4249, 5811b		
368.		1,4-Cyclopentanedione, 2-hydroxy-3,5,5-trimethyl-	568b, 4249		
369.	120-92-3	Cyclopentanone {adipic ketone}	299, 314, 568b, 722, 1063–1066, 1068–1074, 1140, 1238, 1348–1350, 1354, 1365, 1371, 1374, 1375a, 1377, 1378, 1416, 1418, 1419, 1586, 1589, 1634, 2506, 2507, 2508, 2543, 2545, 2570, 2731, 2735, 2761, 2762, 2765, 2767, 2773, 2777, 2799a, 2857, 3255, 3308, 3410, 3530, 3553, 3557, 3797, 3897, 4249, 4360, 4570a, 5034, 5770, 5811b	404, 568b, 2386, 4249	642, 1354, 1375a, 1377, 1378, 2244, 2506 (0), 2507 (0), 3401, 3402, 3404, 4249

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

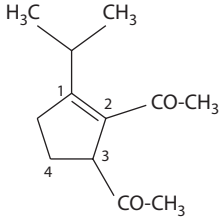
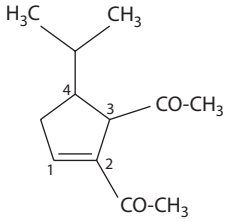
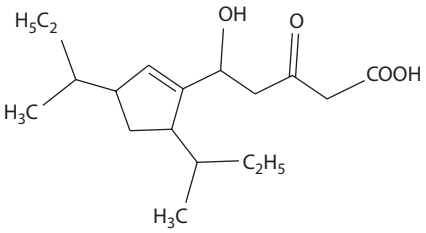
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
370.	55713-44-5	Cyclopentanone, 2,2-dimethyl-4-(2-oxopropyl)-		4249, 4780	
371.	1121-33-1	Cyclopentanone, 2,4-dimethyl-	568b, 4249		
372.	20030-85-7	Cyclopentanone, 2,4-dimethyl- {isomer}	568b, 4249		
373.	4041-09-2	Cyclopentanone, 2,5-dimethyl-	3559		
374.	4971-18-0	Cyclopentanone, 2-ethyl-	4570a		
375.	10264-55-8	Cyclopentanone, 3-ethyl-	1368, 4249		
376.		Cyclopentanone, 2-ethylidene-	2387, 4249		
377.	473-84-7	Cyclopentanone, 2-hydroxy-	5811b		3404, 3405, 4249
378.	28631-88-1	Cyclopentanone, methyl-	1215, 3530, 4249, 4800, 5811b		
379.	1120-72-5	Cyclopentanone, 2-methyl-	642, 1365, 1371, 1422, 2387, 2545, 2777, 3255, 4249, 5770		2387
380.		Cyclopentanone, 2-(1-methylpropyl)-	4570a		
381.	1757-42-2	Cyclopentanone, 3-methyl-	299, 1140, 1348–1350, 1354, 1365, 1371, 1375a, 1360, 1375a, 1378, 1419, 1586, 1589, 2543, 2545, 2765, 2767, 2777, 3255, 3410, 4249, 4570a, 5770		642, 1354, 1360, 1375a, 1378, 4249
382.		Cyclopentanone, 3-methyl- {isomer}	5770		
383.		Cyclopentene, 2-acetyl-4-hydroxy-4-(1-methylethyl)-		3543	
384.		Cyclopentene, 2,3-diacetyl-1-(1-methylethyl)- 		3543	
385.		Cyclopentene, 2,3-diacetyl-4-(1-methylethyl)- 		3543, 3545	
386.	28750-51-8	3-Cyclopentene-1,2-dione	1367, 4249, 5811b	5811b	
387.		3-Cyclopentene-1,2-dione, 3,4-dimethyl-	91, 2570		
388.	2687-69-6	3-Cyclopentene-1,2-dione, 3,5-dimethyl-	91, 1378, 2570, 2769, 4249		1378, 4249
389.		3-Cyclopentene-1,2-dione, 3-ethyl-4-methyl-	91, 1378, 2543, 2773, 4249		1378, 4249

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
390.	10130-95-7	3-Cyclopentene-1,2-dione, 3-methyl-	91, 1375, 1375b, 2387, 4249		
391.	66309-79-3	3-Cyclopentene-1,2-dione, 4-methyl-	91, 2769, 4249		
392.	930-60-9	4-Cyclopentene-1,3-dione		568b, 2917a, 4249	3401
393.		4-Cyclopentene-1,3-dione, 2,4-dimethyl-	568b, 4249		
394.	18515-43-0	4-Cyclopentene-1,3-dione, 4,5-dimethyl-	2767, 2769, 3404, 4249, 5811b		3404, 4249
395.	53109-18-5	1-Cyclopentene-1-pentanoic acid, δ-hydroxy-3,5-bis(1-methylpropyl)-β-oxo- 		4249	
396.	28982-58-3	Cyclopentenone	1375a, 1377, 1378, 2508, 4249		1375a, 1377, 1378
397.	930-30-3	2-Cyclopenten-1-one {cyclopenten-3-one}	299, 568b, 1063–1066, 1068–1074, 1099, 1338, 1339, 1352, 1365, 1371, 1378, 1422, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2628, 2629, 2636, 2731, 2735, 2773, 2777, 2857, 3255, 3397, 3410, 3530, 3559, 4249, 5034, 5811b	568b, 2386, 4249	1378, 2387, 2506, 2507, 2244, 3401, 3402, 3404, 3405, 4249
398.		2-Cyclopenten-1-one, C_3-alkyl-	1063–1066, 1068–1074, 1365, 1371, 2543, 2570, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 3410, 3559, 4249		
399.		2-Cyclopenten-1-one, C_4-alkyl-	1365, 1371, 2543, 2570, 2767, 2775		
400.	72692-71-8	2-Cyclopenten-1-one, dimethyl-	312, 1360, 1371, 1375a, 2761, 2762, 2765, 2766, 2773, 2777, 3255, 3410, 4249		1360, 1375a
401.	65462-39-7	2-Cyclopenten-1-one, ethyl-	5811, 5811a, 5811b		
402.	61205-39-8	2-Cyclopenten-1-one, ethyl-2-hydroxy-	92, 93		
403.		2-Cyclopenten-1-one, ethylmethyl-	1371, 2761, 2762, 2765, 2766, 2777, 4249		
404.	65452-01-9	2-Cyclopenten-1-one, methyl-	2570, 5811b		
405.		2-Cyclopenten-1-one, phenyl-	1378, 2506, 2507		1378, 2506, 2507

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

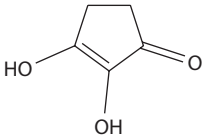
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
406	65436-85-3	2-Cyclopenten-1-one, propyl-	5811, 5811a, 5811b		
407	82000-05-3	2-Cyclopenten-1-one, trimethyl-	2775, 2777, 5811a		
408	17190-74-8	2-Cyclopenten-1-one, 2-(2-butenyl)-4-hydroxy-3-methyl-		404	
409	78210-65-8	2-Cyclopenten-1-one, 2-(2-furanyl)-	568b, 1587, 4249, 5811b		
410	61892-84-0	2-Cyclopenten-1-one, 2-(2-oxopropyl)-	568b, 1350, 1352, 1354, 1375a, 1360, 1375a, 2767, 2769, 3553, 4249, 5811b		1354, 1360, 1375a
411.	80-72-8	2-Cyclopenten-1-one, 2,3-dihydroxy- {reductic acid} 	92, 93, 1352, 1375a, 1377, 1882, 2939, 3127, 3302, 3797, 4079, 4249, 5811b		1375a, 1377, 3402
412.	1121-05-7	2-Cyclopenten-1-one, 2,3-dimethyl-	568b, 1075, 1063–1066, 1068–1074, 1099, 1360, 1365, 1371, 1375a, 1378, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2628, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 3255, 3397, 3410, 3553, 3557, 3559, 4249, 4570a, 5811b	404, 568b, 937, 1256, 2389, 2544, 4249, 5811b	1360, 1375a, 1378, 2387, 2506, 2507
413.	3779-64-4	2-Cyclopenten-1-one, 2,3-dimethyl-4-(1-methylethyl)-	1352, 3553, 4249, 5811b		
414.	61893-14-9	2-Cyclopenten-1-one, 2,3-dimethyl-5-(1-methylethyl)-	1352, 3553, 4249, 5811b	404	
415.	28790-86-5	2-Cyclopenten-1-one, 2,3,4-trimethyl-	3557, 4249, 4570a, 5811b	404	
416.	54562-24-2	2-Cyclopenten-1-one, 2,3,5-trimethyl-	568b, 1075, 1063–1066, 1068–1074, 1352, 1360, 1364, 1371, 1375a, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2769, 2773, 2775, 2777, 3410, 3557, 3559, 4249		1360, 1375a
417.	66309-82-8	2-Cyclopenten-1-one, 2,4,5-trimethyl-	568b, 1378, 2767, 2769, 3557, 4249		1378
418.	23048-13-7	2-Cyclopenten-1-one, 2,4-dimethyl-	568b, 1352, 1360, 1375a, 1587, 2543, 2545, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 3255, 3410, 4249, 4570a, 5811b		1360, 1375a
419.	4041-11-6	2-Cyclopenten-1-one, 2,5-dimethyl-	568b, 1063–1066, 1068–1074, 1365, 1371, 2543, 2761, 2762, 2765, 2766, 2769, 2773, 2775, 3410, 4249, 4570a, 5811b		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
420.	2931-10-4	2-Cyclopenten-1-one, 2-ethyl-	299, 1352, 1364, 1371, 1378, 2545, 2767, 2775, 3688, 4064, 4249, 4570a		1378
421.	5682-72-4	2-Cyclopenten-1-one, 2-ethyl-3-methyl-	568b, 1063–1066, 1068–1074, 1352, 1364, 1371, 1378, 1586, 2506, 2507, 2767, 2777, 3410, 3557, 4249, 5811b		1378, 2506, 2507, 4249
422.	78210-64-7	2-Cyclopenten-1-one, 2-ethyl-5-methyl-	568b, 1364, 1371, 1587, 2775, 2777, 3410, 4249, 5811b		
423.	10493-98-8	2-Cyclopenten-1-one, 2-hydroxy-	93, 5811, 5811a, 5811b		
424.	29798-72-9	2-Cyclopenten-1-one, 2-hydroxy-3-(1-butyl)-	93, 5811, 5811b		
425.	80-71-7	2-Cyclopenten-1-one, 2-hydroxy-3-methyl- {methylcyclopentenolone}	92, 93, 596, 597, 1099, 1133, 1375, 1375b, 1586, 1958, 1960, 2327c, 2337, 2387, 2493, 2601a, 3255, 3266, 3553, 3555, 3557, 4249, 5034, 5811b	174b, 1053, 2337, 2389, 2544, 3266, 3370, 3430, 3555, 4249, 5811b	2387, 3402, 3404
426.	109682-92-0	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylbutyl)-	93, 5811b		
427.	109682-91-9	2-Cyclopenten-1-one, 2-hydroxy-3-(3-methylbutyl)-	93, 5811b		
428.	109682-81-7	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-(1-methylethyl)-	93, 5811b		
429.	55277-47-9	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylethyl)-	93, 5811, 5811a, 5811b		
430.	29798-73-0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylpropyl)-	93, 5811, 5811a, 5811b		
431.	25684-05-3	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylpropyl)-	93, 5811, 5811a, 5811b		
432.	109682-89-5	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-propyl-	93, 5811b		
433.	109682-85-1	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-5-propyl-	92, 93, 1586, 5811b		
434.	15899-72-6	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-	93, 5811, 5811a, 5811b		
435.	109682-88-4	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-3-propyl-	93, 5811b		
436.	55007-08-4	2-Cyclopenten-1-one, 2-hydroxy-3-pentyl-	93		
437.	25684-04-2	2-Cyclopenten-1-one, 2-hydroxy-3-propyl-	92, 93, 1352, 1586, 1587, 4249, 5811b		
438.	82147-26-0	2-Cyclopenten-1-one, 2-hydroxy-4-propyl-	92, 93, 568b, 1587, 4249, 5811b		
439.	61205-40-1	2-Cyclopenten-1-one, 2-hydroxypropyl-	4249	4249	
440.	109682-87-3	2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl-	93, 5811b		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
441.	22323-97-3	2-Cyclopenten-1-one, 2-methoxy-	5811, 5811a, 5811b		3404, 4249
442.	14189-85-6	2-Cyclopenten-1-one, 2-methoxy-3-methyl-	1371, 2543, 2773, 2775, 3410, 4249		
443.	1120-73-6	2-Cyclopenten-1-one, 2-methyl-	299, 568b, 1063–1066, 1068–1074, 1099, 1360, 1365, 1371, 1375a, 1378, 1958, 1960, 2493, 2506, 2507, 2543, 2545, 2731, 2735, 2761, 2762, 2765, 2766, 2773–2775, 2777, 2857, 3255, 3397, 3410, 3530, 4054, 4249, 4570a, 5770, 5811b	568b, 2386, 4249	1360, 1375a, 1378, 2506, 2507, 3402
444.	5760-58-7	2-Cyclopenten-1-one, 2-methyl-3-propyl-	3387, 4249		
445.	61892-83-9	2-Cyclopenten-1-one, 2-methyl-4-(1-methylethyl)-	568b, 1352, 3553, 4249, 5811b		
446.	31089-17-5	2-Cyclopenten-1-one, 2-methyl-5-(1-methylethyl)-	1352, 3553, 4249, 5811b		
447.	66309-80-6	2-Cyclopenten-1-one, 2-methyl-5-methylene-	2769, 4249		
448.	24105-07-5	2-Cyclopenten-1-one, 2-propyl-	1352, 1422, 2506, 2507, 4054, 4249, 5811b	5811b	2506, 2507
449.		2-Cyclopenten-1-one, 3-(2-furanyl)-	2543, 2773, 2775, 4249		
450.	1619-28-9	2-Cyclopenten-1-one, 3-(1-methylethyl)-	568b, 1587, 4249, 5811b		
451.	21835-00-7	2-Cyclopenten-1-one, 3,4-diethyl-2-hydroxy-	93, 5811, 5811a, 5811b		
452.	30434-64-1	2-Cyclopenten-1-one, 3,4-dimethyl-	568b, 1075, 1352, 1360, 1371, 1375a, 1378, 1587, 2506, 2507, 2570, 2761, 2762, 3410, 4249, 4570a, 4633, 5770, 5811b		1360, 1375a, 1378, 2506, 2507, 4249
453.	21835-00-7	2-Cyclopenten-1-one, 3,4-dimethyl-2-hydroxy-	92, 93, 1586, 5811, 5811a, 5811b		
454.	72692-76-3	2-Cyclopenten-1-one, 3,4-dimethyl-2-(1-methylethyl)-		3547	
455.	52808-97-6	2-Cyclopenten-1-one, 3,5-diethyl-2-hydroxy-	92, 93, 1586, 5811, 5811a, 5811b		
456.	931-22-6	2-Cyclopenten-1-one, 3,5-dimethyl-	299, 568b, 1352, 1360, 1364, 1371, 1375a, 1378, 2543, 2545, 2570, 2761, 2762, 2767, 2773, 2775, 2777, 2769, 3410, 4249	404, 568b, 4249	1360, 1375a, 1378, 4249
457.	109682-90-8	2-Cyclopenten-1-one, 3,5-dimethyl-4-ethyl-2-hydroxy-	93		
458.	21834-98-0	2-Cyclopenten-1-one, 3,5-dimethyl-2-hydroxy-	93, 1364, 1586, 5811, 5811a, 5811b		
459.		2-Cyclopenten-1-one, 3,5-dimethyl-2-(1-methylethyl)-		3547	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

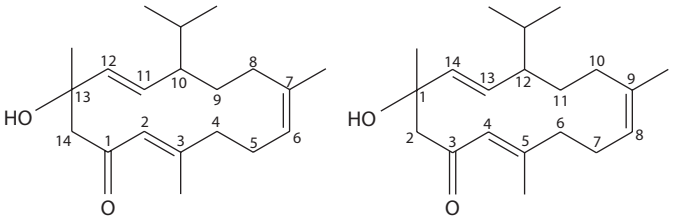
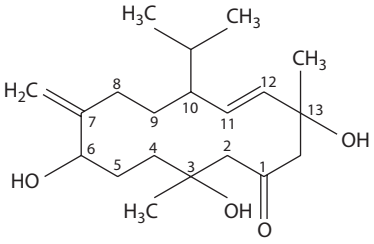
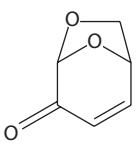
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
460.	5682-69-9	2-Cyclopenten-1-one, 3-ethyl-	568b, 1063–1066, 1068–1074, 1352, 1375, 1375b, 1378, 1586, 2387, 2506, 2507, 2543, 2545, 2570, 2767, 2773, 2775, 3557	404, 568b, 4249	1378, 2387, 2506, 2507
461.	21835-01-8	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- {ethylcyclopentenolone}	92, 93, 1063–1066, 1068–1074, 1133, 1364, 1367, 2857, 3266, 4249	172a, 174b, 1053, 1133, 2917a, 3266, 4249	3402
462.	42348-12-9	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-4-methyl-	93, 5811, 5811a, 5811b		
463.	58228-72-1	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-5-methyl-	93, 5811, 5811a, 5811b		
464.		2-Cyclopenten-1-one, 3-ethyl-2-methoxy-	1367, 4249		
465.	41496-77-9	2-Cyclopenten-1-one, 3-ethyl-2-methyl-	568b, 1352, 1360, 1375a, 1378, 2543, 2545, 2761, 2762, 2765–2767, 2773, 2775, 3557, 4249	404, 568b, 4249	1360, 1375a, 1378, 4249
466.	78210-63-6	2-Cyclopenten-1-one, 3-ethyl-4-hydroxy-	568b, 1587, 4249, 5811b		
467.		2-Cyclopenten-1-one, 3-ethyl-4-methyl-	568b, 1378, 4249		1378, 4249
468.		2-Cyclopenten-1-one, 3-ethyl-5-methyl-	1360, 1375a, 1378		1360, 1375a, 1378
469.	5870-63-3	2-Cyclopenten-1-one, 3-hydroxy-2-methyl-		3072a, 3430, 5811b	
470.	2758-18-1	2-Cyclopenten-1-one, 3-methyl-	568b, 1063–1066, 1068–1074, 1339, 1352, 1360, 1364, 1365, 1375, 1375a, 1375b, 1378, 1586, 2387, 2493, 2543, 2570, 2628, 2762, 2765–2767, 2773, 2775, 2777, 2857, 3255, 3397, 3410, 3530, 3553, 3557, 3559, 4249, 4570a, 5811b	404, 568b, 2386, 2389, 2544, 4249, 5811b	1360, 1375a, 1378, 2387, 4249
471.	3727-35-3	2-Cyclopenten-1-one, 3-methyl-2-(2-oxopropyl)-	568b, 1352, 2769, 3553, 5811b	568b, 2389, 2544, 4249, 5811b	
472.		2-Cyclopenten-1-one, 3-methyl-2-(1,3-pentadienyl)-	4570a		
473.	488-10-8	2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (*Z*)-		4096a, 5811b	
474.		2-Cyclopenten-1-one, 3-(2-oxopropyl)-	2767, 3553, 4249		
475.	3810-26-2	2-Cyclopenten-1-one, 3-phenyl-	2775		
476.	35953-18-5	2-Cyclopenten-1-one, 3-propyl-	568b, 1422, 2506, 2507, 2775, 3650, 4249, 5811b		2506, 2507
477.	30434-65-2	2-Cyclopenten-1-one, 3,4,4-trimethyl-		2917a	
478.	24156-95-4	2-Cyclopenten-1-one, 3,5,5-trimethyl-	5811, 5811a, 5811b		
479.		2-Cyclopenten-1-one, 4-acetoxy-3-methyl-	568b, 4249		
480.		2-Cyclopenten-1-one, 4-acetyl-3,5,5-trimethyl-	568b. 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
481.	28017-62-1	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-	93, 5811, 5811a, 5811b		
482.	71387-71-8	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-3-methyl-	93, 5811b		
483.	71278-13-2	2-Cyclopenten-1-one, 4-ethyl-2-methyl-	1352, 2767, 3557, 4249		
484.	30434-68-5	2-Cyclopenten-1-one, 4-ethyl-3-methyl-	568b, 4249		
485.	10288-24-1	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-	568b, 1586, 2767, 3553, 3557, 4249		
486.	23415-96-7	2-Cyclopenten-1-one, 4-methyl-	1371, 3410, 4249		
487.	66309-81-7	2-Cyclopenten-1-one, 4-methyl-3-(1-propenyl)-	1352, 2767, 2769, 4249		
488.	53263-58-4	2-Cyclopenten-1-one, 5-ethyl-2-hydroxy-3-methyl-	92, 93, 1586, 5811, 5811a, 5811b		
489.	70919-26-5	2-Cyclopenten-1-one, 5-hydroxy-		4249	3401, 3402, 3405, 4249
490.	70919-27-6	2-Cyclopenten-1-one, 5-hydroxy-3-methyl-	1371, 1586, 2767, 2774, 3553, 4249		
491.	14963-40-7	2-Cyclopenten-1-one, 5-methyl-	1075, 1365, 1371, 2545, 2775, 3410, 4249		
492.	14320-37-7	3-Cyclopenten-1-one	1422, 4249		
493.		3-Cyclopenten-1-one, 3-(1-methylethyl)-		3547, 4249	
494.	90660-18-7	4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-(1-methylethyl)-,		4249, 4811, 5811b	
495.	119613-98-8	5,10-Cyclotetradecadien-1-one, 7,9-dihydroxy-7,11-dimethyl-4-(1-methylethyl)-, [4S-(4R*,5*E*,7R*,9S*,10*E*)]-		4249, 5811b	
496.	149312-90-3	2,6,11-Cyclotetradecatrien-1-one, 5,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-, [5S-(2*E*,5R*,6*E*,10R*,11*E*,13R*)]-		4249	
497.	98064-74-5	2,5,11-Cyclotetradecatrien-1-one, 7,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-, [7S-(2*E*,5*E*,7R*,10R*,11*E*,13R*)]-		4098, 4249, 5811b	
498.	149312-89-0	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-, [6S-(2*E*,6R*,7*E*,9R*,11S*,12*E*)]-		4249	
499.	149403-72-5	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-, [6S-(2*E*,6R*,7*E*,9S*,11S*,12*E*)]-		4249	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
500.	41429-54-3	2,6,11-Cyclotetradecatrien-1-one, 13-hydroxy-3,7,13-trimethyl-10-(1-methylethyl)- = 4,8,13-Cyclotetradecatrien-1-ol-3-one,-1,5,9-trimethyl-12-(1-methylethyl)-, 	1364	671, 1149, 1149a, 1591, 4089, 4249, 4401, 4780, 5811b	
501.		1-Cyclotetradecen-1-one, 3,6,13-triol-3,13-dimethyl-7-methylene-10-(1-methylethyl)- 		94a	
502.	59286-28-1	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*Z,E*)- H_3C-CO-$(CH_2)_2$-CH[CH$(CH_3)_2$]-CH═CH-C(CH_3)═CH-COOH		2, 736, 1156, 4090, 4249	
503.	58315-84-7	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, [S-(*E,E*)]-		2, 736, 1156, 4090, 4249	
504.	59262-52-1	2,7-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*E,E*)- H_3C-CO-CH═CH-CH[CH$(CH_3)_2$]-(CH_2)2-CH(CH_3)═CH-COOH		2, 731, 738, 1156, 4090, 4249	
505.		Decanoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-	2092, 4249	2092, 4249	
506.	693-54-9	2-Decanone {methyl octyl ketone}	568b, 2570, 2769, 3410, 4249	568b, 1662, 4249	
507.	60924-66-5	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-		737, 4249	
508.	129777-23-7	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-, [R-[R*,S*-(*E*)]]-		737, 4249, 5811b	
509.	77288-98-3	6-Decen-2-one, 8,10-dihydroxy-8-methyl-5-(1-methylethyl)-		4249, 4948	
510.	1210-35-1	5*H*-Dibenzo[*a,d*]cyclohepten-5-one, 10,11-dihydro-	278, 4249		
511.	37112-31-5	6,8-Dioxabicyclo[3.2.1]oct-2-en-4-one, (1S)- {levoglucosenone} 	1350, 1354, 1375a, 1377, 2388, 2777, 4249, 5811b	3430, 5811b	1350, 1375a, 1377, 2387, 2388, 4249

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

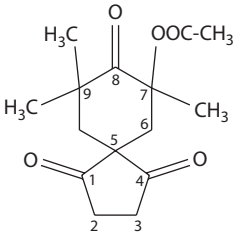
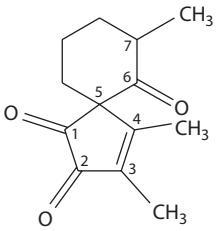
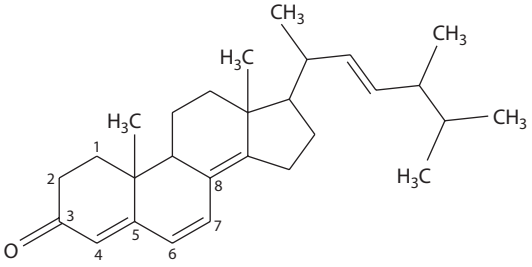
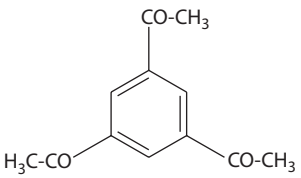
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
512.	162188-91-2	1,4-Dioxaspiro[4.5]decan-8-one, 7-(acetyloxy)-7,9,9-trimethyl-, (±)- 	4249		
513.	41059-94-3 51607-05-7	1,6-Dioxaspiro[4.5]dec-3-en-2-one, 3,4,7-trimethyl- 		568b, 1087, 4249, 5811, 5811b	
514.		2,4-Dodecadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-		9	
515.	117232-64-1	5,10-Dodecadien-2-one, 9-hydroxy-6,11-dimethyl-		3285, 4249, 5811b	
516.	6175-49-1	2-Dodecanone $H_3C\text{-}(CH_2)_9\text{-}CO\text{-}CH_3$	3387, 4249		
517.	19254-69-4	Ergosta-4,6,8(14),22-tetraen-3-one, (22*E*)- 		334, 3866, 4249	
518.	80736-41-0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R,23R,24S)-		4249	
519.	121468-15-3	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3β,5α,22R,23R,24S)-		429c	
520.	92751-21-8	Ergostan-6-one, 3,22,23-trihydroxy-, (3β,5α,22R,23R,24S)-		429c	
521.	87734-68-7	Ergostan-6-one, 3,22,23-trihydroxy-, (3α,5α,22R,23R,24S)-		429c	
522.	134-81-6	Ethanedione, diphenyl- {benzil} $C_6H_5\text{-}CO\text{-}CO\text{-}C_6H_5$	568b, 3553, 4249, 5811b		
523.		Ethanone, 1-(alkyl-1*H*-pyrrolyl)-	2773		
524.	6004-60-0	Ethanone, 1-cyclopentyl-	5034		
525.	765-43-5	Ethanone, 1-cyclopropyl-	5770		
526.	78210-69-2	Ethanone, 1-(1,2-dihydro-2-methyl-3-pyridinyl)-	568b, 1587, 4249, 5811b		
527.		Ethanone, 1-(1,2-dihydro-1*H*-pyrrolyl)-	568b, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
528.		Ethanone, 1-(1-ethyl-1*H*-pyrrol-3-yl)-	568b, 4249		
529.	117210-49-8	Ethanone, 1-(1,4,4a,5,6,7,8,8a-octahydro-4a,8,8-trimethyl-2-naphthalenyl)-, (4aR-*trans*)-		4249, 5811b	
530.	932-66-1	Ethanone, 1-(1-cyclohexen-1-yl)-	37, 38, 4249, 4425		
531.		Ethanone, 1-(dimethylphenyl)- {dimethylacetophenone}	2570		
532.	26444-19-9	Ethanone, 1-(methylphenyl)- {methylacetophenone}	1427, 2387, 2570, 4249, 5811b		2387
533.	78249-87-3	Ethanone, 1-(methylpyridinyl)- {two isomers}	1587, 4249, 4570a, 5811, 5811a, 5811b		
534.		Ethanone, 1-(methyl-1*H*-pyrrolyl)-	2543, 2761, 2765–2767, 2773, 3557, 4249		
535.	941-98-0	Ethanone, 1-(1-naphthalenyl) {1′-acetonaphthone}	5811, 5811a, 5811b		
536.	20583-33-9	Ethanone, 1-(1*H*-pyrazol-3-yl)-		4249	
537.	25016-16-4	Ethanone, 1-(1*H*-pyrazol-4-yl)-		984, 4249	
538.	1072-83-9	Ethanone, 1-(1*H*-pyrrol-2-yl)- {2-acetylpyrrole; methyl 2-pyrrolyl ketone}	568b, 1360, 1371, 1375a, 1375, 1375b, 1428, 1586, 1587a, 2337, 2387, 2543, 2545, 2570, 2731, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3059, 3266, 3397, 3410, 3444, 3553, 3555, 3557, 4249, 4407, 5811b	120, 172a, 174b, 404, 568b, 937, 965, 1053, 1063–1066, 1068–1074, 1590a, 1854, 2337, 2386, 2389, 2544, 2861a, 2862, 2917a, 2939, 3188, 3198, 3215, 3217, 3266, 3354, 3543, 3545, 3547, 3555, 3560, 3561, 3797, 3905, 3974a, 4249, 5811b	1360, 1375a, 2387
539.	1072-82-8	Ethanone, 1-(1*H*-pyrrol-3-yl)- {3-acetylpyrrole; methyl 3-pyrrolyl ketone}	568b, 1371, 1586, 1587, 2543, 2767, 2769, 2773, 2775, 3255, 3410, 3553, 3557, 4249	568b, 3549, 4249	
540.	711-79-5	Ethanone, 1-(1-hydroxy-2-naphthalenyl)-	4249	3430, 5811b	
541.	20970-50-7	Ethanone, 1-(1-methyl-1*H*-imidazol-5-yl)-	568b, 1587, 1590, 2775, 4249, 5811b		
542.	37687-18-6	Ethanone, 1-(1-methyl-1*H*-pyrazol-4-yl)-	3553, 4249		
543.	932-16-1	Ethanone, 1-(1-methyl-1*H*-pyrrol-2-yl)-	568b, 1360, 1375a, 2387, 3491, 4249, 4570a, 5811b	568b, 984, 1248, 3201, 3215, 3491, 3974a, 4249	1360, 1375a, 2387
544.	932-62-7	Ethanone, 1-(1-methyl-1*H*-pyrrol-3-yl)-	568b, 1587, 3491, 4249, 4570a, 5811b	568b, 937, 1248, 3491, 3974a, 4249	
545.	70987-81-4	Ethanone, 1-(1,2,3-trimethyl-2-cyclopenten-2-yl)-	2601a	2917a	
546.	779-90-8	Ethanone, 1,1′,1″-(1,3,5-benzenetriyl) tris- {1,3,5-triacetylbenzene} 		4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

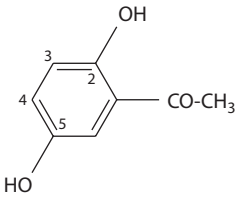
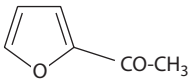
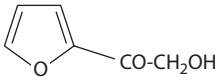
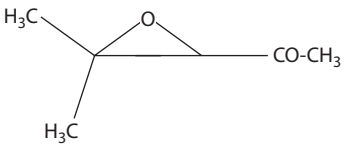
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
547.		Ethanone, 1-(2-alkylphenyl)-	2761, 4249		
548.	55041-85-5	Ethanone, 1-(2,3-dihydro-1*H*-pyrrolizin-5-yl)-	568b, 2543, 2773, 4249	568b, 3547, 4249	
549.		Ethanone, 1-(2,3-dihydrothiophen-2-yl)-	568b, 4249		
550.	19005-95-9	Ethanone, 1-(2,4,5-trimethyl-1*H*-pyrrol-3-yl)-	2543, 2773, 4249		
551.	1667-01-2	Ethanone, 1-(2,4,6-trimethylphenyl)-	5811b		
552.	85213-22-5	Ethanone, 1-(2,5-dihydro-1*H*-pyrrol-2-yl)- {2-acetylpyrroline}		2917a	
553.		Ethanone, 1-(2,5-dihydro-5-methyl-1*H*-pyrrol-3-yl)-	2767		
554.	490-78-8	Ethanone, 1-(2,5-dihydroxyphenyl)- 	568b, 1884, 3553, 3557, 3712, 4249, 5811b		
555.	1500-94-3	Ethanone, 1-(2,5-dimethyl-1*H*-pyrrol-3-yl)-	1375, 1375b, 2767, 3410, 3557		
556.	1197-92-8	Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-		3547, 4249	
557.	699-83-2	Ethanone, 1-(2,6-dihydroxyphenyl)-	3712		
558.	1192-62-7	Ethanone, 1-(2-furanyl)- {2-acetylfuran} 	37, 38, 339, 568b, 1140, 1215, 1238, 1338, 1339, 1365, 1371, 1378, 1419, 1427, 1586, 1590, 1958, 1960, 2337, 2387, 2506, 2507, 2543, 2545, 2570, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 3255, 3397, 3410, 3530, 3555, 3797, 4249, 4407, 4570a, 5034, 5811b	404, 568b, 937, 953, 984, 1590, 1590a, 2337, 2339a, 2386, 2389, 2544, 2917a, 3188, 3547, 3555, 3561, 4249	1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404
559.	19859-79-1	Ethanone, 1-(2-furanyl)-2-(acetyloxy)-	568b, 1375, 1375b, 1586, 2767, 3553, 3557, 5811b		
560.	17678-19-2	Ethanone, 1-(2-furanyl)-2-hydroxy- 	568b, 3553, 3557, 4249, 5811b	568b, 3797, 4249	3402, 3404, 3405, 4249
561.	703-98-0	Ethanone, 1-(2-hydroxy-3-methoxyphenyl)-	568b, 1375, 1375b, 3712, 4249		
562.	6921-64-8	Ethanone, 1-(2-hydroxy-4-methylphenyl)-		568b, 547, 4249	
563.	1450-72-2	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	2601a, 4249	937, 4249	
564.	703-23-1	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-	2570, 3712		
565.		Ethanone, 1-(2-hydroxy-6-methylphenyl)-		2338	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
566.	118-93-4	Ethanone, 1-(2-hydroxyphenyl)-	1238, 1360, 1375a, 1378, 1586, 1884, 2327c, 2387, 2767, 3557, 3712, 3797, 4036, 5811b	120, 2862, 2939, 3059, 4249, 5811b	1360, 1375a, 1378, 2387, 3395
567.	78210-66-9	Ethanone, 1-(2-methyl-1*H*-imidazol-4-yl)-	568b, 1587, 4249, 5811b		
568.	577-16-2	Ethanone, 1-(2-methylphenyl)- {2-methylacetophenone}	1360, 1371, 1375a, 1586, 2506, 2507, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3557, 4249, 5811b	404, 1254, 2336, 2389, 2544, 3550, 5811b	1360, 1375a, 2506, 2507
569.		Ethanone, 1-[2-methyl-5-(1-methylethyl)-phenyl]-		3973	
570.	1122-62-9	Ethanone, 1-(2-pyridinyl)- {2-acetylpyridine}	1099, 1360, 1371, 1375a, 1587, 1949, 2234, 2543, 2727, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2939, 3056, 3255, 3266, 3398, 3491, 3557, 4249, 4570a, 5034, 5811b	937, 1053, 1949, 2336, 2337a, 2339a, 2359, 2724, 2917a, 2939, 3056, 3204, 3215, 3266, 3491, 3550, 3974a, 4159a, 4249	1360, 1375a
571.	60026-20-2	Ethanone, 1-(2-pyrrolidinyl)- {2-acetylpyrrolidine}	2727, 2775, 3410, 3491, 3650, 4159	937, 1154, 2095, 2389, 2544, 3219, 3491, 3550, 3560, 3561, 3974a	
572.	24295-03-2	Ethanone, 1-(2-thiazolyl)-		172a, 174b, 1053, 3266, 3370	
573.	88-15-3	Ethanone, 1-(2-thienyl)-		937, 4249	
574.		Ethanone, 1-[2,3-dihydro-2-(1-methylethyl)-inden-4-yl]-		3547, 4249	
575.		Ethanone, 1-[3,4-dihydro-6-(1-methylethyl)-inden-4-yl]-pyran-2-yl]-		3547, 4249	
576.		Ethanone, 1-(3,4-dihydro-4-methylpyrazin-2-yl)-		3547, 4249	
577.	1197-09-7	Ethanone, 1-(3,4-dihydroxyphenyl)-	3712	5811b	
578.	1131-62-0	Ethanone, 1-(3,4-dimethoxyphenyl)-	2570, 2769, 4249, 5811b	1256, 4249, 5811b	
579.	4478-63-1	Ethanone, 1-(3,3-dimethyloxiranyl)- {mesityl oxide epoxide}		404	
					
580.	89-74-7	Ethanone, 1-(2,4-dimethylphenyl)-		603**,** 1053, 3266, 3370	
581.	3637-01-2	Ethanone, 1-(3,4-dimethylphenyl)-	1586, 2767, 2769, 3266, 3557, 4249		
582.	51863-60-6	Ethanone, 1-(3,5-dihydroxyphenyl)-	4249	5811b	
583.	117210-50-1	Ethanone, 1-(3a,4,5,6,7,7a-hexahydro-3a,7,7-trimethyl-1*H*-inden-2-yl)-, (3aR-*trans*)-		4249, 5811b	
584.	66611-15-2	Ethanone, 1-(3-benzofuranyl)-	568b, 1587, 4249, 5811b		
585.	22699-70-3	Ethanone, 1-(3-ethylphenyl)-	1586, 2767, 3557, 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

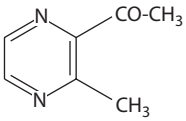
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
586.	14313-09-8	Ethanone, 1-(3-furanyl)-	2767, 2769, 4249		
587.	3420-59-5	Ethanone, 1-(3-hydroxy-2-furanyl)- {isomaltol}		2917a	
588.		Ethanone, 1-(3-hydroxy-2-methoxyphenyl)-	1360, 1375a		1360, 1375a
589.	6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-	1375, 1375b, 1586, 1884, 2767, 2769, 3557, 3712, 4249		
590.	33414-49-2	Ethanone, 1-(3-hydroxy-4-methylphenyl)-	2769, 3557, 3712, 4249		
591.	121-71-1	Ethanone, 1-(3-hydroxyphenyl)-	615, 1360, 1375, 1375a, 1375b, 1378, 1586, 1884, 1971, 2178, 2767, 2939, 3059, 3302, 3557, 3712, 3797, 4036, 4249, 4319, 5811b		1360, 1375a, 1378, 3395, 4249
592.	586-37-8	Ethanone, 1-(3-methoxyphenyl)-	796, 1626, 2939, 4249		
593.	72693-15-3	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-	3553, 4249, 5811b		
594.	72709-76-3	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-	4249		
595.	585-74-0	Ethanone, 1-(3-methylphenyl)- {3-methylacetophenone}	1586, 2767, 3557, 4249, 5811b	2339a	
596.	23787-80-6	Ethanone, 1-(3-methylpyrazinyl)- {2-acetyl-3-methylpyrazine} 	1587a, 3491, 4249, 4570a	937, 2337, 3219, 3491, 3547, 3974a, 4249	
597.	350-03-8	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine; methyl 3-pyridyl ketone}	568b, 761, 1075, 1078, 1083, 1360, 1364, 1371, 1375a, 2224, 2234, 2270, 2493, 2543, 2724, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 2939, 3054, 3058, 3059, 3062, 3255, 3266, 3308, 3386, 3397, 3398, 3410, 3499, 3505, 3553, 3797, 4249, 5034, 5811b	120, 404, 568b, 937, 1053, 1086, 1223, 1225, 1662, 1854, 2339a, 2359, 2386, 2389, 2544, 2917a, 2939, 3266, 3430, 3547, 3905, 3973, 3974a, 3983a, 4249, 5079, 5720, 5811b	1360, 1375a
598.	25343-57-1	Ethanone, 1-[3-(1,4,5,6-tetrahydropyridinyl)]-		2917a	
599.	27300-27-2	Ethanone, 1-[3-(3,4,5,6-tetrahydropyridinyl)]-		2917a	
600.	59576-31-7	Ethanone, 1-(4,6-dimethyl-2-pyridinyl)-	568b, 1587, 4249, 5811b		
601.	37920-25-5	Ethanone, 1-(4-butylphenyl)-	2570, 2767, 2769, 2777, 4249		
602.	1676-63-7	Ethanone, 1-(4-ethoxyphenyl)-	2487		
603.	66309-77-1	Ethanone, 1-(4-ethyl-2,3-dimethylphenyl)-	1586, 2767, 2769, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
604.	493-33-4	Ethanone, 1-(4-hydroxy-2-methoxyphenyl)-	1360, 2761, 2762, 3712, 4249		
605.	2478-38-8	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	3712	404, 3430, 5811b	
606.	498-02-2	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)- {acetovanillone}	568b, 1360, 1364, 1375, 1375a, 1375b, 1586, 1884, 2327c, 2765–2767, 2769, 2773, 3557, 3712, 4249, 5811b	404, 568b, 938, 2386, 2917a, 3430, 3767a, 4249	1360, 1375a
607.	99-93-4	Ethanone, 1-(4-hydroxyphenyl)-	615, 1238, 1364, 1375, 1375b, 1586, 1884, 1971, 2387, 2570, 2939, 3059, 3302, 3712, 3797, 4249, 4319, 5811b	3988, 5811b	2387, 3395
608.	100-06-1	Ethanone, 1-(4-methoxyphenyl)- {acetanisole}	336, 616, 1626, 2939, 3224, 3266, 4249, 5811b	172a, 174b, 336, 1053, 2389, 2544, 3266, 3370, 4249	
609.	2524-90-5	Ethanone, 1-(4-methyl-1*H*-imidazol-2-yl)-	568b, 1351, 3553, 4249, 5811b		
610.	122-00-9	Ethanone, 1-(4-methylphenyl)- {4-methylacetophenone}	568b, 1132, 1360, 1371, 1375, 1375a, 1375b, 1426, 1427, 2387, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3266, 3410, 3557, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 937, 1053, 1156, 2339a, 2386, 2389, 2544, 2917a, 3266, 3370, 3547, 3973, 4090, 4249	1360, 1375a, 2387
611.	59576-26-0	Ethanone, 1-(4-methyl-2-pyridinyl)-	568b, 1587, 4249, 5811b		
612.	1122-54-9	Ethanone, 1-(4-pyridinyl)- {4-acetylpyridine}	568b, 1587, 2234, 4249, 5034, 5811b	568b, 2359, 2917a, 4249	
613.	38205-66-2	Ethanone, 1-(4-thiazolyl)- {4-acetylthiazole}	568b, 1587, 3266, 4249, 5811b		
614.	32974-92-8	Ethanone, 1-(5-ethylpyrazinyl)-		1053, 3266	
615.	23328-91-8	Ethanone, 1-(5-methyl-1*H*-imidazol-2-yl)-	568b, 4249		
616.	6982-72-5	Ethanone, 1-(5-methyl-1*H*-pyrrol-2-yl)- {2-acetyl-5-methylpyrrole}	568b, 1375, 1375b, 1586, 1587a, 2337, 2570, 2767, 2775, 3553, 3557, 4159, 4249, 5811b	568b, 2337, 2389, 2544, 3205, 3219, 3491, 3543, 3560, 3561, 4249, 5811b	
617.	1193-79-9	Ethanone, 1-(5-methyl-2-furanyl)- {2-acetyl-5-methylfuran}	568b, 1427, 1586, 2337, 2570, 2731, 2735, 2767, 2775, 3553, 3555, 3557, 4249, 4570a, 5811b	404, 568b, 965, 1053, 1662, 2337, 2339a, 2386, 2389, 2544, 3188, 3205, 3219, 3266, 3543, 3547, 3555, 3560, 3561, 3905, 4249, 5811b	
618.		Ethanone, 1-(5-methyl-2-furanyl)-2-hydroxy- = Furan, 2-(1-oxo-2-hydroxyethyl)-5-methy-	568b, 4249		
619.	42972-46-3	Ethanone, 1-(5-methyl-3-pyridinyl)-	568b, 1587, 2727, 3266, 3491, 4249, 5811b	568b, 3266, 4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

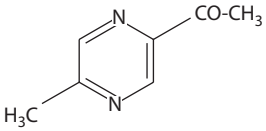
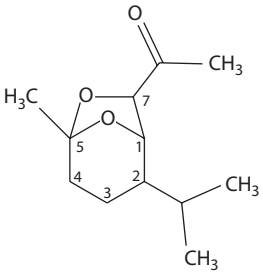
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
620.	22047-27-4	Ethanone, 1-(5-methylpyrazinyl)- {2-acetyl-5-methylpyrazine} 	1587a, 3266	937, 3215, 3491, 3547, 3974a	
621.	78210-67-0	Ethanone, 1-(5-propyl-1*H*-imidazol-4-yl)-	5811b 568b, 1587, 4249, 5811b		
622.	6940-57-4	Ethanone, 1-(6-methyl-2-pyridinyl)-	1587, 4249, 5811b		
623.	36357-38-7	Ethanone, 1-(6-methyl-3-pyridinyl)-	568b, 1371, 2731, 2735, 4249	5811b	
624.	22047-26-3	Ethanone, 1-(6-methylpyrazinyl)- {2-acetyl-6-methylpyrazine}	1587a, 937, 3491	2337, 3204, 3205, 3215, 3219, 3547, 3974a, 4249, 5811b	
625.	61891-76-7	Ethanone, 1-(dihydro-3,4-dimethylpyrrol-2-yl)-	568b, 3553, 4249		
626.	78249-86-2	Ethanone, 1-(dimethylpyridinyl)-	1587, 4249, 4570a, 5811b		
627.	25496-14-4	Ethanone, 1-(ethylphenyl)-	642, 4249		
628.	25154-45-4	Ethanone, 1-(furanyl)-	3404, 4249, 5811b		
629.	692-73-0	Ethanone, 1-(hydroxymethylphenyl)-	1586, 2570, 2767, 4249		
630.	70587-92-7	Ethanone, 1-(hydroxyphenyl)-	2777, 4249		642, 4249
631.	71278-10-9	Ethanone, 1-(methyl-2-furanyl)-	1427, 4249		
632.	74430-25-4	Ethanone, 1-(methylfuranyl)-	4249	5811b	
633.	1333-52-4 93-08-3	Ethanone, 1-(2-naphthalenyl)- {methyl naphthyl ketone}	568b, 626, 2761, 2762, 3266, 3797, 4249	568b, 1053, 3266	
634.	25252-64-6	Ethanone, 1-(tetrahydro-2-furanyl)-	4249		
635.	121198-50-3	Ethanone, 1-(tetrahydrofuranyl)-	2387	5811b	2387
636.	13678-73-4	Ethanone, 1-[1-(2-furanylmethyl)-1*H*-pyrrol-2-yl]-		404, 568b, 3547, 3555, 4249	
637.	22583-61-5	Ethanone, 1-[2-(1,1-dimethylethyl)phenyl]-	4249, 4800		
638.	112523-81-6	Ethanone, 1-[2,3,3a,4,6a,7,8,9,9a,9b-decahydro-5,9a-dimethyl-7-(1-methylethyl)-1*H*-cyclopent[*a*]azulen-3-yl]-, [3R-(3α,3aα,6aβ,7β,9aα,9bβ)]-	4249	4249, 5811b	
639.	152186-01-1	Ethanone, 1-[2,3,3a,4,6a,7,8,9,9a,9b-decahydro-5,9a-dimethyl-7-(1-methylethyl)-1*H*-cyclopent[*a*]azulen-3-yl]-, (3α,3aα,6aβ,7β,9aα,9bβ)-(±)-		429b	
640.	1767-84-6	Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-		2917a	
641.	94390-73-5	Ethanone, 1-[2-methyl-5-(1-methylethyl)-2,5-cyclohexadien-1-yl]-	4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
642.	1202-08-0	Ethanone, 1-[2-methyl-5-(1-methylethyl)phenyl]-		4249	
643.	51297-35-9	Ethanone, 1-[3-(1-ethyl-2-methylpropyl)oxiranyl]-		4249	
644.	38552-75-9	Ethanone, 1-[2-(1-methylethenyl)cyclopentyl]-		5811b	
645.	31577-86-3 43219-68-7	Ethanone, 1-[3-(1-methylethenyl)cyclopentyl]- {two isomers detected}		404, 937, 1156, 2389, 2544, 3206, 3219, 4090, 4249, 5811b	
646.	120056-06-6	Ethanone, 1-[3-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl) oxiranyl]-, [1S- [1α(2S*,3R*),2β,4a		4249, 5811b	
647.		Ethanone, 1-[4-(2,6-dimethylpyridinyl)]-	1587, 4249		
648.	937-30-4	Ethanone, 1-(4-ethylphenyl	5811, 5811a, 5811b		
649.	55087-82-6	Ethanone, 1-[5-(hydroxymethyl)-2-furanyl]-	568b, 1586, 2767, 3553, 3557, 4249, 5811b		
650.	52812-41-6 102518-81-0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]- 		404, 940, 942, 3546, 3547, 3555, 3561, 4249, 5811, 5811b	
651.	57934-85-7 102518-82-1	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-, (exo,exo)-(±)-		4249, 4573, 5811, 5811b	
652.	123695-66-9	Ethanone, 1-[6-hydroxy-6-methyl-3-(1-methylethyl)-2-cyclohexen-1-yl]-	4249		
653.	823-76-7	Ethanone, 1-cyclohexyl-		38, 4249, 5811b	
654.	57276-33-2	Ethanone, 1-cyclopropyl-2-(3-pyridinyl)-	568b, 1587, 4249, 5811b		
655.	98-86-2	Ethanone, 1-phenyl- {acetophenone}	37, 38, 568b, 1075, 1238, 1360, 1364, 1371, 1375a, 1426, 1427, 1586, 1949, 2337, 2387, 2506, 2507, 2731, 2735, 2767, 2773, 2775, 2777, 2799a, 3266, 3397, 3410, 3553, 3557, 3559, 4036, 4249, 4570a, 5811b	172a, 174b, 568b, 937, 984, 1053, 1254, 1256, 1662, 1949, 1980, 2283, 2337, 2339, 2339a, 2386, 2389, 2544, 2917a, 3188, 3205, 3219, 3266, 3370, 3543, 3547, 3560, 3561, 3905, 4249, 5811b	1360, 1375a, 2387, 2506, 2507, 3401
656.	2243-35-8	Ethanone, 1-phenyl-2-(acetyloxy)-		4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

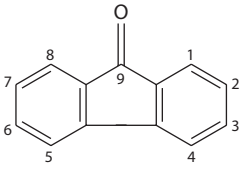
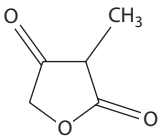
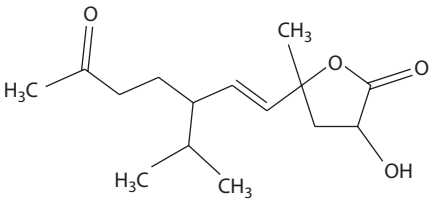
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
657.	22047-25-2	Ethanone, 1-pyrazinyl- {acetylpyrazine}	568b, 1587, 1587a, 2470, 3266, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1207, 2337, 3204, 3202, 3205, 3215, 3219, 3266, 3370, 3491, 3547, 3550, 4249, 5811b	
658.	119-53-9	Ethanone, 1,2-diphenyl-2-hydroxy- C_6H_5-CHOH-CO-C_6H_5		1053, 3266	
659.	574-06-1	Ethanone, 1,2-diphenyl-2-(acetyloxy)- {benzoin acetate}	2601a		
660.	582-24-1	Ethanone, 2-hydroxy-1-phenyl- C_6H_5-CO-CH_2OH	5811, 5811b		
661.	463-51-4	Ethenone {ketene} $H_2C{=}CO$	610, 1183, 1305 [not found]	662	
662.	27134-14-1	Fluoren-9-one, ethyl-	246, 247, 4249, 5811b		
663.	27134-15-2	Fluoren-9-one, ethylmethyl-	246, 247, 4249, 5811b		
664.	486-25-9	9*H*-Fluoren-9-one 	246, 247, 568b, 662, 1375a, 1377, 1586, 2543, 2570, 2596a, 2767, 2773, 3255, 3410, 3557, 4249, 5811b	568b, 3547, 4249	1375a, 1377, 4249
665.	27134-13-0	9*H*-Fluoren-9-one, dimethyl- {five isomers detected)	246, 247, 662, 4249, 5811b		
666.	79147-47-0	9*H*-Fluoren-9-one, methyl {two isomers detected}	662, 5811a		
667.	5501-37-1	9*H*-Fluoren-9-one, 1-methyl-	246, 247, 4249, 5811b		
668.	2840-51-9	9*H*-Fluoren-9-one, 2-methyl-	246, 247, 2767, 3557, 4249, 5811b	3547, 4249	
669.	1705-89-1	9*H*-Fluoren-9-one, 3-methyl-	246, 247, 2570, 2767, 3557, 4249, 5811b		
670.	4269-05-0	9*H*-Fluoren-9-one, 4-methyl-	246, 247, 2767, 3557, 4249		
671.	32529-53-6	2-Furancarboxaldehyde, 5-acetyl-	568b, 1140, 2570, 4249	568b, 2389, 2544, 3547, 4249, 5811b	
672.	1192-51-4	2,4(3*H*,5*H*)-Furandione, 3-methyl- 	5811, 5811a, 5811b		
673.		2(3*H*)-Furanone, acetyl-	2767, 3557		
674.	517-23-7	2(3*H*)-Furanone, 3-acetyldihydro-	568b, 1360, 1375, 1375a, 1375b, 2767, 3553, 3557, 4249, 5811b		1360, 1375a

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
675.	7400-67-1	2(3*H*)-Furanone, 4-acetyldihydro-	568b, 1375, 1375b, 2767, 3553, 3557, 4249		
676.	29393-32-6	2(3*H*)-Furanone, 5-acetyldihydro-	568b, 1354, 1360, 1375, 1375a, 1375b, 2387, 2761, 2762, 2765–2767, 2777, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 4249	1354, 1375a, 1360, 1375a, 2387, 3404, 3405
677.	160115-54-8	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1E,3S*)]]-		4249	
678.	160224-93-1	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5α(1E,3S*)]]-		4249	
679.	38273-97-1	2(3*H*)-Furanone, dihydro-3,3-dimethyl-5-(2-oxopropyl)-		568b, 2389, 2544, 3218, 3543, 3546, 4249, 5811b	
680.	60016-73-1	2(3*H*)-Furanone, dihydro-(2-oxopropyl)-	4249	2544, 4249, 5811b	
681.	71385-84-7	2(3*H*)-Furanone, dihydro-3-(2-oxopropyl)-	568b, 3553, 3557	568b, 2389, 2544	3405, 4249
682.	65331-00-2	2(3*H*)-Furanone, dihydro-4-(2-oxopropyl)-	1586, 2767, 3557, 4249		
683.	61892-49-7	2(3*H*)-Furanone, dihydro-5-(1-oxopropyl)-	568b, 1586, 2767, 3553, 3557, 4249, 5811b		
684.	158815-71-5	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1E,3S*)]]- 		4249, 5811b	
685.		2(3*H*)-Furanone, dihydro-5-methyl-5-(3-oxobutyl)-		3543	
686.	133561-47-4	2(3*H*)-Furanone,dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-		5811, 5811b	
687.	129742-48-9	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-, (*E*)-(+)-		4249, 5811b	
688.	72507-34-7	2(3*H*)-Furanone, dihydro-5-[1-methyl-4-(1-methylethyl)-7-oxo-2-octenyl]-		4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

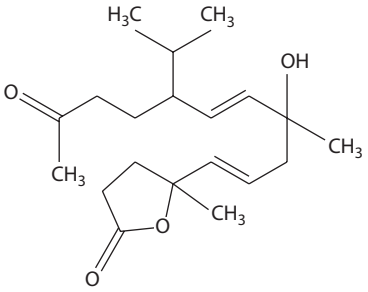
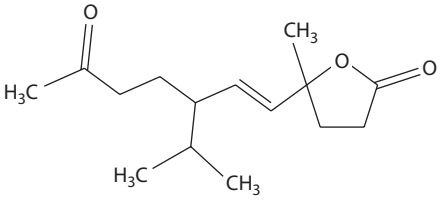
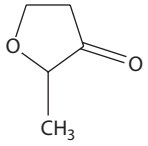
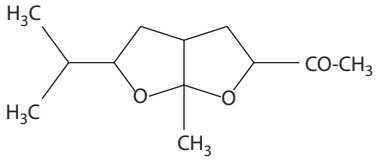
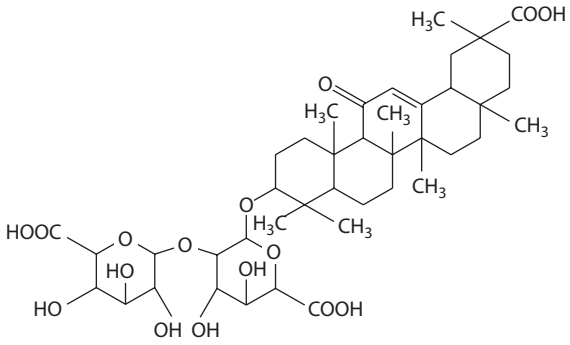
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
689.	102734-52-1	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5S-[5R*(1E,4R*,5E,7R*)]]- 		453, 4089, 5811b	
690.	102734-53-2	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5S-[5R*(1E,4S*,5E,7R*)]]-		4089, 5811b	
691.	102734-54-3	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5R-[5R*(1E,4S*,5E,7S*)]]-		4089, 5811b	
692.	102734-55-4	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5R-[5R*(1E,4R*,5E,7S*)]]-		4089, 5811b	
693.	80744-25-8	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-		4249, 4947	
694.		2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl- {stereoisomer}		4249, 4947	
695.	57213-51-1	2(3*H*)-Furanone, dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]- 		8, 9, 909, 943, 1151, 1156, 4090, 4249	
696.		2(5*H*)-Furanone, acetyl-	3557		
697.	80436-91-5	2(5*H*)-Furanone, 3-acetyl-	4249		
698.	38260-27-4	2(5*H*)-Furanone, 4-acetyl-	4249		
699.	61892-53-3	2(5*H*)-Furanone, 5-acetyl-	568b, 2767, 3553, 4249, 5811b		
700.	61892-42-0	2(5*H*)-Furanone, 3-acetyl-4-methyl-	568b, 4249, 5811b		
701.	150669-57-1	2(5*H*)-Furanone, 4-methyl-5-(3-oxobutyl)		2934b	
702.		2(5*H*)-Furanone, 5-methyl-4-(3-oxo-4-methylpentyl)-		3543	
703.	3511-31-7	3(2*H*)-Furanone	4249	5811b	
704.	22929-52-8	3(2*H*)-Furanone, dihydro-	4249	5811b	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

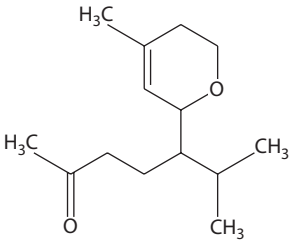
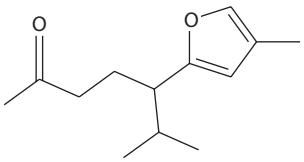
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
705.	33909-95-4	3(2*H*)-Furanone, dihydro-2,5-dimethyl-, (*E*)-			2388, 4249
706.	33794-61-5	3(2*H*)-Furanone, dihydro-2,5-dimethyl-, (*Z*)-			2388, 4249
707.	3188-00-9	3(2*H*)-Furanone, dihydro-2-methyl- {2-methyltetrahydrofuran-3-one} 	1371, 2735, 3266, 3410, 4249, 5770, 5811b	984, 1590a, 2336, 2389, 2544, 2917a, 3188, 3266, 3547, 3555, 4249, 5811b	3404, 4249
708.	89364-27-2	3(2*H*)-Furanone, dihydro-4-methyl-	4249	5811b	
709.		3(2*H*)-Furanone, dihydro-5-methyl-5-propyl-		3547, 4249	
710.	14400-67-0	3(2*H*)-Furanone, 2,5-dimethyl-	1075, 2775, 4249		
711.	27538-09-6	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl-		174b, 3266	
712.	17678-20-5	3(2*H*)-Furanone, 4-hydroxy-2-(hydroxymethyl)-5-methyl-	1375, 1375b, 4249		
713.	3658-77-3	3(2*H*)-Furanone, 4-hydroxy-2,5-dimethyl- {furaneol}	568b, 1063–1066, 1068–1074, 1364, 1370, 1371, 1882, 2493, 2570, 2601a, 2767, 3266, 3397, 4249, 4407, 5811b	172a, 174b, 568b, 1053, 2917a, 3266, 3370, 4249, 5811b	
714.	484-20-8	7*H*-Furo[3,2-*g*][1]benzopyran-7-one, 4-methoxy-		898a	4249, 4513
715.		Furo[3,2-*b*]furan (3*H*), tetrahydro-2-acetyl-3a-methyl-5-(1-methyl)- 		3543, 3545	
716.	1405-86-3	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid; glycyrrhizin} 		174e, 242, 743, 1356, 1361, 1671, 2313a, 3390, 3555, 4623, 5019, 5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
717.	53596-04-0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated 3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated; glycyrrhizin ammoniated}		172a, 174b, 1053, 3266	
718.	58-05-9	*L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-		429b	
719.	6704-02-5	5,9,13,17,21,25,29-Hentriacontaheptaen-2-one, 6,10,14,18,22,26,30-heptamethyl-	1352, 2769	1352, 2015, 4249	
720.	502-73-8	16-Hentriacontanone $H_3C\text{-}(CH_2)_{14}\text{-}CO\text{-}(CH_2)_{14}\text{-}CH_3$	2170, 2270, 2939, 3302, 3562, 3797, 4030, 4249, 4319, 5079, 5811b	2079, 3036, 4249, 5079	
721.	32304-17-9	5,9,13,17,21,25-Heptacosahexaen-2-one, 6,10,14,18,22,26-hexamethyl-, (all-*E*)-	1352, 2769	1352, 2015, 4249	
722.	542-50-7	14-Heptacosanone $H_3C\text{-}(CH_2)_{12}\text{-}CO\text{-}(CH_2)_{12}\text{-}CH_3$		1894, 4249	
723.	79-78-7	1,6-Heptadien-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {allylionone}		1053, 3266	
724.	504-20-1	2,5-Heptadien-4-one, 2.6-dimethyl-		568b, 4249	
725.		3,5-Heptadien-2-one, 6-methyl-, (*Z*)-	2570	2339a	
726.	1604-28-0	3,5-Heptadien-2-one, 6-methyl-, (*E*)- $(H_3C)_2{=}C{=}CH\text{-}CH{=}CH\text{-}CO\text{-}CH_3$	568b, 2506, 2507, 2570, 4249, 5811b	172a, 174b, 404, 568b, 937, 1053, 1156, 2338, 2339a, 2386, 2389, 2544, 3186, 3188, 3266, 3370, 3905, 3547, 4090, 4098a, 4249, 5811b	2506 (0), 2507 (0)
727.		4,6-Heptadien-2-one		5777	
728.		4,6-Heptadien-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methylfuranyl)-		3547, 4249	
729.	2363-85-1	Heptanal, 2-oxo- $H_3C\text{-}(CH_2)_4\text{-}CO\text{-}CH{=}O$	568b, 4249		
730.	96-04-8	2,3-Heptanedione $H_3C\text{-}(CH_2)_3\text{-}CO\text{-}CO\text{-}CH_3$	1238, 3902, 4249, 4570a		
731.	7307-02-0	2,4-Heptanedione $H_3C\text{-}(CH_2)_2\text{-}CO\text{-}CH_2\text{-}CO\text{-}CH_3$	1371, 3410, 4249		
732.	3002-23-1	2,4-Heptanedione, 6-methyl- $(H_3C)_2{=}CH\text{-}CH_2\text{-}CO\text{-}CH_2\text{-}CO\text{-}CH_3$		3186, 4249	
733.	1703-51-1	2,5-Heptanedione	4249		
734.		2,5-Heptanedione, 4-(1-methylethyl)-		3543	
735.	13901-85-4	2,5-Heptanedione, 6-methyl- $(H_3C)_2{=}CH\text{-}CO\text{-}(CH_2)_2\text{-}CO\text{-}CH_3$	5811b	568b, 1156, 2338, 3186, 3188, 3219, 3543, 3545, 3547, 3561, 4090, 4249	
736.	13505-34-5	2,6-Heptanedione $H_3C\text{-}CO\text{-}(CH_2)_3\text{-}CO\text{-}CH_3$	568b, 3553, 4249, 5811b	404, 568b, 3543, 3546, 3547, 3560, 3561, 4048, 4249	
737.		2,6-Heptanedione, 3-methyl- $H_3C\text{-}CO\text{-}CH(CH_3)\text{-}(CH_2)_2\text{-}CO\text{-}CH_3$		3545	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
738.	59262-53-2	Heptanoic acid, 3-(1-methylethyl)-6-oxo-, (S)-		731, 738, 1156, 3858, 4090, 4249	
739.	39815-78-6	Heptanoic acid, 3-oxo-, methyl ester		4249	
740.	3128-07-2	Heptanoic acid, 6-oxo-	3410, 3553, 4248		
741.	110-43-0	2-Heptanone {methyl pentyl ketone}	1238, 2002, 2461, 2773, 3266, 4249	172a, 174b, 1053, 2337, 2339a, 2389, 2544, 3186, 3188, 3266, 3370, 4249, 5811b	
742.	52812-44-9	2-Heptanone, 5-(3-acetyloxiranyl)-6-methyl-		940, 942, 4249, 5811b	
743.	52812-43-8	2-Heptanone, 5-[3-(1-hydroxy-1-methylethyl)oxiranyl]-6-methyl-	2545	940, 942, 4249	
744.		2-Heptanone, 5-(2,3-dihydro-4-methyl-6-pyranyl)-6-methyl-		943, 944	
745.		2-Heptanone, 5-(5,6-dihydro-4-methyl-2-pyranyl)-6-methyl- 		943, 944	
746.	541-85-5	2-Heptanone, 5-methyl-		568b, 4249	
747.	121269-00-9	2-Heptanone, 6-(5-methyl-2-furanyl)-		941, 1256, 3547, 4249, 4780, 5811b	
748.	72693-12-0	2-Heptanone, 6-hydroxy-	3553, 4249		
749.	928-68-7	2-Heptanone, 6-methyl-	1371, 5811b	404, 2095, 2917a, 5811b	
750.	41059-93-2	2-Heptanone, 6-methyl-5-(4-methyl-2-furanyl)- {solanofuran} 		943, 1087, 1662, 3547, 5811b	
751.	106-35-4	3-Heptanone {ethyl butyl ketone} $H_3C\text{-}CH_2\text{-}CO\text{-}(CH_2)_3\text{-}CH_3$	1238, 1239, 1360, 1375a, 2702, 2761, 2765, 2766, 3251, 3302, 4249, 5811b	58, 3474, 4249	1360, 1375a
752.	19549-83-8	3-Heptanone, 2,6-dimethyl-	4570a		
753.	123-19-3	4-Heptanone {butyrone; dipropyl ketone} $H_3C\text{-}(CH_2)_2\text{-}CO\text{-}(CH_2)_2\text{-}CH_3$	112, 568b, 1140, 1238, 1418, 1419, 1971, 2079, 2088, 2170, 2270, 2337, 2702, 2939, 3302, 3308, 3797, 4249, 5079, 5811b	568b, 2704, 4249, 5079	
754.	108-83-8	4-Heptanone, 2,6-dimethyl-	568b, 1238, 1378, 4249		1378, 4249

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

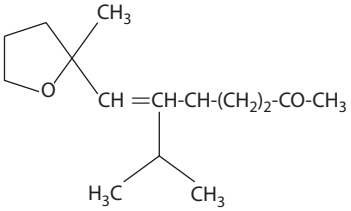
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
755.		4-Heptanone, 5-hydroxy-	568b, 4249		
756.	21504-51-8	3-Heptene-2,5-dione, 6-methyl-	5811b	568b, 1156, 3560, 3561, 4090, 4249	
757.	499-84-3	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo- H_3C-CO-$(CH_2)_2$-C[$CH(CH_3)_2$]═CH-COOH		731, 736, 738, 936, 930, 1156, 1256a, 2092, 4090, 4249	
758.	41654-06-2	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)-		736, 1156, 2092, 4090, 4249, 5811b	
759.	63892-03-5	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*Z*)-		736, 1156, 2092, 4090, 4249	
760.	41654-07-3	4-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)- H_3C-CO-CH═CH-CH[$CH(CH_3)_2$]-CH_2-COOH	2092	731, 738, 1156, 2092, 4090, 4249, 5811b	
761.	409-02-9	Heptenone, methyl-		2283, 4249	
762.		2-Hepten-4-one CH_3-$(CH_2)_2$-CO-CH═CH-CH_3		1053, 3266	
763.	1119-44-4	3-Hepten-2-one CH_3-$(CH_2)_2$-CH═CH-CO-CH_3		1053, 3266, 3370	
764.	133561-46-3	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-		5811, 5811b	
765.	129742-47-8	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-, [R-(*E*)]-		4249, 5811b	
766.	57283-79-1	3-Hepten-2-one, 5-ethyl-6-methyl-		2917a, 3854	
767.	50767-76-5	3-Hepten-2-one, 5-ethyl-6-methyl-, (*E*)-		1662, 2339a, 3547, 4249	
768.		3-Hepten-2-one, 5-(1-methylethyl)-		568b, 1156, 1662, 3547, 4090	
769.	2009-74-7	3-Hepten-2-one, 6-methyl-	1365, 2387, 4249	3973	2387
770.	152209-54-6	3-Hepten-2-one, 5-(1-methylethyl)-7-[2-methyl-3-(3-methyl-5-oxo-3-hexenyl)oxiranyl]-, [2S-[2α(3E,5R*),3β(*E*)]]-		4249	
771.	110-93-0	5-Hepten-2-one, 6-methyl-	568b, 1371, 1949, 2545, 2773, 2775, 3410, 4249, 5811b	172a, 404, 568b, 937, 984, 1053, 1063–1066, 1068–1074, 1256, 1590a, 1615, 1854, 1949, 2015, 2095, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3188, 3266, 3370, 3905, 3547, 4249, 5811b	
772.	57782-60-2	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)- 		568b, 944, 3545, 3547, 4098a, 4249, 5811b	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
773.	104669-35-4	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-4-hydroxy-2-methyl-2-furanyl)-		232, 943, 944, 1156, 3852, 4090, 4249, 4780, 5811b	
774.	160115-55-9	6-Hepten-2-one, 7-[4-(acetyloxy)tetrahydro-5-hydroxy-2-methyl-2-furanyl]-5-(1-methylethyl)-		4249	
775.	117210-48-7	6-Hepten-2-one, 7-[tetrahydro-2-methyl-5-(1-methylethyl)-2-furanyl]-		4249, 5811b	
776.	18787-63-8	2-Hexadecanone	2601a	2094, 4249, 5811b	
777.	60026-26-8	7-Hexadecen-6-one, 3,7,11,15-tetramethyl-		2389, 2544, 4249, 5811b	
778.	90-65-3	2,5-Hexadienoic acid, 3-methoxy-5-methyl-4-oxo-	3760, 4249	3760, 4249, 5811b	
779.	15303-46-5	Hexanal, 2-(1-methylethyl)-5-oxo-		568b, 2917a, 3547, 4249	
780.	2363-84-0	Hexanal, 2-oxo- $H_3C\text{-}(CH_2)_3\text{-}CO\text{-}CH{=}O$	3902, 4249		
781.	25346-59-2	Hexanal, 4-oxo- $H_3C\text{-}CH_2\text{-}CO\text{-}(CH_2)_2\text{-}CH{=}O$		1980	
782.	3184-35-8	Hexanedioic acid, 2-oxo-	3302, 4249	1312	
783.	3848-24-6	2,3-Hexanedione $H_3C\text{-}CO\text{-}CO\text{-}(CH_2)_3\text{-}CH_3$	568b, 1238, 3902, 4249, 5770		
784.	110-13-4	2,5-Hexanedione {acetonylacetone}	568b, 1238, 1364, 2775, 3553, 4249, 5811b	568b, 2917a, 3186, 3188, 3547, 4249	3402, 3404
785.	61892-85-1	2,5-Hexanedione, 3-hydroxy-	568b, 2767, 3553, 3557, 4249, 5811b		
786.	4437-50-7	2,5-Hexanedione, 3-methyl-	3553, 4249, 5811b		
787.	4437-51-8	3,4-Hexanedione $H_3C\text{-}CH_2\text{-}CO\text{-}CO\text{-}CH_2\text{-}CH_3$	1238, 4570a, 5811b		3404, 4249
788.		3,4-Hexanedione, 2-methyl-	4570a		
789.	2543-54-6	Hexanoic acid, 2-(1-methylethyl)-5-oxo-		9, 936, 940, 1156, 1257, 2092, 2389, 2544, 3767a, 4090, 4249, 5811b	
790.	16825-90-4	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, (S)-	568b, 3559, 4249	5811b	
791.	1842-56-4	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, methyl ester		3858	
792.	6818-07-1	Hexanoic acid, 4-methyl-5-oxo-	568b, 4249		
793.	30414-55-2	Hexanoic acid, 5-methyl-3-oxo-, methyl ester		3858, 4249	
794.	41654-04-0	Hexanoic acid, 5-methyl-4-oxo-	2092, 4249	2092, 4249	
795.	3249-68-1	Hexanoic acid, 3-oxo-, ethyl ester	5811		
796.	1117-74-4	Hexanoic acid, 4-oxo-	568b, 3553, 4249, 5811b	568b, 1980, 4249	
797.	3128-06-1	Hexanoic acid, 5-oxo-	568b, 3553, 4249, 5811b		
798.	13984-57-1	Hexanoic acid, 5-oxo-, ethyl ester	5811		
799.		Hexanone	5777		
800.	14360-50-0	1-Hexanone, 1-(2-furanyl)-	2767, 2769, 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

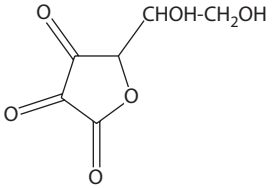
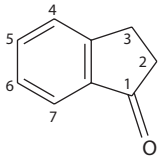
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
801.	591-78-6	2-Hexanone {butyl methyl ketone} $H_3C\text{-}(CH_2)_3\text{-}CO\text{-}CH_3$	112, 568b, 1140, 1238, 1348–1350, 1354, 1365, 1375a, 1418, 1419, 1589, 1637, 2337, 2570, 2767, 3219, 3308, 3396, 3559, 4249, 4570a, 5770, 5811b	568b, 984, 4249	1354, 1375a
802.	72693-13-1	2-Hexanone, 5,6-dihydroxy-	3553, 4249	4249	
803.	56745-61-0	2-Hexanone, 5-hydroxy-	2767, 4249		
804.	2550-21-2	2-Hexanone, 3-methyl-		5811, 5811b	
805.	105-42-0	2-Hexanone, 4-methyl-	5811		
806.	110-12-3	2-Hexanone, 5-methyl-	568b, 4249, 5811		
807.	68208-73-1	2-Hexanone, 6-hydroxy-5-methyl-	2570, 4249		
808.	589-38-8	3-Hexanone {ethyl propyl ketone}	568b, 1140, 1238, 1365, 1418, 1419, 2002, 2767, 3219, 3308, 3559, 4249, 4570a, 5770, 5811b	568b, 984, 2336, 4249	
809.	623-56-3	3-Hexanone, 5-methyl-	5811, 5811a, 5811b		
810.	4436-75-3	3-Hexene-2,5-dione		2917a	
811.	763-93-9	3-Hexen-2-one	568b, 1371, 1587, 3410, 4249, 5811b		
812.	5166-53-0	3-Hexen-2-one, 5-methyl-	1360, 1375a, 2761, 2765, 3266, 4249	1053, 1662, 2336, 3186, 3188, 3266, 3550, 4249	1360, 1375a
813.	1821-29-0	3-Hexen-2-one, 5-methyl-, (*E*)-		568b, 1248, 1662, 3186, 3188, 4249	
814.	25659-22-7	4-Hexen-3-one	568b, 4249		
815.	17325-90-5	4-Hexen-3-one, 4,5-dimethyl-		984	
816.	109-49-9	5-Hexen-2-one	348, 4249, 5811b	2917a	
817.	55615-04-8	5-Hexen-2-one, 4,5-dimethyl-		4249	
818.	121197-12-4	5-Hexen-3-one, 4,5-dihydroxy-	4249	5811b	
819.	33124-69-5	threo-2,3-Hexodiulosonic acid, γ-lactone {2,3-diketogulonic acid, γ-lactone} 		4249	
820.	490-83-5	*L*-threo-2,3-Hexodiulosonic acid, γ-lactone {*L*-2,3-diketogulonic acid, γ-lactone}		429b	
821.	1415-93-6	Humic acids		2665a	
822.	606-23-5	1*H*-Indene-1,3(2*H*)-dione	663, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
823.	30286-23-8	Indenone, dihydro-	4249		
824.	72692-87-6	Indenone, 1,3(or 2,3)-dihydrodimethyl-	4249, 5811b		
825.	480-90-0	1*H*-Inden-1-one	2543, 2773		
826.	83-33-0	1*H*-Inden-1-one, 2,3-dihydro-{1-indanone} 	568b, 1364, 1375, 1375a, 1375b, 1377, 1378, 1586, 2506, 2507, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3410, 3553, 3557, 4249, 5034, 5811b		642, 1375a, 1377, 1378, 2506, 2507, 3401, 4249
827.	71278-03-0	1*H*-Inden-1-one, 2,3-dihydrodimethyl- {six isomers detected}	661, 1378, 1586, 2543, 2570, 2761, 2762, 2765–2767, 2767, 2773, 2775, 3557, 4249		1378
828.	66309-83-9	1*H*-Inden-1-one, 2,3-dihydro-2,6-dimethyl-	1586, 2767, 2769, 3557, 4249		
829.	17714-57-7	1*H*-Inden-1-one, 2,3-dihydro-3,5-dimethyl-	2387, 2543, 2570, 2761, 2762, 2765–2767, 2769, 2773, 4249		2387
830.	5037-60-5	1*H*-Inden-1-one, 2,3-dihydro-4,7-dimethyl-	568b, 1586, 2769, 3557, 4249		
831.	71278-04-1	1*H*-Inden-1-one, 2,3-dihydro-ethyl-	1378, 2005, 4249		1378
832.	57878-30-5	1*H*-Inden-1-one, 2,3-dihydro-5-hydroxy-3-methyl-		2917a	
833.	72692-69-4	1*H*-Inden-1-one, 2,3-dihydro(methoxymethyl)-	1586, 2767, 3557, 4249		
834.	65436-86-4	1*H*-Inden-1-one, 2,3-dihydromethyl- {four isomers detected}	312, 1360, 1375a, 1378, 1586, 2543, 2570, 2767, 2773, 2775, 2777, 3557, 5811b		1360, 1375a, 1378
835.	17496-14-9	1*H*-Inden-1-one, 2,3-dihydro-2-methyl-	1360, 1375a, 1586, 2543, 2761, 2762, 2765–2767, 2769, 2773, 2777, 3557, 4249		1360, 1375a
836.	6072-57-7	1*H*-Inden-1-one, 2,3-dihydro-3-methyl-	568b, 1360, 1375a, 1586, 2387, 2506, 2507, 2543, 2570, 2761, 2762, 2765–2767, 2773, 2777, 3557, 4249, 5811b		1360, 1375a, 2387, 2506, 2507
837.	24644-78-8	1*H*-Inden-1-one, 2,3-dihydro-4-methyl-	3650, 4249, 5811b		
838.	4593-38-8	1*H*-Inden-1-one, 2,3-dihydro-5-methyl-	3557, 3650, 4249, 5811b		3402
839.	24623-20-9	1*H*-Inden-1-one, 2,3-dihydro-6-methyl-	3557, 3650, 4249, 5811b		
840.	66288-51-5	1*H*-Inden-1-one, 2,3-dihydrotrimethyl- {three isomers detected}	1586, 2570, 2767, 2769, 3557, 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

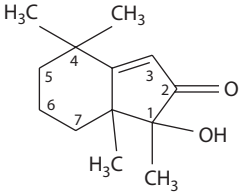
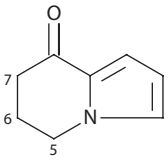
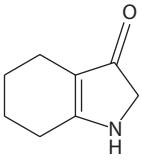
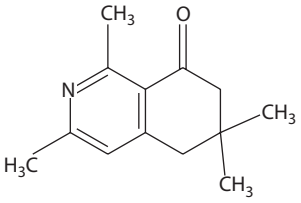
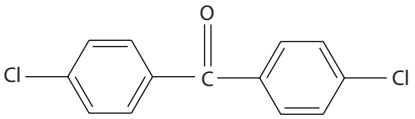
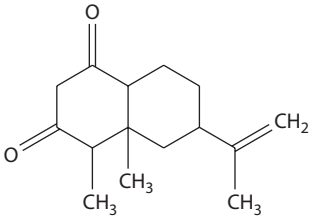
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
841.	54789-23-0	1*H*-Inden-1-one, 2,3-dihydro-3,3,5,7-tetramethyl-	1371, 3410	404	
842.	35322-84-0	1*H*-Inden-1-one, 2,3-dihydro-3,4,7-trimethyl-	1371, 4249		
843.	22303-81-7	1*H*-Inden-1-one, 3-methyl-	2388, 4249		
844.	615-13-4	2*H*-Inden-2-one, 1,3-dihydro-	568b, 3255, 3553, 3557, 4249		
845.		2*H*-Inden-2-one, dimethyl-	278, 1586, 2767, 4249		
846.		2*H*-Inden-2-one, methyl-	1586, 2767		
847.	39815-71-9	2*H*-Inden-2-one, 1,4,5,6,7,7a-hexahydro-1-hydroxy-1,4,4,7a-tetramethyl- 		937, 3219, 4249, 5811b	
848.	35656-49-6	1*H*-Indolepropanoic acid, α-oxo-		4249	
849.	392-12-1	1*H*-Indole-3-propanoic acid, α-oxo-		429b, 4249, 4943	
850.	54906-44-4	8(5*H*)-Indolizinone, 5,6,7,8-tetrahydro- {5-oxocyclohexa[] pyrrole} 	568b, 1587, 2775, 4249, 5811b	404, 568b, 1157, 3491, 3547, 4249	
851.	55041-88-8	8(5*H*)-Indolizinone, 6,7-dihydro-2-methyl-		3547, 4249	
852.	58074-25-2	3*H*-Indol-3-one, 2,3,4,5,6,7-hexahydro- {4,5,6,7-tetrahydro-3-indolinone} 		2917a	
853.	8013-90-9	Ionone {see 3-buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- and 3-buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)-}	2767		
854.		5,6-Isoquinolinedione, 7,8-dihydro-1,3,7,7-tetramethyl-		4249, 4967	
855.	55713-38-7	8(5*H*)-Isoquinolinone, 6,7-dihydro-1,3,6,6-tetramethyl- [6,7-dihydro- or 5,6,7,8-tetrahydro-?] 		938, 939, 1090, 3491, 4249	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
856.	88125-11-5	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 1a,2,3,4,7a,7b-hexahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,7aα,7bα)]-		4249, 4812	
857.	105300-09-2	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 1a-[(β-*D*-glucopyranosyloxy)methyl]octahydro-5,7b-dimethyl-, [1aR		4249, 5811b	
858.	125537-96-4	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 3-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,3β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
859.	125537-95-3	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 4-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
860.	105300-10-5	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 5-[(β-*D*-glucopyranosyloxy)methyl]octahydro-1a,7b-dimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
861.	88848-60-6	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 6-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy] octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,6β,7aα,7bα)]-		4249, 4717, 5811b	
862.	68690-84-6	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		1255, 3547, 4249, 5811b	
863.	5293-97-0	Methanone, bis(2-chlorophenyl)-	2570, 4249	2389, 2544, 4249	
864.	90-98-2	Methanone, bis(4-chlorophenyl)- 	707, 708, 713, 714, 2570, 4249	4249, 5811b	
865.	24966-13-0	Methanone, cyclopropyl-3-pyridinyl-	568b, 1587, 4249, 5811b		
866.	119-61-9	Methanone, diphenyl- {benzophenone} C_6H_5-CO-C_6H_5	278, 568b, 3266, 4249	172a, 174b, 568b, 1053, 2339a, 3266, 3370	
867.	5162-03-8	Methanone, (2-chlorophenyl)phenyl-		2917a	
868.	16709-30-1	Methylcarbamic acid, 2,2-dimethyl-3(2*H*)-oxobenzofuran-7-yl ester		5811, 5811b	
869.	68982-27-4	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-oxo-, [1R-(1α,4aβ,8aα)]-		4249	
870.	60026-23-5	1,3(2*H*,5*H*)-Naphthalenedione, 6,7,8,8a-tetrahydro-4,8a-dimethyl-6-(1-methylethenyl- 		5811, 5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

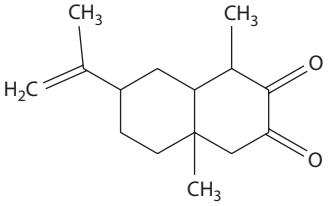
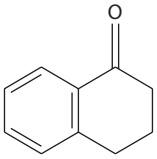
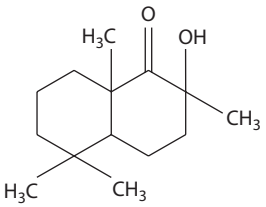
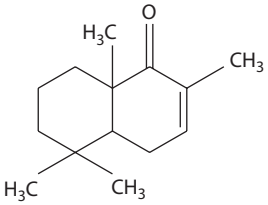
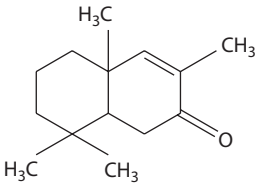
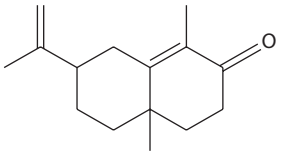
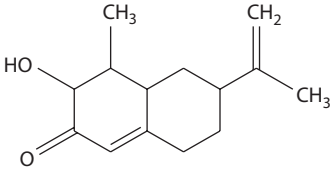
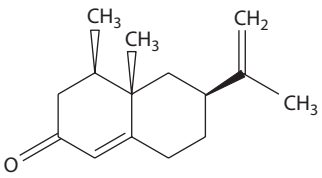
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
871.	117769-22-9	2,3-Naphthalenedione, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)- 		4249, 5811b	
872.	88125-12-6	2,3-Naphthalenedione, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)-		2544, 4249	
873.	133480-20-3	Naphthalenone, hexahydro-8-methyl-(1-methylethenyl)-		5811, 5811b	
874.	529-34-0	1(2*H*)-Naphthalenone, 3,4-dihydro- {1-tetralone} 	278, 568b, 3553, 4249, 5811b		
875.	117210-52-3	1(2*H*)-Naphthalenone, 3,4-dihydro-5-methyl-3-(1-methylethenyl)-		4249, 5811b	
876.	27410-97-5	1(2*H*)-Naphthalenone, 3,4-dihydro-4,5,7-trimethyl-	2570, 2769, 4249		
877.	41720-93-8	1(2*H*)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-3-hydroxy-4,4a-dimethyl-6-(1-methylethenyl)-, [3R-(3α,4α,4aβ,6β)]-		4249	
878.	52811-60-6	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl- 	5811b	3545, 3560, 3561, 4101, 4249	
879.	55497-93-3	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [2R- (2α,4aα,8aβ)]-		4249, 5811b	
880.	25487-94-9	1(4*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)- 		5, 151, 1660a, 4249, 5811b	
881.	57601-69-1	1(4*H*)-Naphthalenone, 2-hydroxy-4,4,7-trimethyl-		568b, 3547, 4249	
882.	117472-47-6	1(4*H*)-Naphthalenone, 5,6,7,8-tetrahydro-8-methyl-5-(1-methylethenyl)-		4249, 4967, 5811b	
883.	29210-91-1	2(1*H*)-Naphthalenone, 3,4-dihydro-4,4,7-trimethyl-	2570, 2769, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
884.	55733-01-2	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4,4a,8,8-pentamethyl-, (4aS-*trans*)-		3547, 4249, 5811b	
885.	76739-26-9	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4,4a,8,8-pentamethyl-		3547, 4249	
886.		2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3-hydroxy-3,4a,8,8-tetramethyl- {two isomers reported}		3545, 3547, 4249	
887.	51020-10-1	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4a,8,8-tetramethyl-, (4aR-*trans*)- {isonordimenone} 		13, 1660a, 1662, 3547, 4249, 4780, 5811b	
888.	72446-33-4	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4a,8,8-tetramethyl-4-(3-oxobutyl)-, (4aS-*trans*)-		4249, 5811b	
889.	14506-68-4	2(1*H*)-Naphthalenone, 1-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-5,5,8a-trimethyl-, [1R-[1α(R*),4aβ,8aα]]-		4249	
890.	57567-07-4	2(1*H*)-Naphthalenone, 8-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-4,4,8a- trimethyl-7-methylene-		1248, 4249, 4780	
891.	473-08-5	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)- {bicyclo[4.4.0]dec-1-en-3-one, 2,6-dimethyl-9-isopropenyl-} 	2769	1156, 2389, 4090	
892.	60026-22-4	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)- {6-epicyperone-1}	312, 1586**,** 2543, 2661, 2765–2767, 2773, 2775, 3557, 4249	2544, 4249, 5811b	
893.	55051-94-0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-3-hydroxy-4-methyl-6-(1-methylethenyl)-, [3R-(3α,4β,4aβ,6α)]- 		1156, 4090, 4249, 4455, 5811b	
894.	4674-50-4	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4α,4aα,6β)]- {bicyclo[4.4.0]dec-1-en-3-one, 5,6-dimethyl-8-isopropenyl-} (nootkatone) 	568b, 4249, 4570a	404, 568b, 1590a, 2386, 4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

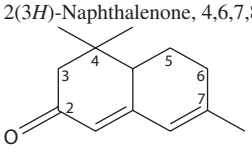
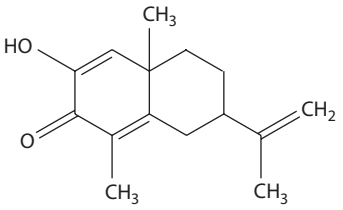
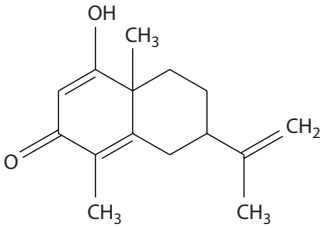
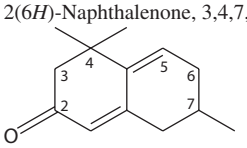
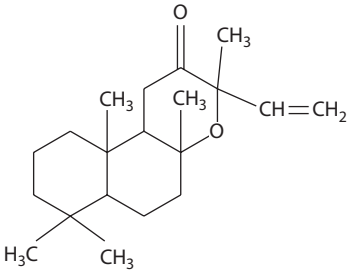
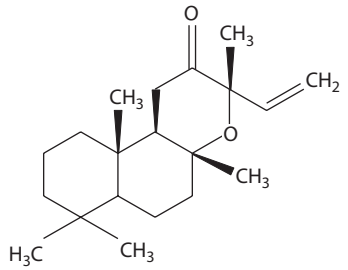
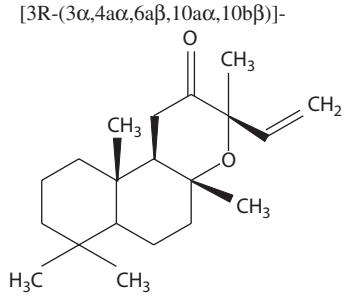
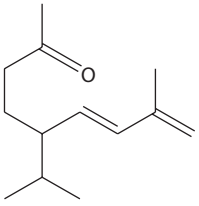
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
895.	102977-86-6	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,8-dimethyl-7-(1-methylethenyl)-		4159b	
896.	38044-00-7	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-		2544, 4249, 5811b	
897.	5835-19-8	2(3*H*)-Naphthalenone, 4,4a,5,6-tetrahydro-4,4,7-trimethyl		4249, 5811, 5811a	
898.	39815-74-2	2(3*H*)-Naphthalenone, 4,6,7,8-tetrahydro-4,4,7-trimethyl- 		1149, 1149a, 3199, 3205, 3219, 4249, 4780, 5811b	
899.	17081-85-5	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-1,4a-dimethyl-7-(1-methylethenyl)-(4aS-*cis*)- {1,2-dehydro-α-cyperone}		5811, 5811b	
900.	68420-60-0	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-3-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)- 		1156, 3212, 4090	
901.	38043-97-9	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-4-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-, (4aR-*cis*)- {1-keto-α-cyperone} 	2761, 2762, 2777	1156, 2389, 3205, 3211, 3219, 4090, 5811b	
902.		2(6*H*)-Naphthalenone, 3,4,7,8-tetrahydro-4,4,7-trimethyl- 		1149, 1149a, 3219	
903.	38017-17-3	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl- {8,13-epoxylabd-14-en-12-one} 		5811, 5811b	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
904.	37551-73-8	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]- 		11, 1156, 2308, 4090, 4249	
905.	37551-74-9	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aα,6aβ,10aα,10bβ)]- 		11, 1156, 4090, 4249	
906.	68985-12-6	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-		2094, 4249	
907.	6809-52-5	5,9,13,17-Nonadecatetraen-2-one, 6,10,14,18-tetramethyl-	1352, 2767, 2769, 4249	1352, 2015, 4249	
908.	817-88-9	3,7-Nonadien-2-one, 4,8-dimethyl-		2339a	
909.		3,8-Nonadien-2-one, 4,8-dimethyl-		2339a	
910.	123695-65-8	5,7-Nonadien-2-one, 8-hydroxy-5-(1-methylethyl)-, (*E,Z*)-	4249		
911.	39012-18-5	5,7-Nonadien-2-one, 8-methyl-5-(1-methylethyl)- {isosolanone}	802, 803, 2722, 2767, 3557	937, 940, 1156, 4090, 5811b	
912.	60714-16-1	6,8-Nonadien-2-one, 6-methyl-5-(1-methylethenyl)-		2917a	
913.	40286-47-3	6,8-Nonadien-2-one, 8-methyl-5-(methylethyl)-		5811, 5811b	
914.	2278-53-7	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [R-(*E*)]-	2767, 4249	937, 943, 1156, 4090, 4249	
915.	1937-54-8	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [S-(*E*)]- {solanone} 	69, 568b, 802, 803, 1352, 1360, 1364, 1365, 1375, 1375a, 1375b, 1586, 2045, 2387, 2506, 2507, 2545, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 2857, 2871, 3224, 3266, 3297, 3302, 3308, 3410, 3557, 3559, 3648, 4249, 4336, 5811b	9, 69, 404, 537, 543a, 568b, 671, 908, 909, 911, 943, 1053, 1063–1066, 1068–1074, 1149, 1149a, 1156, 1254, 1256, 1257, 1352, 1550, 1590a, 1591, 1961, 2282, 2338, 2339a, 2386, 2389,	1360, 1375a, 2387, 2506, 2507

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

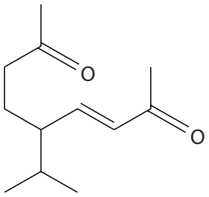
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [S-(*E*)]- {solanone} (cont.)		2544, 2786, 2914, 3188, 3198, 3215, 3219, 3266, 3354, 3543, 3545, 3547, 3549, 3550, 3560, 3561, 3648, 3905, 3973, 4090, 4098a, 4249, 4336, 5811b	
916.	54868-48-3	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, (*E*)-		2917a	
917.		Nonane, 4-acetyl-2,6,8-trimethyl-			1378
918.		2,5-Nonanedione		404	
919.		2,7-Nonanedione, 8-hydroxy-8-methyl-5-(1-methylethyl)-		3543, 4249	
920.	55023-57-9	2,8-Nonanedione, 5-(1-methylethyl)- {norsolanadione} 	2387	9, 537, 908, 909, 940, 942, 1149, 1149a, 1156, 1254, 1591, 2338, 2386, 2786, 4090, 4098a, 4249	2387
921.	38284-28-5	2,5,8-Nonanetrione		568b, 937, 2336, 2389, 2544, 4249, 5811b	
922.	6064-52-4	Nonanoic acid, 4-oxo-		568b, 908, 2092, 2389, 2544, 3219, 3331, 3767a, 4249, 5811b	
923.	821-55-6	2-Nonanone $H_3C\text{-}(CH_2)_6\text{-}CO\text{-}CH_3$	297, 568b, 3266, 4249	172a, 174b, 568b, 1053, 1662, 2339a, 3266, 3626, 4249	
924.	58002-07-6	2-Nonanone, 6,7-epoxy-8-hydroxy-5-(1-methylethyl)-		2917a	
925.	55023-54-6	2-Nonanone, 8-hydroxy-5-(1-methylethyl)-		940, 1149, 1149a, 1156, 4090, 4249	
926.	123-18-2	4-Nonanone, 2,6,8-trimethyl-			1378, 4249
927.		5-Nonanone, 2,8-dimethyl-7,8-epoxy-		3545	
928.	17609-32-4	3,5,7-Nonatrien-2-one		404	
929.		2-Nonenal, 2,3-dimethyl-8-oxo-		2917a	
930.	38372-56-4	3-Nonene-2,8-dione {norsolanadione}	1375, 1375b, 4249	3219, 3550	
931.	35953-21-0 60619-46-7 101159-09-5	3-Nonene-2,8-dione, 5-(1-methylethyl)-, [S-(*E*)]- {oxysolanone}	568b, 671, 1360, 1371, 1375, 1375a, 1375b, 1586, 2570, 2761, 2762, 2765–2767, 2775, 3410, 3557, 4249, 5811b	404, 568b, 937, 943, 1063–1066, 1068–1074, 1156, 1256, 1590a, 2386, 2389, 2544, 3215, 3219, 3329, 3356, 3543, 3545, 3547, 3549, 3560, 3561, 3973, 4090, 4249, 5811b	1360, 1375a

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
932.	68985-18-2	2-Nonen-4-one, 3-methyl-, (*E*)-		404, 947, 2339a, 4249	
933.	65017-85-8	2-Nonen-4-one, 8-hydroxy-3-methyl-, (*E*)-		231, 4249	
934.	122881-64-5	3-Nonen-8-one, 1,2-dihydroxy-2-methyl-5-(1-methylethyl)-		5811, 5811b	
935.		5-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-		3543, 4249	
936.	55023-59-1	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-		936, 940, 1149, 1149a, 1156, 1256, 2092, 4090, 4249, 5811b	
937.	57934-86-8	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-,(*E*)-(±)-		940, 942, 1156, 4090, 4249	
938.	60828-13-9	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (6*E*)-		5811, 5811b	
939.	55023-52-4	6-Nonen-2-one, 8-hydroxy-5-(1-methylethyl)-		940, 942, 1156, 4090, 4249	
940.	77288-95-0	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [R-[R*,S*-(*E*)]]-		738, 1156, 4090, 4249, 4948	
941.	77288-96-1	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [S-[R*,R*-(*E*)]]-		738, 1156, 4090, 4249, 4948	
942.	3452-09-3	1-Nonyne $HC{\equiv}C\text{-}(CH_2)_6\text{-}CH_3$	1822, 4249		
943.	18444-66-1	19-Norlanosta-1,5,23-triene-3,11,22-trione, 25-(acetyloxy)-2,16,20-trihydroxy-9-methyl-, (9β,10α,16α,23*E*)-		4249	
944.	17278-28-3	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3α,9β,10α,16α,23*E*)-		4249	
945.	89647-62-1	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3β,9β,10α,16α,23*E*)-		4249	
946.	38284-27-4	3,5-Octadien-2-one		404, 937, 2389, 2544, 4249, 5811b	
947.	30086-02-3	3,5-Octadien-2-one, (*E,E*)-		2339a, 4249, 4573a	
948.	585-25-1	2,3-Octanedione	568b, 1238, 3559, 3902, 4249	404, 568b, 937, 2336, 2389, 2544, 4249	
949.	65716-44-1	2,7-Octanedione, 3,3-dimethyl-		404, 568b, 947, 4249, 4780	
950.	96937-51-8	Octanoic acid, oxo-	3741, 3743, 4249, 4897		
951.	1674-37-9	1-Octanone, 1-phenyl- {octanophenone}	5811		
952.	111-13-7	2-Octanone {hexyl methyl ketone}	568b, 1371, 3105, 3219, 3224, 3266, 3308, 4249	59, 568b, 1053, 2339a, 3266, 4249, 4434	
953.	102488-04-4	2-Octanone, 3,3-dimethyl-7-hydroxy		5811, 5811b	
954.	65716-45-2	2-Octanone, 3,3-dimethyl-7-hydroxy-, (±)-		230, 1156, 4090	
955.	106-68-3	3-Octanone {ethyl amyl ketone}		568b, 1187, 2339a, 4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

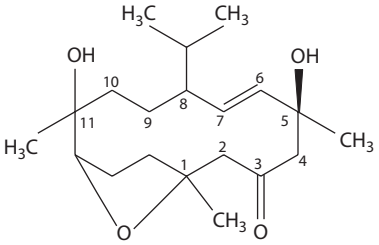
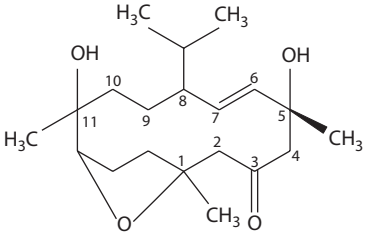
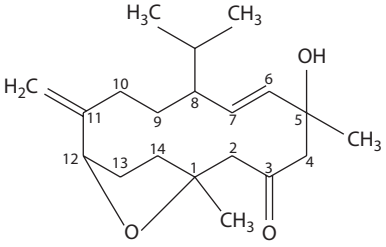
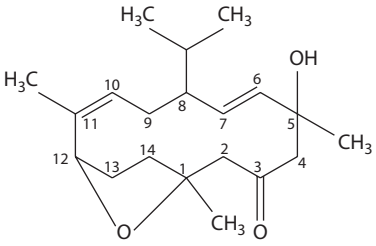
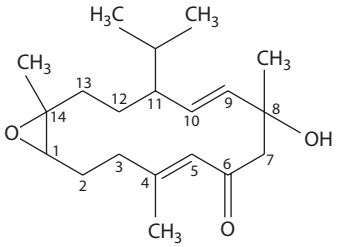
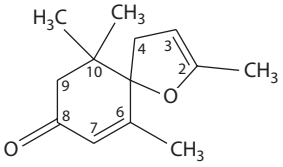
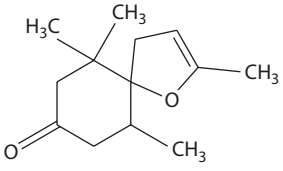
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
956.		2-Octenoic acid, 4-(1-methylethyl)-7-oxo-		731, 738, 1156, 4090, 4249	
957.	1669-44-9	3-Octen-2-one		568b, 1053, 3266, 4249	
958.	14129-48-7	4-Octen-3-one		404	
959.	124354-88-7	Octen-4-one, 2,6-dimethyl-, monoepoxy derivative		4249, 5811b	
960.	471-53-4	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-	3390, 4249		
961.	38284-11-6	7-Oxabicyclo[4.1.0]heptane-2,5-dione, 1,3,3-trimethyl-		1157, 4249, 5811b	
962.	10276-21-8	7-Oxabicyclo[4.1.0]heptan-2-one, 4,4,6-trimethyl-	568b, 4249		
963.	17024-44-1	6-Oxabicyclo[3.1.0]hexan-4-one, 1-methyl-	568b, 4249		
964.	98064-77-8	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,11R*, 		4089, 4091, 4249, 5811b	
965.	98167-33-0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,11S*,12S*)]- 		4089, 4098, 4249	
966.	98064-76-7	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5-hydroxy-1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,1 		943, 3352, 4089, 4091, 4098, 4249, 5811b	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
967.	58947-96-9	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-2-one, 8-hydroxy-8,12-dimethyl-5-(1-methylethyl)-		4249	
968.	98064-75-6	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-3-one, 5-hydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,10E, 		3219, 3971, 4089, 4091, 5811b	
969.	119613-99-9	15-Oxabicyclo[12.1.0]pentadec-9-en-5-one, 11,13-dihydroxy-1,11-dimethyl-8-(1-methylethyl)-, [1S-(1R*,8R*,9E,11R*,13S*,14S*)]-		4249, 5811b	
970.	98064-73-4	15-Oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one, 8-hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4E,8R*,9E,11R*, 		9, 12, 235, 236, 1156, 3971, 4089–4091, 5811b	
971.	72962-43-7	β-homo-7-Oxaergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R,23R,24S)-		429c, 4249	
972.	80722-28-7	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl- 		4249, 5811b	
973.	85248-56-2	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-, (*S*)- {8,9-dehydrotheaspirone}		5811, 5811b	
974.	38713-26-7	1-Oxaspiro[4.5]dec-2-en-8-one, 2,6,6,10-tetramethyl- 		937, 4249	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

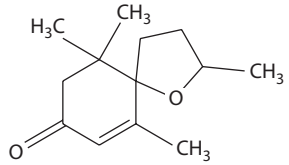
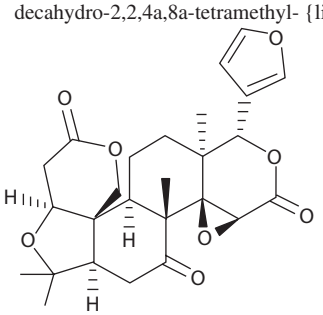
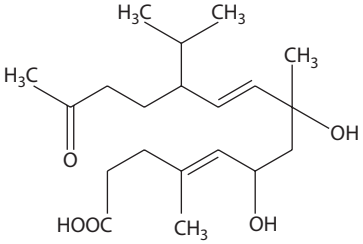
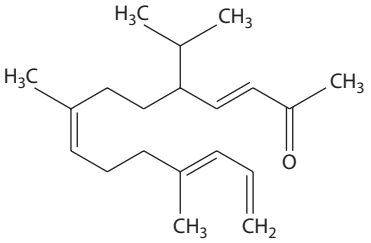
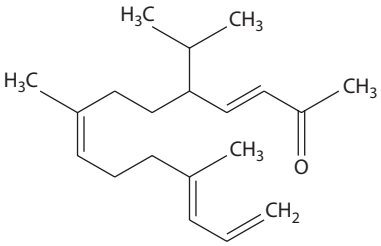
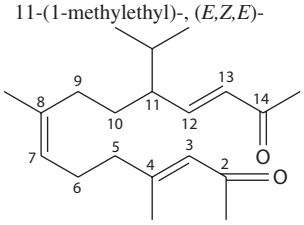
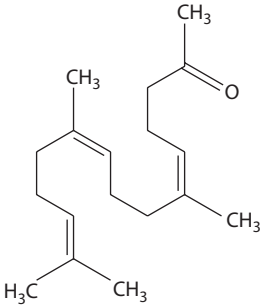
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
975.	19377-59-4	1-Oxaspiro[4.5]dec-6-en-8-one, 2,6,10,10-tetramethyl- 		937, 4249	
976..	1180-71-8	11*H*,13*H*-Oxireno[*d*]pyrano[4′,3′:3,3a]isobenzofuro[5,4-f][2]benzopyran-4,6,13(2H,5aH)-trione,8-(3-furyl) decahydro-2,2,4a,8a-tetramethyl- {limonin} 	5811, 5811a, 5811b		
977.	102673-27-8	4,9-Pentadecadienal, 6-(acetyloxy)-8-hydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4E,6R*,8R*,9E,11S*)]-		4249	
978.	95360-16-0	4,9-Pentadecadienal, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4E,6R*,8S*,9E,11S*)]-		4249	
979.	102734-47-4	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-		5811b	
980.	70898-33-8 102734-49-6	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)- 14-oxo- {isomer} 	2722	943, 2098, 2722, 4089, 4249, 5811, 5811b	
981.	102734-50-9	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl- 11-(1-methylethyl)-14-oxo-,methylester,[6R-(4E,6R*,8S*,9E,11S*)]-		3973, 3974a	
982.	102734-51-0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl- 11-(1-methylethyl)-14-oxo-,methylester,[6R-(4E,6R*,8R*,9E,11S*)]-		3973, 3974a	
983.	152209-55-7	6,11-Pentadecadien-2-one, 8,10,15-trihydroxy-8,12-dimethyl-5-(1-methylethyl)-, [5S-(5R*,6E,8R*,10S*,11E)]-		4249	
984.	2345-28-0	2-Pentadecanone $H_3C\text{-}(CH_2)_{12}\text{-}CO\text{-}CH_3$		947, 1240a, 4098a, 4249	
985.	502-69-2	2-Pentadecanone, 6,10,14-trimethyl- {phytone; hexahydrofarnesyl acetone} $H\text{-}[CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_2]_3\text{-}CH_2\text{-}CO\text{-}CH_3$	568b, 802, 803, 1375, 1375b, 2601a, 2775, 3219, 3287, 3308, 3557, 4249, 4570a, 5811b	404, 537, 543a, 568b, 1256, 1590a, 2339a, 2386, 2389, 2544, 2917a, 3545, 3547, 3549, 3550, 3560, 3561, 3905, 3971, 3973, 3974a, 4098a, 4249, 5811b	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
986	16825-16-4	2-Pentadecanone, 6,10,14-trimethyl-, [R-(R*,R*)]-	5811b	4249, 5811b	
987.	81345-07-5	3,8,12,14-Pentadecatetraen-2-one, 8,12-dimethyl-5-(1-methylethyl)-, (*E,E,E*)- 	2053, 4089, 4249, 5811b		
988.	81345-08-6	3,8,12,14-Pentadecatetraen-2-one, 8,12-dimethyl-5-(1-methylethyl)-, (*E,Z,E*)- 	2053, 4089, 4249		
989.	41429-55-4	3,7,12-Pentadecatriene-2,14-dione, 4,8-dimethyl-11-(1-methylethyl)-, (*E,Z,E*)- 		9, 943, 4089, 4249, 4409, 4573	
990.	57760-50-6	3,7,12-Pentadecatriene-2,14-dione, 4,8-dimethyl-11-(1-methylethyl)-, [S-(*E,E,E*)]-		9, 4249, 4573, 5811b	
991.	762-29-8	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl- {farnesyl acetone} {three isomers} 	568b, 810, 1063–1066, 1068–1074, 2761, 2762, 2765–2767, 2777, 2872, 3557, 4249, 5811b	404, 543a, 568b, 1256, 1590a, 2015, 2338, 2339a, 2386, 2389, 2544, 2917a, 3545, 3547, 3549, 3550, 3560, 3561, 3971, 4098a, 4249, 5811b	
992.	1117-52-8	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (*E,E*)-	1075, 5811b	2917a, 5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

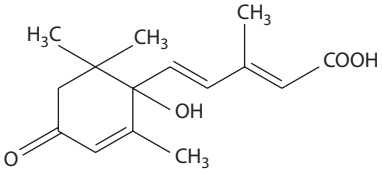
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
993.	21293-29-8 14375-45-2	2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-, [S-(*Z,E*)]- {abscisic acid} 		1156, 1206a,, 2864a, 3216, 3218, 3973, 4090, 5811b	
994.	7332-93-6	Pentanal, 2-oxo- CH_3-$(CH_2)_2$-CO-CH═O	1238, 3902, 4249		
995.	626-96-0	Pentanal, 4-oxo- CH_3-CO-$(CH_2)_2$-CH═O	3988a		3402, 3404, 3405
996.	328-50-7	Pentanedioic acid, 2-oxo- {α-ketoglutaric acid} HOOC-$(CH_2)_2$-CO-COOH	1238, 1310, 2939, 3059, 3302, 4249	120, 1310, 1312, 2939, 3797, 3973, 3974a, 4249, 5651, 5811b	
997.	52786-29-5	1,4-Pentanedione, 1-(2-furanyl)-	568b, 2570, 3553, 4249, 5811b		
998.	600-14-6	2,3-Pentanedione H_3C-CH_2-CO-CO-CH_3	314, 568b, 1140, 1232, 1238, 239, 1348–1350, 1354, 1374, 1375a, 1375a, 1377, 1378, 1418, 1419, 1586, 1589, 1590, 2002, 2079, 2337, 2387, 2469, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 2939, 3266, 3302, 3308, 3341, 3557, 3559, 3797, 3901, 4249, 4570a, 5770, 5811b	172a, 174b, 568b, 1053, 2917a, 3266, 5811b	1354, 1375a, 1375a, 1377, 1378 2244, 2387, 2506, 2507, 3401, 3402, 3404
999.	7493-58-5	2,3-Pentanedione, 4-methyl- H_3C-$CH(CH_3)$-CO-CO-CH_3	1238, 1375a, 1377, 3902, 4249		1375a, 1377
1000.	123-54-6	2,4-Pentanedione H_3C-CO-CH_2-CO-CH_3	5811b	2917a	3404, 4249
1001.	927-56-0	Pentanenitrile, 4-oxo- H_3C-CO-$(CH_2)_2$-CN	4249		
1002.	96937-54-1	Pentanoic acid, methyl-oxo-	3741, 3743, 4249, 4897, 5811b		
1003.	96937-53-0	Pentanoic acid, oxo-	3741, 3743, 4249, 4897		
1004.	54031-97-9	Pentanoic acid, 2-hydroxy-4-oxo-		4249, 4845	
1005.	6641-83-4	Pentanoic acid, 2-methyl-4-oxo-	568b, 3553, 4249, 5811b		
1006.	6376-59-6	Pentanoic acid, 2-oxo-, methyl ester	4249, 4800		
1007.	6628-79-1	Pentanoic acid, 3-methyl-4-oxo-	568b, 3553, 4249, 4897		
1008.	10191-25-0	Pentanoic acid, 3-oxo-	3553, 4249	2389, 2544, 4249	
1009.	123-76-2	Pentanoic acid, 4-oxo- {levulinic acid} H_3C-CO-$(CH_2)_2$-COOH	565, 568b, 741, 1099, 1103, 1237, 1238, 1360, 1375, 1375a, 1375b, 1586, 1882, 2088, 2570, 2761, 2762, 2765–2767, 2939, 3059, 3060, 3061, 3224, 3255, 3266, 3302, 3308, 3394, 3496, 3553, 3557, 4249, 4319, 4897, 5811b	307, 569, 568b, 570, 833, 1053, 1103, 1312, 3060, 3266, 4249, 5811b	1360, 1375a, 3393, 3402, 3404, 3405

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

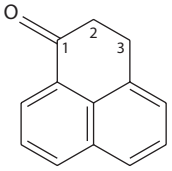
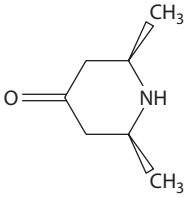
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1010.	539-88-8	Pentanoic acid, 4-oxo-, ethyl ester {ethyl levulinate} H_3C-CO-$(CH_2)_2$-COO-CH_2-CH_3	1238	1053, 3266	
1011.	624-45-3	Pentanoic acid, 4-oxo-, methyl ester {methyl levulinate} H_3C-CO-$(CH_2)_2$-COO-CH_3	1238	3266, 3543, 3560, 3561, 3858, 4249	
1012.	106-60-5	Pentanoic acid, 5-amino-4-oxo-		2024a, 4249, 4869	
1013.	66274-27-9	Pentanoic acid, 5-hydroxy-4-oxo-, methyl ester	3904, 4249, 5811b		3404
1014.	27154-67-2	Pentanone	3530, 4249, 5034		
1015.	63072-44-6	Pentanone, methyl-	642, 4249		
1016.	1009-14-9	1-Pentanone, 1-phenyl-	2570, 2769, 4249		
1017.	107-87-9	2-Pentanone H_3C-$(CH_2)_2$-CO-CH_3	112, 173a, 299, 299, 568b, 1063–1066, 1068–1074, 1140, 1238, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1378, 1412–1414, 1416, 1418, 1419, 1586, 1589, 1637, 1947, 2337, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 2782, 2804, 2858, 2939, 3254, 3255, 3266, 3302, 3308, 3508, 3530, 3557, 3901, 4052, 4056, 4162, 4249, 4319, 5770	172a, 174b, 568b, 647, 1053, 2337, 2389, 2544, 2722, 3266, 3797, 3973, 3974a, 4249, 5811b	1354, 1375a, 1378, 2506, 2507, 2244, 4052, 4056
1018.	64502-89-2	2-Pentanone, 1-hydroxy- H_3C-$(CH_2)_2$-CO-CH_2OH	5811b		3402, 3404, 4249
1019.	4161-60-8	2-Pentanone, 4-hydroxy- H_3C-CHOH-CH_2-CO-CH_3	2769, 3557, 4249	2339a	
1020.	123-42-2	2-Pentanone, 4-hydroxy-4-methyl- {diacetone alcohol} $(H_3C)_2$═C(OH)-CH_2-CO-CH_3	568b, 1378, 2767, 2769, 2773, 3397, 3555, 3559, 4249, 5770, 5811b	568b, 2356, 4249, 4867, 5811b	1378
1021.	565-61-7	2-Pentanone, 3-methyl- H_3C-CH_2-CH(CH_3)-CO-CH_3	1140, 1365, 1419, 1589, 3797, 4249, 5811b	5811b	
1022.	108-10-1	2-Pentanone, 4-methyl- $(H_3C)_2$═CH-CH_2-CO-CH_3	314, 568b, 1140, 1238, 1365, 1418, 1419, 2002, 2545, 2767, 3308, 4249, 5770, 5811b	568b, 647, 1662, 3186, 3188, 3974a, 4249	
1023.	5349-62-2	2-Pentanone, 4-methyl-1-phenyl-		1053, 3266	
1024.	5185-97-7	2-Pentanone, 5-(acetyloxy)-	5811b	568b, 3561, 4249	
1025.	1071-73-4	2-Pentanone, 5-hydroxy-	568b, 4249	568b, 4249	
1026.	1567-93-7	2-Pentanone, 5-hydroxy-3-methyl-	2774, 4249		
1027.	66309-84-0	2-Pentanone, 5-hydroxy-4-methyl-	2570, 2769, 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1028.	96-22-0	3-Pentanone H_3C-CH_2-CO-CH_2-CH_3	112, 314, 564, 568b, 605, 722, 1140, 1238, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1388–1390, 1412–1414, 1416, 1418, 1419, 1586, 1668, 2079, 2088, 2170, 2270, 2293, 2310, 2543, 2545, 2570, 2591, 2702, 2706, 2765, 2767, 2777, 2782, 2804, 2887, 2939, 3105, 3254, 3302, 3308, 3396, 3557, 3797, 4257, 4249, 4319, 5079, 5770, 5811b	568b, 984, 2339a, 2704, 3188, 3973, 4249, 5079, 5811b	1354, 1375a, 1375a, 1377, 2244
1029.	66735-69-1	3-Pentanone, 1-(methylthio)-	4570a		
1030.	565-80-0	3-Pentanone, 2,4-dimethyl- $(H_3C)_2$═CH-CO-CH═$(CH_3)_2$	1140, 1418, 1419, 2003, 3219, 3308, 3797, 4249, 5811b		
1031.	565-69-5	3-Pentanone, 2-methyl- $(H_3C)_2$═CH-CO-CH_2-CH_3	1140, 1418, 1419, 2387, 2506, 2507, 2570, 2775, 3219, 3308, 3797, 4249, 5811b	3186, 3188, 4249	2387, 2506, 2507
1032.	21978-49-4	5,9,13,17,21,25,29,33-Pentatriacontaoctaen-2-one, 6,10,14,18,22,26,30,34-octamethyl-, (all-*E*)-	1352, 2769	1352, 2015, 4249, 5811b	
1033.	91238-45-8	4-Pentene-2,3-dione	4249	5811b	
1034.	1629-58-9	1-Penten-3-one H_3C-CH_2-CO-CH═CH_2	314, 1140, 1365, 1418, 1419, 2506, 2507, 2777, 2857, 3308, 3797, 4249, 4570a, 5770, 5811b	1157, 1248, 2336, 2917a, 4092, 4249	2506, 2507
1035.	3712-68-8	1-Penten-3-one, 2,4-dimethyl-		2917a	
1036.	104-27-8	1-Penten-3-one, 1-(4-methoxyphenyl)-		1053, 3266	
1037.	25044-01-3	1-Penten-3-one, 2-methyl- H_3C-CH_2-CO-C(CH_3)═CH_2	2506, 2507, 4249, 5811b		2506 (0), 2507 (0)
1038.		2-Penten-4-one, 2,3-dimethyl- $(H_3C)_2$═C═C(CH_3)-CO-CH_3	1364		
1039.	625-33-2	3-Penten-2-one H_3C-CH═CH-CO-CH_3	1063–1066, 1068–1074, 1348–1350, 1354, 1365, 1371, 1375a, 1587, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 3559, 4249, 4570a, 5770	3186, 3188, 4249	1354, 1375a, 2244, 2506, 2507, 3401
1040.	3102-33-8	3-Penten-2-one, (*E*)		568b, 2917a, 4249	
1041.	1118-66-7	3-Penten-2-one, 4-amino- H_3C-C(NH_2)═CH-CO-CH_3	3559		
1042.	565-62-8	3-Penten-2-one, 3-methyl- H_3C-CH═C(CH_3)-CO-CH_3	3824, 4249		
1043.	141-79-7	3-Penten-2-one, 4-methyl- {mesityl oxide} $(H_3C)_2$═C═CH-CO-CH_3	1053, 1238, 3266, 4249, 5770	404, 1053, 2339a, 3217, 3266, 4249	
1044.	13891-87-7	4-Penten-2-one H_2C═CH-CH_2-CO-CH_3	1140, 1419, 1589, 2506, 2507, 2777, 3797, 4249, 5811b		2506 (0), 2507 (0), 3401

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1045.	127-42-4	4-Penten-3-one, 5-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {ethyl-α-ionone}		172a, 174b, 1053, 3266	
1046.	488-84-6	*D*-erythro-2-Pentulose {xylulose} = *D*-ribulose 488-84-6 $HOCH_2$-CO-$(CHOH)_2$-CH_2OH		429b, 4249, 4712	
1047.	24218-00-6	*D*-erythro-2-pentulose, 1,5-bis(dihydrogen phosphate)		4249	
1048.	518-85-4	1*H*-Phenalen-1-one, 2,3-dihydro- 	278, 279, 4249		
1049.	20239-99-0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, [3S- (3α,4β,21β)]-		4249, 4445, 4844	
1050.		Pheophytin, 10-hydroxy-		5517	
1051.	3147-18-0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2E,7S*,11S*),4β,21β]]- {pheophytin B}		4249, 4445, 5517	
1052.	15664-29-6	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, [3S-(3α,4β,21β)]- {pheophorbide A}		4249, 4445, 5517	
1053.	603-17-8	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2E,7S*,11S*),4β,21β]]- {pheophytin A}		3626a, 4249, 4445, 5517	
1054.	62784-01-4	Piperidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-	5811, 5811a, 5811b		
1055.	13200-35-6	4-Piperidinone, 2,6-dimethyl-, *cis*- 	1120, 3559, 4249, 5811b		
1056.	69135-98-4	4-Piperidinone, 2,6-dimethyl-, *trans*-	1120, 4249, 5811b		
1057.	3311-23-7	4-Piperidinone, 2,2,6-trimethyl-, (R)-	1120, 4249, 5811b		
1058.	57-83-0	Pregn-4-ene-3,20-dione		429c, 4249, 4613	
1059.	145-13-1	Pregn-5-en-20-one, 3-hydroxy-, (3β)-		429c, 4249, 4613	
1060.	32378-60-2	Pregnan-20-one, 3-[(1-oxohexadecyl)oxy]-, (3β,5α)-		429c, 4249, 4613	
1061.	78-98-8	Propanal, 2-oxo- {pyruvaldehyde; methylglyoxal} H_3C-CO-CH═O	568b, 1238, 1239, 1491, 2270, 2337, 2939, 3251, 3266, 3302, 3341, 3515, 3553, 4079, 4249, 5680, 5811b	120, 568b, 826a, 2153b, 2337, 2939, 3266, 3797, 3974a, 4079 4249, 5079, 5811b	1228
1062.	997-10-4	Propanal, 2-oxo-3-hydroxy- {reductone} $HOCH_2$-CO-CH═O		3797	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1063	631-66-3	Propanamide, 2-oxo- {pyruvamide} H_3C-CO-CO-NH_2	568b, 1586, 2543, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3553, 3557, 4249, 5811b		
1064	1438-92-2	1,2-Propanedione, 1-(2-furanyl)-	568b, 2765, 2766, 3553, 4249, 5811b	568b, 3547, 4249, 5811b	3402, 3404
1065	2034-60-8	1,2-Propanedione, 1-(4-hydroxy-3-methoxyphenyl)-	4249	5811b	
1066	1197-20-2	1,2-Propanedione, 1-(5-methyl-2-furanyl)-	568b, 3553, 3555, 4249	568b, 3547, 3555, 4249	
1067	579-07-7	1,2-Propanedione, 1-phenyl-	2761, 2762, 2765, 2766, 4249		
1068	631-57-2	Propanenitrile, 2-oxo- H_3C-CO-CN	568b, 642, 4249		
1069	127-17-3	Propanoic acid, 2-oxo- {pyruvic acid} H_3C-CO-COOH	563, 568b, 1310, 2088, 2939, 3059, 3224, 3302, 3308, 3553, 4249, 5811b	69, 120, 172a, 174b, 563, 568b, 1053, 1305a, 1310, 1312, 1923, 2389, 2544, 2939, 3266, 3370, 3797, 3973, 3974a, 4249, 5811b, 5896	
1070	617-35-6	Propanoic acid, 2-oxo-, ethyl ester H_3C-CO-COO-C_2H_5	3410, 4249		
1071.	600-22-6	Propanoic acid, 2-oxo-, methyl ester H_3C-CO-COO-CH_3	568b, 4249, 5811b	5811b	
1072	4151-33-1	Propanoic acid, 2-oxo-, potassium salt		5811b	
1073	3913-50-6	Propanoic acid, 2-oxo-3-(phosphonooxy)-		429b, 4249, 4634	
1074	1113-60-6	Propanoic acid, 3-hydroxy-2-oxo- HOH_2C-CO-COOH		1971, 2939, 3797, 4634, 5777, 5811, 5811b	
1075		1-Propanone, 1-(dimethylhydroxyphenyl)-	3226, 3557, 4249		
1076		1-Propanone, 1-(3,5-dimethyl-4-hydroxyphenyl)-	2767, 4249		
1077	3194-15-8	1-Propanone, 1-(2-furanyl)-	568b, 1587, 2570, 2767, 2773, 4249, 5770, 5811b		
1078		1-Propanone, 1-(3-furanyl)-	2773, 4249		
1079	610-99-1	1-Propanone, 1-(2-hydroxyphenyl)-	1375, 1375b, 2767, 2769, 4249		
1080		1-Propanone, 1-(3-hydroxyphenyl)-	1586, 4249		
1081		1-Propanone, 1-(2-methylphenyl)-	2767, 2769, 4249		
1082	51772-30-6	1-Propanone, 1-(3-methylphenyl)-	2767, 2769, 4249		
1083	5337-93-9	1-Propanone, 1-(4-methylphenyl)-	3387, 4249		
1084		1-Propanone, 1-(4-methyl-2-pyridinyl)-	4570a		
1085	93-55-0	1-Propanone, 1-phenyl- {propiophenone}	568b, 1378, 1427, 1586, 2731, 2735, 2767, 3410, 3557, 4249, 4570a, 5811b	568b, 2336, 2389, 2544, 4249, 5811b	1378
1086	1321-48-8	1-Propanone, 1-phenyl-3-hydroxy-	1586		
1087	3238-55-9	1-Propanone, 1-(2-pyridinyl)-	4570a		
1088		1-Propanone, 1-(2-pyridinyl)-2-methyl-	4570a		
1089	1570-48-5	1-Propanone, 1-(3-pyridinyl)- {pyridyl ethyl ketone}	568b, 761, 916, 1587, 2079, 2107, 2170, 2224, 2228, 2270, 2724, 2731, 2735, 2939, 3054, 3056, 3058, 3062, 3302, 3308, 3444, 3523, 3553, 3708, 4202, 4249, 5079, 5811b	568b, 937, 2359, 2939, 3056, 3444, 3973, 4249, 5079, 5382	
1090	1701-69-5	1-Propanone, 1-(4-pyridinyl)-	568b, 1587, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1091.	1073-26-3	1-Propanone, 1-(1*H*-pyrrol-2-yl)-	568b, 1586, 2767, 3553, 3557, 3650, 4249, 5811b	568b, 2389, 2544, 3547, 4249, 5811b	
1092.	80933-75-1	1-Propanone, 1-[2-(3,4,5,6-tetrahydropyridinyl)]-		2917a	
1093.	67-64-1	2-Propanone {acetone} $H_3C\text{-}CO\text{-}CH_3$-	38, 111, 112, 126a, 126b, 172, 173a, 174b, 174c, 199, 237, 239, 298, 299, 314, 329, 402, 405, 407, 408, 480, 544–546, 564, 568b, 639, 643, 645, 688, 722, 764a, 778, 830a, 892, 893, 929, 966, 1023, 1039, 1051, 1063–1074, 1099, 1140, 1153, 1154, 1167, 1168, 1238, 1239, 1283, 1284, 1329, 1338, 1348–1352, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412, 1413, 1416, 1418, 1419, 1437, 1449, 1489, 1495–1497, 1586, 1589, 1590, 1634, 1637, 1638, 1668, 1674, 1744, 1842, 1875, 1947, 1963, 2002, 2003, 2063, 2079, 2083–2085, 2091, 2133, 2170, 2171, 2252, 2270, 2296, 2301, 2302, 2304, 2305, 2313a, 2337, 2452, 2483, 2519, 2520, 2525, 2543, 2570, 2573–2575, 2591, 2634, 2644, 2702, 2765, 2767, 2777, 2781, 2782, 2800, 2801, 2822, 2857, 2868, 2927, 2939, 2942, 3007, 3059, 3132, 3135, 3136, 3169, 3190, 3251, 3254, 3255, 3257, 3300, 3302, 3306, 3308, 3373, 3396, 3418, 3431, 3436, 3438, 3482, 3493, 3530, 3551, 3553, 3557, 3581–3584, 3692, 3797, 3817, 3844, 3871, 3876, 3880, 3882, 3883, 3897, 3901, 3973, 3992, 4005–4007, 4052, 4056, 4078, 4159, 4162, 4194, 4202, 4249, 4254, 4256, 4257, 4290, 4319, 4360, 5028, 5034, 5079, 5512, 5547, 5554, 5583, 5770, 5811b, 5836, 5869a, 4A02	120, 568b, 647, 984, 1550, 1590, 1668, 2293, 2337, 2339a, 2863, 2866, 2914, 2939, 3626, 3797, 3974a, 4064, 4223, 4225, 4249, 5079, 5811b, 5896	1228, 1354, 1375a, 1377, 1378, 2244, 3401, 4052, 4056

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

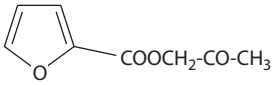
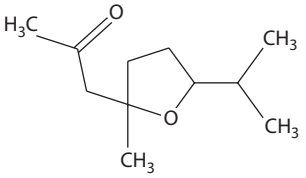
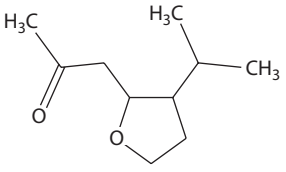
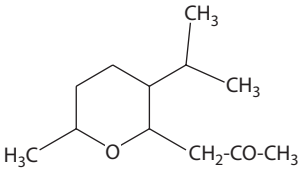
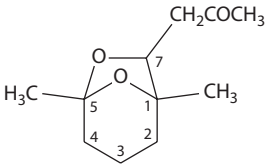
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1094.	592-20-1	2-Propanone, 1-(acetyloxy)- H_3C-CO-CH_2-OOC-CH_3	568b, 1215, 1238, 1375, 1375b, 1378, 2387, 2570, 2731, 2731, 2735, 2777, 3553, 3557, 4249, 5770, 5811b	568b, 2386, 4249, 5811b	1378, 2244, 2387, 3401, 3402, 3404
1095.	298-08-8	2-Propanone, 1-amino- H_3C-CO-CH_2-NH_2	568b, 1371, 1587, 2543, 2773, 3410, 4249, 5811b		
1096.	78-95-5	2-Propanone, 1-chloro- H_3C-CO-CH_2-Cl	2777, 4249, 5811b		
1097.	10258-70-5	2-Propanone, 1-(formyloxy)- H_3C-CO-CH_2-OOC-H	5811b		3402, 4249
1098.	116-09-6	2-Propanone, 1-hydroxy- {acetol} H_3C-CO-CH_2-OH	568b, 1063–1066, 1068–1074, 1360, 1371, 1375a, 2337, 2493, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3397, 3410, 3553, 3555, 3557, 3559, 4249, 5811b	404, 568b, 1590a, 2337, 2339b, 2389, 2544, 2917a, 3549, 3555, 4249, 5811b	1360, 1375a, 2244, 3401, 3402, 3404, 3405
1099.		2-Propanone, 1-hydroxy-, 2-furoyl ester 	1586		
1100.	57-04-5	2-Propanone, 1-hydroxy-3-(phosphonooxy)-		429b	
1101.	122-84-9	2-Propanone, 1-(4-methoxyphenyl)-		172a, 174b, 174b, 568b, 1053, 3266	
1102.	496-49-1	2-Propanone, 1-(1-methyl-2-pyrrolidinyl)-		2917a, 4249	
1103.	103-79-7	2-Propanone, 1-phenyl-	1360, 1375a, 2761, 2765–2767, 4249	937, 3547, 4249	1360, 1375a
1104.	20194-70-1	2-Propanone, 1-(tetrahydro-4-methyl-2*H*-pyran-2-yl)-	568b, 2761, 2762, 2765, 2766, 4249, 5811b	568b, 937, 3188, 3543, 3547, 3560, 3561, 4048, 4249	
1105.		2-Propanone,1-[tetrahydro-(2-methyl-5-methylethyl)-2-furanyl]- 		3219, 3545	
1106.	38713-24-5	2-Propanone,1-[tetrahydro-3-(1-methylethyl)-2-furanyl]-,*trans*- 		404, 568b, 943, 1156, 3205, 3219, 3543, 3547, 3550, 4090, 4249	
1107.	39815-69-5	2-Propanone, 1-[tetrahydro-4-(1-methylethyl)-2-furanyl]-	5811b	3219, 4249	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1108.	39815-68-4	2-Propanone, 1-[tetrahydro-6-methyl-3-(1-methylethyl)-2*H*-pyran-2-yl]- {two isomers reported} 	568b, 2761, 4249, 5811b	404, 568b, 937, 1063–1066, 1068–1074, 1590a, 2386, 2389, 2544, 3188, 3219, 3356, 3543, 3545, 3547, 3550, 3561, 4098a, 4249, 5811b	
1109.		2-Propanone, 1-[tetrahydro-6-methyl-4-(1-methylethyl)-2*H*-pyran-2-yl]-		3217, 4249	
1110.		2-Propanone, 1-(1,5-dimethyl-6,8-dioxabicyclo[3.2.1]oct-7-yl)- 		3547, 4249	
1111.	6975-60-6	2-Propanone, 1-(2-furanyl)-	568b, 3555, 4249, 5811b	568b, 2917a, 3547, 3555, 4249, 5811b	3404
1112.		2-Propanone, 1-[2-hydroxy-5-(1-methylethyl)-2-methyl-1-cyclopentyl]-		3547, 4249	
1113.	13100-05-5	2-Propanone, 1-(2-hydroxyphenyl)-	1586, 1884, 2767, 3553, 3712, 3890, 4249		
1114.	5211-62-1	2-Propanone, 1-(2-methoxyphenyl)-	1586, 3266, 4249		
1115.		2-Propanone, 1-(2-tetrahydrofuranyl)-	1360, 1375a		1360, 1375a
1116.		2-Propanone, 1-(3-hydroxyphenyl)-	1884, 3553, 3712	3186, 3188, 4249	
1117.	18826-61-4	2-Propanone, 1-(3-methylphenyl)-	2767, 3557		
1118.	6302-03-0	2-Propanone, 1-(3-pyridinyl)-	2724, 2727, 2731, 2735, 2939, 3302, 3491	937, 3491	
1119.	96-26-4	2-Propanone, 1,3-dihydroxy-	1371, 4249		
1120.		2-Propanone, 1-(3,4-dihydro-6-methylpyran-2-yl)-		3547, 4249	
1121.	19037-58-2	2-Propanone, 1-(3,5-dimethoxy-4-hydroxyphenyl)-	3553, 3712	5811b	
1122.	16695-72-0	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (*E*)-	2543, 2773, 4249	2389, 2544, 4249, 5811b	
1123.	16695-73-1	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (*Z*)-	2543, 2773	2389, 2544, 5811b	
1124.	2503-46-0 110053-51-5	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	568b, 1364, 1586, 1884, 2570, 2767, 3553, 3557, 3712, 4249, 5811b	568b, 3430, 4249, 5811b	
1125.	770-39-8	2-Propanone, 1-(4-hydroxyphenyl)-	568b, 1364, 3553, 4249, 5811b		
1126.	6304-16-1	2-Propanone, 1-(4-pyridinyl)-	1587, 4249		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

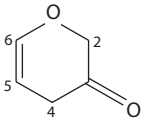
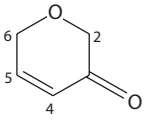
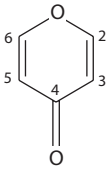
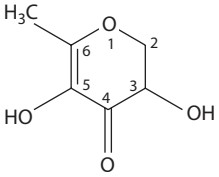
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1127.	13678-74-5	2-Propanone, 1-(5-methyl-2-furanyl)-	2570, 4249	2917a	
1128.	50672-03-2	2-Propanone, 1-[5-(hydroxymethyl)-2-furanyl]-	568b, 1375, 3553, 4249, 5811b		
1129.	2983-65-5	2-Propen-1-one, 1-(4-hydroxy-3-methoxyphenyl)-	4249	5811b	
1130.	94-41-7	2-Propen-1-one, 1,3-diphenyl- {chalcone}	1238, 4249, 4786		
1131.	145917-24-4	2-Propen-1-one, 1,3-di-3-pyridinyl-, (*E*)-		4249	
1132.	551-68-8	*D*-Psicose $HOCH_2$-CO-$(CHOH)_3$-CH_2OH		3667, 4249	
1133.	70898-35-0	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro-6-hydroxy-3-oxo-	1378	2939, 3797, 4249	1378
1134.	112468-46-9	2*H*-Pyran-2,5(6*H*)-dione	4249	5811b	
1135.	28743-04-6	2*H*-Pyran-3(4*H*)-one 	4249	5811b	
1136.	23462-75-1	2*H*-Pyran-3(4*H*)-one, dihydro-	4249, 5811b		3402, 3404, 4249
1137.	121197-11-3	2*H*-Pyran-3(4*H*)-one, dihydro-4-(hydroxymethyl)-	4249	5811b	
1138.	65712-87-0	2*H*-Pyran-3(4*H*)-one, dihydro-6-methoxy-	4249, 5811b		3404, 4249
1139.	43152-89-2	2*H*-Pyran-3(4*H*)-one, dihydro-6-methyl-	3404, 4249		
1140.	98166-23-5	2*H*-Pyran-3(6*H*)-one 	4249	5811b	
1141.	108-97-4	4*H*-Pyran-4-one 	1352, 5811b		
1142.	84302-42-1	4*H*-Pyran-4-one, 2,3-dihydro-	4249	5811b	
1143.	28564-83-2	4*H*-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- 	568b, 1089a, 1134, 1138, 1351, 1352, 1360, 1375, 1375a, 1375b, 1882, 1887a, 2337, 2493, 2524a, 2543, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2857, 3394, 3397, 3553, 3557, 3828, 4249, 5811b	568b, 2339b, 2917a, 3549, 4249, 5811b	1360, 1375a, 3402, 3405
1144.	6380-97-8	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-2-(hydroxymethyl)-	3553, 4249	3430, 5811b	
1145.	38877-21-3	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-6-methyl-	1134, 1138, 4249		

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1146.	131524-09-9	4*H*-Pyran-4-one, 2,6-diethyl-3-hydroxy-	90b, 4249		
1147.	1004-36-0	4*H*-Pyran-4-one, 2,6-dimethyl-	2507, 4249		
1148.	4940-17-4	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-	90b, 4249, 5811b		
1149.	131524-16-8	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-6-methyl-	90b, 4249, 5811b		
1150.	4940-11-8	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy- {ethylmaltol}	90b, 568b, 3266, 4249, 5811b	172a, 174b, 568b, 1053, 3219, 3266, 3370, 4249	
1151.	131524-08-8	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5,6-dimethyl-	90b, 4249, 5811b		
1152.	131524-04-4	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5-methyl-	90b, 4249, 5811b		
1153.	22639-24-3	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-6-methyl-	90b, 4249, 5811b		
1154.	61892-88-4	4*H*-Pyran-4-one, 2-hydroxy-3-methyl-	3410, 3553, 4249		
1155.	61892-87-3	4*H*-Pyran-4-one, 2-hydroxy-5-methyl-	1351, 1352, 3553, 4249		
1156.		4*H*-Pyran-4-one, 2-hydroxymethyl-3,5,6-trihydroxy-	1375a (0), 1377 (0), 4249		1375a, 1377, 4249
1157.		4*H*-Pyran-4-one, 2-methyl-3,5,6-trihydroxy-	1375a (0), 1377 (0)		1375a, 1377
1158.	29943-42-8	4*H*-Pyran-4-one, 2,3,5,6-tetrahydro- = 4*H*-Pyran-4-one, tetrahydro-	568b, 4249		
1159.		4*H*-Pyran-4-one, 2,5-dihydroxy-3-methyl-	1351, 1352		
1160.	488-18-6	4*H*-Pyran-4-one, 3,5-dihydroxy-	568b, 1351, 1375a, 1377, 1586, 2769, 4249		
1161.	61892-86-2	4*H*-Pyran-4-one, 3,5-dihydroxy-2,6-dimethyl-	568b, 1375, 1375b, 2767, 3553, 3557, 4249		
1162.	1073-96-7	4*H*-Pyran-4-one, 3,5-dihydroxy-2-methyl- {5-hydroxymaltol}	568b, 1089a, 1351, 1352, 1360, 1375, 1375a, 1375b, 1377, 1882, 1886, 1887a, 2524a, 2761, 2762, 2765–2767, 2777, 3394, 3410, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 4249, 5811b	1360, 1375a, 1377, 3402, 3404, 3405
1163.		4*H*-Pyran-4-one, 3,5-dihydroxymethyl-2,6-dimethyl-	1375, 1375b, 2767, 4249		
1164.	496-63-9	4*H*-Pyran-4-one, 3-hydroxy-	568b, 1351, 1352, 1375, 1375a, 1375b, 1377, 1586, 2767, 3553, 3557, 4249, 5811b		1375a, 1377, 3401, 3402, 3404, 3405, 4249
1165.	40311-00-0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylethyl)-	90b, 4249, 5811b		
1166.	4940-18-5	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylpropyl)-	90b, 4249, 5811b		
1167.	131524-11-3	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylbutyl)-	90b, 4249, 5811b		
1168.	76015-10-6	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylpropyl)-	90b, 4249, 5811b		
1169.	131524-12-4	4*H*-Pyran-4-one, 3-hydroxy-2-(3-methylbutyl)-	90b, 4249, 5811b		

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

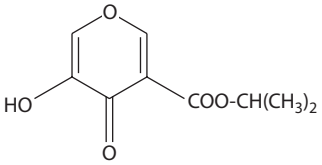
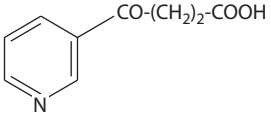
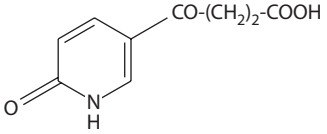
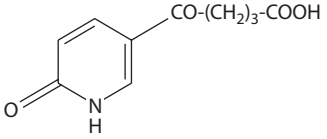
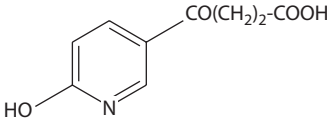
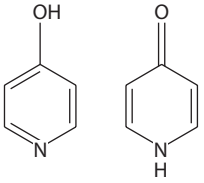
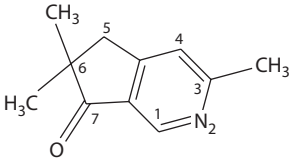
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1170.	131524-05-5	4*H*-Pyran-4-one, 3-hydroxy-2,5,6-trimethyl-	90b, 4249, 5811b		
1171.	131524-02-2	4*H*-Pyran-4-one, 3-hydroxy-2,5-dimethyl-	90b, 4249, 5811b		
1172.	2298-99-9	4*H*-Pyran-4-one, 3-hydroxy-2,6-dimethyl-	90b, 4249, 5811b		
1173.		4*H*-Pyran-4-one, 3-hydroxymethyl-	1582		
1174.	118-71-8	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}	568b, 1131, 1351, 1352, 1375, 1375a, 1375b, 1377, 1378, 1586, 1881, 1884, 2570, 2767, 2777, 3266, 3397, 3553, 3555, 3557, 4249, 5811b	172a, 174d, 568b, 965, 1053, 1590a, 2337, 2339b, 2386, 2389, 2544, 2917a, 3266, 3430, 3543, 3555, 3560, 3561, 5811b	1375a, 1377, 1378, 3401, 3402, 3404, 3405
1175.	131524-10-2	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-6-propyl-	90b, 4249, 5811b		
1176.	131524-13-5	4*H*-Pyran-4-one, 3-hydroxy-2-pentyl-	90b, 4249, 5811b		
1177.	4940-16-3	4*H*-Pyran-4-one, 3-hydroxy-2-propyl-	90b, 4249, 5811b		
1178.	42508-10-1	4*H*-Pyran-4-one, 3-hydroxy-5-methyl-	568b, 4249		
1179.	131524-07-7	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylethyl)-	90b, 4249, 5811b		
1180.	131524-14-6	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylpropyl)-	90b, 4249, 5811b		
1181.	131524-15-7	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(2-methylpropyl)-	90b, 4249, 5811b		
1182.	40861-87-8	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-propyl-	90b, 4249, 5811b		
1183.	50671-50-6	4*H*-Pyran-4-one, 3-methyl-	1375, 1375b, 4249		
1184.	131524-03-3	4*H*-Pyran-4-one, 5-hydroxy-2,3-dimethyl-	90b, 5811b		
1185.	644-46-2	4*H*-Pyran-4-one, 5-hydroxy-2-methyl- = 4*H*-pyran-4-one, 3-hydroxy-6-methyl- {allomaltol}	568b, 1351, 1352, 1364, 2601a, 3553, 4249, 5811b		
1186.	131524-06-6	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-methyl-	90b, 4249, 5811b		
1187.	131524-17-9	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-propyl-	90b. 4249, 5811b		
1188.	499-78-5	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-	1375a (0), 1377 (0)		1375a, 1377
1189.		4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-, (1-methylethyl) ester 	1375a (0), 1377 (0)		1375a, 1377
1190.	76014-80-7	3-Pyridinebutanal, γ-oxo-		4249	
1191.	4192-31-8	3-Pyridinebutanoic acid, γ-oxo- 		1101, 2226, 3444, 4236, 4249, 5508	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1192.	15873-27-5	3-Pyridinebutanoic acid, 1,6-dihydro-γ,6-dioxo- 	4249	1110, 4249, 4709	
1193.	5006-66-6	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-		4249	
1194.	71608-01-0	3-Pyridinepentanoic acid, 1,6-dihydro-δ,6-dioxo- 		1101, 4249, 4945	
1195.	61892-76-0	2-Pyridinol, 5-acetyl-3,4-dihydro- {2(1*H*)-pyridinone, 5-acetyl-3,4-dihydro-}	568b, 3553, 4249		
1196.		2-Pyridinol-5-butanoic acid, γ-oxo- {2(1*H*)-pyridinone-5-butanoic acid, γ-oxo-} 		1101, 4249	
1197.		2-Pyridinol-5-pentanoic acid, δ-oxo- {2(1*H*)-pyridinone-5-pentanoic acid, δ-oxo-}		1101, 4249	
1198.	108-96-3 626-64-2	4-Pyridinol {4(1*H*)-pyridinone} 	568b, 2387, 4249, 4407		
1199.		9*H*-Pyrido[2,3-*a*]indole, 2-acyl-	568b, 4249		
1200.	55713-43-4	7*H*-2-Pyrindin-7-one, 5,6-dihydro-3,6,6-trimethyl- 		69, 939, 943, 3491, 4249	
1201.	72693-01-7	1*H*-Pyrrole-2-acetaldehyde, α-oxo-	568b, 1587, 4249, 5811b		
1202.	78504-05-9	Pyrrolidine, 1-(2-furoyl)-	568b, 4249		
1203.		Pyrrolidine, 1-(2-furoyl-5-methyl)-	568b, 4249		
1204.	32389-40-5	Pyrrolidinecarboxylic acid, oxo-, (S)-		4249, 4543	
1205.	121197-25-9	2,4-Pyrrolidinedione, 3-butyl-5-propylidene-	3429a, 4249	5811b	
1206.	121197-20-4	2,4-Pyrrolidinedione, 5-butyl-3-propylidene-	3429a, 4249	5811b	
1207.	121197-28-2	2,4-Pyrrolidinedione, 3-butylidene-5-(2-methylpropyl)-	3429a, 4249	5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

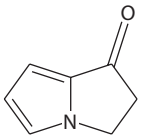
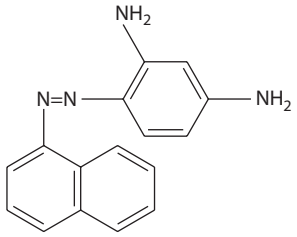
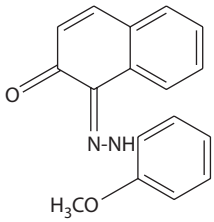
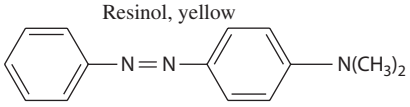
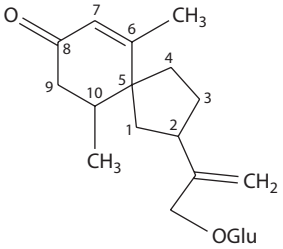
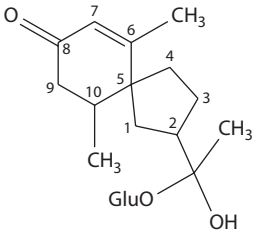
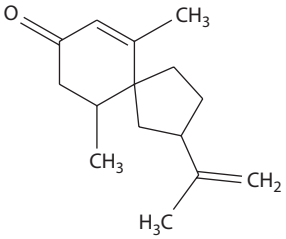
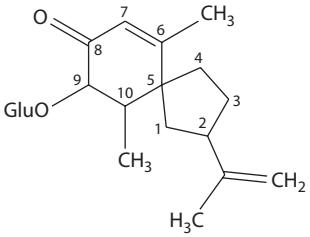
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1208.	121197-18-0	2,4-Pyrrolidinedione, 3-butylidene-5-propyl-	3429a, 4249	5811b	
1209.	121197-17-9	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-(2-methylpropylidene)-	3429a, 4249	5811b	
1210.	121197-22-6	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-propylidene-	3429a, 4249	5811b	
1211.	121197-19-1	2,4-Pyrrolidinedione, 3-(2-methylpropylidene)-5-propyl-	3429a, 4249	5811b	
1212.	121197-15-7	2,4-Pyrrolidinedione, 5-propyl-3-propylidene-	3429a, 4249	5811b	
1213.	17266-64-7	1*H*-Pyrrolizin-1-one, 2,3-dihydro- 	568b, 2775, 4249		
1214.	6416-57-5	Resinol, brown 			5079, 5381
	69772-40-3	Resinol			
		Resinol, red 			
	60-11-7	Resinol, yellow 			
1215.	62574-27-0	Spiro[4.5]dec-6-en-8-one, 2-[1-[(β-*D*-glucopyranosyloxy) methyl]ethenyl]-6,10-dimethyl- 		77, 1156, 4090, 4249	

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1216.	62574-29-2	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl- 		77, 1156, 4090, 4249	
1217.	62623-87-4	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-		77, 1156, 4090, 4249	
1218.	54878-25-0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-2-(1-methylethenyl)-, [2R-[2α,5α(R*)]]- 		1156, 1253, 4090, 4249	
1219.		Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethenyl)-		4249, 4611	
1220.		Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethyl)-		4249, 4611	
1221.	18444-79-6	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethylidene)-, (5R-*cis*)-		3547, 4249	
1222.	62574-25-8	Spiro[4.5]dec-6-en-8-one, 9-(β-*D*-glucopyranosyloxy)-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]- 		77, 1156, 4090, 4249	
1223.	117407-01-9	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6,10-dimethyl-2-(1- methylethenyl)- {spirovetivan A}		5811, 5811b	
1224.	117332-54-4	Spiro[4.5]dec-6-en-8-one,2-[1-(hydroxymethyl)ethenyl]-6-methyl- {spirovetivan B}		5811, 5811b	

(*continued*)

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

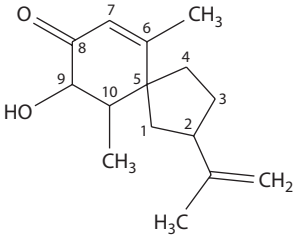
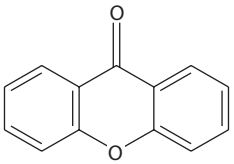
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1225.	62623-88-5	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]- 		1156, 4090, 4249, 4717	
1226.	58879-40-6	1,13-Tetradecadien-3-one		2917a	
1227.	540-09-0	12-Tricosanone $[H_3C\text{-}(CH_2)_{10}]_2{=}C{=}O$	722, 4249		
1228.	66309-85-1	5,9,13,17,21-Tricosapentaen-2-one, 6,10,14,18,22-pentamethyl-	1352, 2769	1352, 2015, 4249	
1229.	129777-24-8	3,7-Tridecadiene-2,12-dione, 6-hydroxy-6-methyl-9-(1-methylethyl)-		2544, 4249, 5811b	
1230.	60593-18-2	3,8-Tridecadiene-2,12-dione, 8-methyl-5-(1-methylethyl)-, [S-(*E,E*)]-		4249	
1231.	593-08-8	2-Tridecanone $H_3C\text{-}(CH_2)_{10}\text{-}CO\text{-}CH_3$		947, 1053, 3266, 4098a, 4249	
1232.	117210-51-2	2-Tridecanone, 4,8,12-trimethyl-		4249, 5811b	
1233.	122855-83-8	5,10,12-Tridecatrien-2-one, 6,12-dimethyl-9-(1-methylethyl)-		5811, 5811b	
1234.	59573-83-0	5,10,12-Tridecatrien-2-one, 6,12-dimethyl-9-(1-methylethyl)-, [S-(*E,E*)]- $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}CH{=}C(CH_3)\text{-}(CH_2)_2\text{-}CH[CH(CH_3)_2]\text{-}CH{=}CH\text{-}C(CH_3){=}CH_2$		943, 944, 1156, 4090, 4249, 5811b	
1235.	22986-69-2	17-Tritriacontanone	2170, 3562, 5079		
1236.		5,8-Undecadien-2-one, 6,10-dimethyl-		3543	
1237.	65017-84-7 133561-45-2	5,8-Undecadien-2-one, 6,10-dimethyl-10-hydroxy- (*E,E*)-		231, 1156, 4090, 4098a, 4249, 5811, 5811b	
1238.	689-67-8	5,9-Undecadien-2-one, 6,10-dimethyl-		404, 1156, 2761, 4090, 4249, 5811b	
1239.	3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (*E*)-{geranylacetone} $H(CH_2\text{-}C(CH_3){=}CH\text{-}CH_2)_2\text{-}CH_2\text{-}CO\text{-}CH_3$	568b, 1360, 1375a, 1586, 1949, 2570, 2761, 2762, 2765, 2766, 2777, 3266, 4249, 5811b	172a, 174b, 404, 568b, 1053, 1256, 1590a, 1949, 2015, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3188, 3215, 3217, 3219, 3266, 3329, 3354, 3370, 3545, 3547, 3549, 3550, 3560, 3561, 3905, 3973, 4098a, 4249, 5811b	1360, 1375a

TABLE 3.13 (continued)
Ketones in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1240.	3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (*Z*)- {nerylacetone}	2761, 2762, 2765, 2766, 4249	404, 2386, 2389, 2544, 2917a, 4249, 5811b	
1241.	74233-43-5	5,10-Undecadien-2-one, 6,10-dimethyl-9-hydroxy-		5811b	
1242.	152209-56-8	6,10-Undecadien-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-2-methyl-2-furanyl)-		4249	
1243.	51297-36-0	8,10-Undecadien-4-one, 2,10-dimethyl-7-(1-methylethyl)-,(*E*)-(±)- $(H_3C)_2$═CH CH_2-CO-$(CH_2)_2$-CH[$CH(CH_3)_2$]-CH═CH-C(CH_3)═CH_2		1156, 4090	
1244.	112-12-9	2-Undecanone {methyl nonyl ketone} H_3C-$(CH_2)_8$-CO-CH_3	1238, 3266, 4249	172a, 174b, 297, 404, 937, 1053, 2282, 3266, 4249	
1245.	1604-34-8	2-Undecanone, 6,10-dimethyl- {tetrahydrogeranylacetone}	568b, 2767, 2769, 4249, 5811b	404, 568b, 1256, 2389, 2544, 3547, 4249, 5811b	
1246.	927-49-1	6-Undecanone		404	
1247.	141-10-6	3,5,9-Undecatrien-2-one, 6,10-dimethyl- {pseudoionone}	2767, 5811b	1156, 2389, 2544, 3547, 4090, 4249, 5811b	
1248.	3548-78-5	3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (*E,E*)- {pseudoionone}		568b, 937, 1156, 2339a, 3218, 4090, 4249	
1249.	13927-47-4	3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (*E,Z*)- {pseudoionone}		568b, 1156, 3218, 4090, 4249	
1250.	133561-48-5	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-		5811, 5811b	
1251.	129777-22-6	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-, (*E*)-		4249, 5811b	
1252.	29093-90-1	5-Undecen-2-one, 10-hydroxy-6,10-dimethyl-		4249, 5811b	
1253.	160115-56-0	6-Undecen-2-one, 10-(acetyloxy)-8,11-dihydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-5-hydroxy-2-methyl-2-furanyl)-		4249	
1254.	90-47-1	9*H*-Xanthen-9-one {xanthone} 		246, 247, 4249	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

TABLE 3.14
Chronology of Studies on Aldehydes and Ketones in Tobacco Smoke

Year	Event
1843	Acrolein (propenal) was first identified as a component in the destructive distillate from fat by Redtenbacher (3093b)
1859	Formaldehyde (methanal) was discovered by Butlerov (3A02)
1867	Formaldehyde was rediscovered by A.W. Von Hofmann (3A24)
1904	Thomas (3912) reported the presence of formaldehyde in cigarette smoke
1909	From his toxicologic study of cigarette smoke, Lehmann (2343) reported the presence of formaldehyde in cigarette smoke
1926	Neuberg and Kobel in their study of the aldehydes reported the presence of several aldehydes, including formaldehyde (2702a)
1927	Neuberg and Ottenstein (2706) report the presence of formaldehyde in tobacco smoke
1931	Neuberg and Burkard (2701) reported the presence of formaldehyde, acetaldehyde, butyraldehyde (butanal), 3-hydroxybutyraldehyde (3-hydroxybutanal, aldol), benzaldehyde, 3-pentanone, and 4-heptanone in cigarette smoke
1932	McNally (2524) reported the presence of formaldehyde and acrolein (propenal) in tobacco smoke
1933	Pfyl (2937) confirmed the finding of Neuberg and Burkard (2701) on the presence of acetaldehyde in tobacco smoke
1936	In his study of the irritant factors in cigarette smoke, Bogen (1936) classified formaldehyde, acetaldehyde, and acrolein (propenal) as "irritant factors" in cigarette smoke and rated formaldehyde as a major contributor to cigarette smoke irritation
1937	Prentiss (2988a) reported that acrolein (propenal) was a powerful lachrymator; even at 3 ppm (7 mg/m^3) acrolein was reported to be highly irritating to the conjunctiva and to the respiratory tract
1939	Proetz (2991a) attributed ciliastasis on upper respiratory tract mucosa of rabbits exposed to cigarette smoke to the aldehydes in the smoke
1939	Ribeiro (3126) reported the presence of acrolein (propenal) in tobacco smoke
1939	Wenusch (4202) reported 2-furaldehyde and acetone in cigarette smoke
1939	Roffo (3324) reported 2-furaldehyde in cigarette smoke
1939	Schmalfuss (3475) reported biacetyl (2,3-butanedione) in tobacco smoke
1940	Smirnov et al. (3A19) listed 3-pentanone as a tobacco smoke component
1954	In his catalog of the components of tobacco smoke reported to mid-1954, Kosak (2170) provided references to reports in tobacco smoke of the following aldehydes: formaldehyde [Neuberg and Ottenstein (2706), Neuberg and Burkard (2702), McNally (2524)], acetaldehyde [Neuberg and Burkard (2702), Pfyl (2937)], butyraldehyde (butanal) [Neuberg and Burkard (2702)], acrolein (propenal) [McNally (2524)], benzaldehyde [Neuberg and Burkard (2702)], and 2-furaldehyde [Wenusch (1939), Roffo (3324)]. Kosak also cataloged reports on the following ketones in tobacco smoke: 3-pentanone (diethyl ketone) [Neuberg and Burkard (2702)], 4-heptanone (dipropyl ketone) [Neuberg and Burkard (2702)], 17-tritriacontanone (dipalmityl ketone) [Schürch and Winterstein (3562)], and 2,3-butanedione (biacetyl) [Schmalfuss (3475)]
1955	In his study of the vapor phase of cigarette MSS, Laurene (2293) identified acrolein (propenal)
1956	Buyske et al. (564) reported butyraldehyde (butanal) and crotonaldehyde (2-butenal) in cigarette MSS
1959	In their review of the components of tobacco and tobacco smoke, Johnstone and Plimmer (1971) listed 18 aldehydes and ketones in tobacco smoke
1959	In anticipation of their possible utility in the identification of aldehydes and ketones that might be present in the MSS from an all-tobacco and/or an all-cellulose cigarette, Fredrickson et al. (1238) prepared over 90 2,4-dinitrophenylhydrazone derivatives for use as standards and cataloged their infrared spectra. The spectral data were used several years later by Fredrickson et al. to identify numerous aldehydes and ketones in tobacco smoke (1239)
1961	Guillerm et al. (1451a) reported the ciliastatic activity of acetaldehyde and acrolein (propenal) in liquid and in vapor form in an in vitro system. They also reported the synergistic ciliastatic activity of these two aldehydes in cigarette MSS exposure studies
1963	Horton et al. (3A11) reported that exposure of mice via inhalation to formaldehyde induced hyperplasia and metaplasia in the lung and typical hyperplastic changes in the trachea, but the tracheal tissue changes did not progress to invasive carcinoma
1963	Kensler and Battista (2083, 2084) reported significant ciliatoxicity for formaldehyde and acrolein, and their levels in cigarette MSS were reduced by passage of the smoke through a charcoal-containing filter
1963	In a study with human ciliated tonsillar epithelium, George (3A09) reported not only was phenol a strong ciliastat but also that acrolein (propenal) was an even stronger ciliastat
1963	Murphy et al. (3A17) reported that exposure of guinea pigs to low concentrations of acrolein (propenal) resulted in an increase in total respiratory flow resistance plus decreased respiratory rates and increased tidal volume
1964	Even though the Advisory Committee to the U.S. Surgeon General (3999) reported that formaldehyde and acrolein (propenal) were two of the components of cigarette MSS considered to be inhibitors of ciliastatic transport activity, the Committee concluded: No one of these [ciliastatic components] occurs at levels high enough to produce the effect noted for smoke
1964	Laurene et al. (2305) described an analytical method for the quantitative determination of acetaldehyde, acrolein (propenal), and acetone in cigarette MSS. Subsequently, an improvement in the analytical procedure for these three carbonyl components was reported by Laurene and Harbin (2302)
1964	From their study of the pyrogenesis of acrolein (propenal) from glycerol, Doihara et al. (1023) and others deduced that a tobacco smoking product that contains glycerol as a humectant has an enhanced potential for the formation and release of acrolein (propenal) during smoking [see Wynder and Hoffmann (4337)]

TABLE 3.14 (continued)
Chronology of Studies on Aldehydes and Ketones in Tobacco Smoke

Year	Event
1965	In testing the ciliatoxicity of cigarette MSS aldehydes to clam gill cilia, Wynder et al. (4330) reported that formaldehyde, acrolein (propenal), and crotonaldehyde (2-butenal) showed the highest toxicity. They also reported that acrolein was about twice as ciliatoxic as phenol in the clam gill cilia test [see also Wynder and Hoffmann (p. 253 in (4332)]. In addition to their aldehyde ciliatoxicity results, Wynder et al. (4330) also noted the serious error introduced into the results obtained in their study of the ciliatoxicity of low-molecular-weight acids in tobacco smoke
1965	To quantitate the level of formaldehyde in cigarette MSS, Newsome et al. (2782) reported on a colorimetric method involving chromatropic acid
1965/1966	Walker and Kiefer (4109) examined the effect of cigarette MSS vapor phase on clam gill cilia. Removal of the acrolein region from the chromatographed vapor phase resulted in a significant reduction in the ciliastatic activity. Contrary toxicity results were reported for the same MSS in which the levels of acrolein (propenal) and acetaldehyde were reduced by 66% and 82%, respectively, by a "hydrazide" filter. The ciliastatic activity of the vapor phase of the "hydrazide" filtered MSS was, within experimental error, the same as that of the unfiltered smoke. Wynder and Hoffmann (4337) offer a possible explanation for these contradictory results: acrolein administered alone is quite toxic, but in the cigarette smoke vapor phase, its effect is "masked" or "neutralized" by other smoke components (identity not specified)
1966	In their study of the levels of acrolein, acetaldehyde, acetone, hydrogen cyanide, nitrogen oxides, nicotine, and total solids in pipe tobacco MSS, Harbin and Laurene (1497) reported that the acrolein delivery increased as the glycerol level was increased by addition but the acrolein delivery leveled off when the glycerol addition exceeded 6%
1967	Wynder and Hoffmann (4337) discussed the conversion of the glycerol, used as a humectant in tobacco smoking products, to acrolein (propenal) during the smoking process
1968	In their study of the ciliastatic components of cigarette smoke MSS vapor phase, Dalhamn et al. (892, 893) reported that the absorption of the vapor-phase ciliastats by the fluids coating the oral cavity resulted in significant reductions of acetaldehyde (60%) and acetone (56%), i.e., significant levels of these in vitro ciliastats failed to reach the ciliated lung tissue and thus were unable to exert the ciliatoxicity asserted by some investigators
1968	In his review of the components of tobacco and tobacco smoke, Stedman (3797) listed references to some 46 aldehydes and ketones in tobacco smoke
1970	Martin and Thacker (2478) described the quantitation of several aldehydes (piperonal, ethylvanillin, vanillin) used as flavorants in cigarette tobacco
1971	Despite the reported findings of Dalhamn et al. (892, 893), the Royal College of Physicians (3363) noted that acrolein (propenal) was one of the most important ciliastatic components of tobacco smoke, possibly contributing to the causes of pulmonary disease by interfering with the self-cleansing mechanism of the lung and thereby allowing more prolonged contact between the lining of the bronchial tubes and the carcinogenic agents in the smoke
1971/1973	From their study of 85 mm nonfiltered cigarettes made from each of four varieties of flue-cured tobacco, Rathkamp et al. (3087, 3088) reported that the MSS acetaldehyde deliveries ranged from 800 to 1280 μg/cig; the acrolein (propenal) deliveries ranged from 51 to 102 μg/cig
1972	The U.S. Surgeon General (4003) classified formaldehyde as a suspected contributor to the health hazard of smoking and acrolein (propenal) as a probable health hazard in cigarette smoke
1972	Testa and Joigny (3885) reported that the per cigarette delivery of acrolein (propenal) from a cigarette made from black tobacco was 65.7 μg
1975	Tsuchiya et al. (3986a) reported that the levels of formaldehyde in fruits and vegetables ranged from 3.4 μg/g in spinach to 17.3 μg/g in apples
1976	Kitchen et al. (2111b) noted that the most significant exposure to formaldehyde is generally industrial, but formaldehyde occurs naturally in many foodstuffs, e.g., fruits and vegetables
1976	OSHA standards for exposure to air contaminants require an employee's exposure to acrolein (propenal) not exceed an 8 h time-weighted average of 0.25 mg/m^3 (0.1 ppm) in the workplace air, in any 8 h shift, during a 40 h work week
1976	Extensive experimental smoking in an unventilated room provided index levels for acrolein (propenal) that accumulated during the cigarette smoking. The industrially permitted threshold limit value (TLV) for acrolein (0.1 ppm; 0.25 mg/m^3) was only exceeded under experimental conditions where a large number of cigarettes were burned in a closed room [Weber et al. (3A25)]
1977	In his discussion of the vapor phase of cigarette MSS, Norman (2799a) listed per cigarette deliveries of 1200 and 70 μg for acetaldehyde and acrolein (propenal), respectively
1977	Mansfield et al. (2456) described an analytical method to quantitate formaldehyde in cigarette MSS
1977	In their study of the effect of inhaled acrolein (propenal) on the tumorigenicity of benzo[*a*]pyrene or *N*-nitrosodiethylamine, Feron and Kruysse (3A08) conducted inhalation and intratracheal experiments with two groups of 18 male and 18 female 6 week old Syrian hamsters. One group was exposed to 9.2 mg/m^3 (4 ppm) of acrolein in air (7 h/day, 5 day/week, 52 week). The other group was similarly exposed to acrolein via inhalation but received an intratracheal installation of 0.9% saline. All animals alive at 81 week were sacrificed. Only one female had a tracheal papilloma. Tumors at other sites were not increased *vs*. untreated controls
1977	In its assessment of tobacco smoke components reported to be ciliastatic, the Royal College of Physicians (3364) reported that acrolein (propenal) appeared to be the most important

(*continued*)

TABLE 3.14 (continued)
Chronology of Studies on Aldehydes and Ketones in Tobacco Smoke

Year	Event
1979	According to the Chemical Industrial Institute of Toxicology (CIIT) (3A04), data supporting the tumorigenicity of formaldehyde were first reported on October 8, 1979 [see Battelle Institute (3A01)]
1979	U.S. Surgeon General (4005) reported acrolein (propenal) to be one of the major toxic agents in the vapor phase of unaged cigarette MSS
1980	Swenberg et al. (3A21) reported the induction of squamous-cell carcinomas in the nasal cavities of rats exposed to cigarette MSS plus 15 ppm of formaldehyde in chambers, 30 h/week for 18 months. The authors noted that reported per cigarette deliveries for formaldehyde ranged from 20 to 90 µg; for acrolein (propenal), deliveries ranged from 10 to 40 µg. Swenberg et al. listed acrolein as a ciliatoxic agent in cigarette MSS
1981	In its report, the Battelle Institute (3A01) described the induction of tumors in rats and mice exposed via inhalation to formaldehyde
1981	According to NIOSH, workers who smoke cigarettes are exposed to additional levels of formaldehyde since cigarette MSS contains as much as 40 ppm of formaldehyde by volume. It was deduced that an individual who smokes a pack a day (20 cigarettes) would inhaled 0.38 mg of formaldehyde, whereas occupational exposure at 3 ppm could result in a daily intake of 29.0 mg (3A04)
1982	Dalbey (3A06) reported that 88 male Syrian hamsters exposed to 70 ppm of formaldehyde vapor (5 h/day, 5 days/week) for their lifetime showed no detectable respiratory tract tumors. No respiratory tract tumors were observed in a similar inhalation experiment involving male hamsters exposed to 30 ppm of formaldehyde (5 h/day, 1 day/week) for their lifetime
1982	In its assessment of the literature on formaldehyde, the IARC (3A13) reported that it considered the evidence sufficient that formaldehyde was carcinogenic to rats. However, the IARC also stated that the epidemiological data [to that time] did not provide adequate evidence to assess the carcinogenicity of formaldehyde in man
1982	The U.S. Surgeon General (4010) reported that formaldehyde and acrolein (propenal) were "tumorigenic" and each was "a major toxic agent" in the vapor phase of cigarette MSS
1982	In a discussion of low-delivered doses of alleged carcinogenic compounds, Starr (3789b) note: Even though formaldehyde has been demonstrated to be mutagenic/genotoxic in test systems of one kind or another, we do not know that is in the human case. Formaldehyde is a major chemical building block in our society. Its outright ban would cause dramatic changes in society [also see Starr in Clary et al. (3A05)]
1982	At the Chemical Industrial Institute of Toxicology (CIIT) meeting, Fayerweather stated: "When the epidemiological studies are viewed as a whole, the data suggest that formaldehyde has not been responsible for producing cancer in man." [see Fayerweather in Clary et al. (3A05)]
1983	Jenkins et al. (1932) at the Oak Ridge National Laboratory (ORNL) analyzed the MSS from 32 commercial brands of cigarettes marketed in the United States for their deliveries of specific smoke components. Included was acrolein (propenal) whose deliveries ranged from 33 to 141 µg/cig
1983	Kerns et al. (2086b) reported significant increases in squamous-cell carcinomas of the nasal cavity were observed in both strains of rats after inhaling highly cytotoxic doses of formaldehyde. However, no carcinomas were observed in mice after inhaling the same dose. In other studies to evaluate the carcinogenicity of formaldehyde, mice and hamsters were exposed via inhalation, rats via subcutaneous injection, and rabbits via exposure in oral tanks. The results from these studies have been considered inadequate to evaluate the carcinogenic risk to humans (3A06, 3A13)
1984	From its study of formaldehyde, the United States Department of Health and Human Services (USDHHS) (3A23) reported: "The data are sparse and conflicting and do not yet provide persuasive evidence of a causal relation between exposure to formaldehyde and cancer in man. It concluded: Although some epidemiological studies noted that there may be an association between formaldehyde exposure and some forms of cancer, the data from these studies are not sufficient, at this time, for quantitative risk modeling"
1984	The Environmental Protection Agency (EPA) (3A07) noted: "There may be a reasonable basis to conclude that certain exposures to formaldehyde present a significant risk of widespread harm to human beings" This statement contradicts a previous one by the EPA in 1982 that no significant risks to human were expected from formaldehyde
1984	From their assessment of components of indoor air found to be tumorigenic in laboratory animals, Sterling and Arundel (3A20) suggested that formaldehyde was potentially carcinogenic to humans
1984	Theiss et al. (3A22) reported a statistically significant increase in the number of lung adenomas in mice after inhaling air containing 15 ppm of formaldehyde for 18 weeks
1984	Acetaldehyde deliveries ranged from 18 to 2815 µg/cig for nonfiltered cigarettes [Huynh et al. (1853a), Miyake and Shibamoto (2564)]
1985	A proposal to lower the exposure limit of formaldehyde from 5 to 1 ppm was under consideration by OSHA (3A18)
1985	Although formaldehyde was reported by Starr and Gibson (3789b) to be carcinogenic in rats when administered at very high dose levels, IARC found the weight of evidence of its carcinogenicity in humans to be inadequate
1986	The IARC (1870) listed the delivery range for acrolein (propenal) in cigarette MSS vapor phase as 10–110 µg/cig and classified it as a ciliatoxic component
1985/1986	Formaldehyde was reported in two studies to induce aneuploidy [Liang and Brinkley (2363a), Oshimura and Barrett (2868a)]
1986	Brunnemann et al. (500) determined several volatile aldehydes and ketones in tobacco headspace and tobacco smoke by derivatization with 2,4-dinitrophenylhydrazine. Tobacco smoke carbonyl components identified included formaldehyde, acetaldehyde (1000 µg/cig), propionaldehyde (propanal), acrolein (propenal), isobutyraldehyde (2-methylpropanal), crotonaldehyde (2-butenal), methacrolein (2-methylpropenal), benzaldehyde (1 µg/cig), and acetone
1987	Bell et al. (243) used the formation of the 2,4-dinitrophenylhydrazone derivative of formaldehyde in SSS as the means to quantitate the level of formaldehyde in SSS

TABLE 3.14 (continued)
Chronology of Studies on Aldehydes and Ketones in Tobacco Smoke

Year	Event
1987	In its review of formaldehyde, the IARC noted that formaldehyde is carcinogenic and mutagenic only at doses far in excess of that seen in cigarette MSS. Whether formaldehyde is mutagenic at noncytotoxic dose levels remains controversial because of the small number of studies and the variability of the results (3A14). The IARC (3A15) also noted that results from some studies suggest that humans routinely exposed to formaldehyde display increased chromosomal aberrations and sister chromatid exchanges in peripheral lymphocytes. Nevertheless, rodents treated with formaldehyde in vivo gave negative results for chromosomal aberrations and assays for lethal mutations; other rodent studies on DNA damage gave equivocal results
1988	Deluca (929) described a 2,4-dinitrophenylhydrazine procedure for the collection of carbonyl compounds in ETS
1989	Formaldehyde deliveries in MSS vapor phase range from 3.4 µg for filtered cigarettes to 283 µg in unfiltered cigarettes [Schaller et al. (3427), Miyake and Shibamoto (2564)]
1990	Hoffmann and Hecht (1727) included formaldehyde, acetaldehyde, and crotonaldehyde (2-butenal) in their list of 43 tumorigenic components of tobacco and tobacco smoke. Their text accompanying the list plus the authors' disregard of how the tumorigenicity of many of the 43 components was determined experimentally raises serious questions as to why many of the components were listed
1990	The EPA (1148) cited the Hoffmann–Hecht list of 43 tumorigenic components in tobacco and tobacco MSS in their effort to indict ETS as a significant health hazard
1992	In their treatise on ETS, Guerin et al. [(3A10), see p. 197 in (1446)] at ORNL, discussed in detail the levels of formaldehyde in indoor and outdoor air. They noted: "It might be expected that ETS would be an important contributor to indoor air concentrations of formaldehyde because formaldehyde is known to be a constituent of cigarette smoke. Popular commercial cigarettes deliver approximately 20–90 µg of formaldehyde in their MSS and 1–2 mg of formaldehyde in their SSS. While this contribution may at first appear highly significant, it has generally been found to be very minor when compared with other sources"
1992	OSHA ruled that the exposure limit for formaldehyde should be reduced from 3 to 0.75 ppm
1994	OSHA (2825) in its list of 43 tumorigenic components of tobacco smoke included only formaldehyde and acetaldehyde but not crotonaldehyde (2-butenal)
1994	NCI (2683a) reported on the OSHA 1992 ruling that the exposure limit for formaldehyde should be reduced from 3 to 0.75 ppm
1994	Although formaldehyde was reported by Monticello and Morgan (2610a) to be carcinogenic in rats when administered at very high dose levels, IARC found the weight of evidence of its carcinogenicity in humans to be inadequate
1995	Formaldehyde deliveries in MSS vapor phase range from 3.4 µg for filtered cigarettes to 283 µg in unfiltered cigarettes [Schaller et al. (3427), Miyake and Shibamoto (2564)]. Acetaldehyde deliveries ranged from 18 to 2815 µg/cig for nonfiltered cigarettes [Huynh et al. (1853a), Miyake and Shibamoto (2564)]
1996	Green and Rodgman (1373) reviewed presentations during the first half century (1947–1996) of the TCRC on the subject of the identification and quantitation of aldehydes and ketones in cigarette MSS and SSS, as well as in ETS
1997/1998	Hoffmann and Hoffmann (1740, 1741), in their lists of 60 tumorigenic components of tobacco and tobacco smoke, included only two aldehydes—formaldehyde and acetaldehyde. Crotonaldehyde (2-butenal) included in the 1990 Hoffmann–Hecht list (1727) was omitted from the Hoffmann–Hoffmann list (1740), an omission that paralleled the 1994 OSHA list (2825)
1998	According to information from the Environmental Health Center (EHC) (1145a), formaldehyde is usually present at the nonirritating level of about 0.06 ppm
1999	Smith et al. discussed the IARC classification of the tobacco smoke vapor-phase components formaldehyde and acetaldehyde as IARC Group 2A [Smith et al. (3713)] and Group 2B [Smith et al. (3714)] carcinogens, respectively
2003	In a discussion of the various lists of tumorigenic components in tobacco and tobacco smoke issued between 1986 and 2003, Rodgman and Green (3300) and Rodgman (3265) noted that formaldehyde, acetaldehyde, crotonaldehyde (2-butenal), and acrolein (propenal) were included in the majority of them (1217, 1740, 1741, 1743, 1744, 1808, 1870, 2825)
2006	IARC revaluated formaldehyde and classifies it as a Group 1 carcinogen (3A03, 3A16)
	Possibly add statements are the following aldehyde–ketone studies:
2007	Joyeux et al. described a filter-tip procedure for the reduction of formaldehyde and other carbonyl components of cigarette mainstream smoke (4689).
2008	Sharifi et al. described the detection of metabolites of 2-butenal (crotonaldehyde) and 2-propenal (acrolein) in the urine of smokers (5022).
2009	Adam and Mitschke described on analytical method for the determination of vapor-phase components of cigarette smoke by single photon ionization (SPI) and time of flight mass spectrometry (TOFMS): (5034).
2010	In a new listing of cigarette smoke toxicants, Hoffmann and Hoffmann again listed several carbonyl components as hazardous components (5512). Nie et al. described the effect of cigarette paper and filter tips on the delivery of "Hoffmann analytes", among which were included several aldehydes and ketones (5546). Otte and Intorp described a new alternative analytical method for the detemination of several selected volatile "Hoffmann analytes", including carbonyl compounds, in cigarette mainstream smoke (5547). Yip et al. described the analytical determination of the contribution of glycerol added to tobacco to the content of 2-propenal (acrolein) and acetone (2-propanone) in cigarette mainstream smoke (5583).

Note: While many of the following items deal with the identification and quantitation of formaldehyde in cigarette MSS, SSS, and ETS, the evidence for the presence of formaldehyde ($H_2C{=}O$) per se is scant. Data indicate that formaldehyde is present as its hydrate, i.e., as dihydroxymethane [$H_2C(OH)_2$], which in most instances behaves chemically and biologically the same as formaldehyde.

4 Carboxylic Acids

4.1 CARBOXYLIC ACIDS

Numerous organic acids have been identified in tobacco. These volatile, nonvolatile, and amino acids have been discussed in-depth by Tso [see Chapter 24 in (3973)]. The major nonvolatile acids are 2-hydroxy-1,2,3-propanetricarboxylic (citric), hydroxybutanedioic (malic), and ethanedioic (oxalic). The minor nonvolatile acids are hydroxyacetic (glycolic), butanedioic (succinic), propanedioic acid (malonic), butenedioic (*E*) (fumaric acid), and 2-oxopropanoic (pyruvic). The major volatile acids in tobacco are acetic and formic acid, while several minor volatile acids are propanoic, 2-furancarboxylic acid (2-furoic), benzoic, α-methylbutyric, β-methylvaleric, and numerous others. Over 40 amino acids and related compounds have been identified in tobacco [Leffingwell (2337)].

The number of identified carboxylic acids in tobacco and tobacco smoke has escalated greatly since the publication in 1954 by Kosak (2170) of his list of identified components in tobacco smoke. The Kosak list included the following carboxylic acids in tobacco smoke: formic acid, acetic acid, butanoic acid, pentanoic acid (valeric acid), hexanoic acid (caproic acid), 7- and 8-carbon carboxylic acids, butanedioic acid (succinic acid), butenedioic acid (*E*) (fumaric acid), benzoic acid, 2-hydroxy-1,2,3-propanetricarboxylic acid (citric acid), and phenolic acids. Kosak questioned the identification data of many of the acids listed. Johnstone and Plimmer (1971) in their 1959 catalog of tobacco and tobacco smoke components listed 52 specific acids plus a range of saturated aliphatic acids. However, Johnstone and Plimmer listed tobacco and smoke amino acids in a different section of their report and included nicotinic acid and nicotinamide as amino acids [see Table 11 in (1971)]. Also, listed in a third section were such carboxylic acids as 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxycyclohexanecarboxylic acid (chlorogenic acid), 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid (quinic acid), and 3,4,5-trihydroxy-1-cyclohexene-1-carboxylic acid (shikimic acid) [see Table 9 in (1971)]. Similar separation problems are encountered on examination of the various assignments of carboxylic acids in the 1968 review by Stedman [see Tables 9, 10, and 14 in (3797)]. In our report, any compound with a carboxyl group is cataloged in this chapter.

Table 4.1 summarizes the numbers of carboxylic acids and amino acids identified to date in tobacco and tobacco smoke. Their listing and references are presented in subsequent tables.

Despite the number of acids identified in tobacco and tobacco smoke, very few of the tobacco smoke acids have been indicted as toxicants. In 1964, Boyland et al. (4A01) described the induction of a bladder carcinoma in 1 of 16 mice (6.5%) implanted with a cholesterol pellet containing 3-(3,4-dihydroxyphenyl)-2-propenoic acid (caffeic acid). However, the carcinogenicity could not be attributed to the acid when it was observed that 5 of the 77 mice (6.5%) implanted with the cholesterol pellet alone developed bladder carcinomas. While caffeic acid was not included in any of the pre-2001 listings by the International Agency for Research on Cancer (IARC) (1871), Hoffmann and Wynder (1808), Hoffmann and Hecht (1727), Hoffmann et al. (1773), and Hoffmann and Hoffmann (1740, 1741, 1743), it was listed in the two 2001 publications by Hoffmann and Hoffmann (1743) and Research on Cancer (IARC) (1871), Hoffmann and Wynder (1808), Hoffmann and Hecht (1727), and Hoffmann et al. (1744), primarily because of its phenolic nature. In the latter two articles, formic, acetic, and propanoic acids are listed as major mainstream smoke (MSS) vapor-phase components [Table 5.1 in (1743), Table 2 in (1744)], and hexadecanoic acid (palmitic acid), octadecanoic acid (stearic acid), 9-octadecenoic acid (oleic acid), 9,12-octadecadienoic acid (linoleic acid), 9,12,15-octadecatrienoic acid (linolenic acid), and 2-hydroxypropanoic acid (lactic acid) are listed as major MSS particulate-phase components [Table 5.2 in (1743), Table 3 in (1744)].* By inclusion of per cigarette yields from the mid-1950s to the date of the publication, these long-chained saturated and unsaturated acids and lactic acid are listed as major particulate-phase components. No comment is made as to whether that statement about the per cigarette yields of the six acids is valid for cigarettes manufactured post-1995.

The formic, acetic, and propanoic acids listed as major MSS vapor-phase components were defined as ciliastats by Wynder et al. (4304, 4350) in the mid-1960s [see summary graph, p. 254, Table 7.31 in (4332)]. However, Wynder and Hoffmann (4332) were among the first to comment on the fact that all vapor-phase ciliastats are water soluble and therefore may be removed from the smoke stream by solution in the fluids coating the oral cavity. In their 1967 book [see p. 646 in (4332)], they stated:

> In man's manner of smoking, however, volatile components are retained to a significant degree in the oral cavity and may, therefore, be far less important than when tested experimentally.

The validity of their 1967 statement had been demonstrated by the results of studies in 1964 by Rodgman et al. (3306,

* From a comparison of the listings in (1743) and (1744), it should be noted that in the particulate-phase acids listed in (1744), stearic acid has been inadvertently omitted and its per cigarette MSS yield assigned to palmitic acid.

TABLE 4.1
Acids Identified in Tobacco and Tobacco Smoke to Date

Acid Category	Total	Smoke	Tobacco	Tobacco and Smoke	Reference
Carboxylic acids	52	37	43	29	Table 8 in (1971)
	787	380	656	249	Table 4.3
Amino acids	28	4	26	2	Table 11 in (1971)
	117	36	117	36	Table 4.10

4A02) and subsequently in 1968 by Dalhamn et al. (892) on the removal of substantial amounts of water-soluble vapor-phase ciliastats from inhaled MSS by the oral cavity fluids.

It is interesting to note that all but two [formic acid, octadecanoic acid (stearic acid)] of the MSS vapor-phase and particulate-phase acids discussed above—whether identified in tobacco, tobacco smoke, or both—are listed by Doull et al. (1053) as compounds included in the flavor formulations added to a tobacco blend by U.S. cigarette manufacturers to enhance consumer acceptability of the product.

Table 4.2 lists the tobacco and/or smoke carboxylic acids that, according to the Doull et al. listing (1073), are or have been used recently as components in flavor formulations for tobacco. It should also be noticed that the flavor ingredient additions in Table 4.2 include 15 amino acids.

Table 4.3 is a catalog of the carboxylic acids identified to date in tobacco, tobacco smoke, and tobacco substitute smoke. Of the 787 components listed, 380 have been identified in smoke, 656 in tobacco, and 249 in both. Because of the recent interest in several amino acid degradation products generated during the tobacco smoking process, a separate section (Section 4.2) is devoted to the amino acids and a discussion of their behavior during pyrolysis and the smoking process.

4.2 AMINO ACIDS AND RELATED COMPOUNDS

Amino acids, both as free acids and as acids bound within protein molecules, are present in all of the tobacco types (flue-cured, burley, Oriental, Maryland) used in the American tobacco blend.

The diversity and levels of amino acids in various tobaccos have been presented by Gori [see Table 2 in (1329), Table 2 in (1330)] and Tso and Chaplin [see Table 8 in (3975)]. Leffingwell (2337) in his report on nitrogen components of leaf and their relationship to smoking quality in 1976 reported that there were 43 amino acids isolated from tobacco. Examples of amino acids occurring free and/or bound in tobaccos include α- and β-alanine, α- and γ-aminobutyric acid, arginine, aspartic acid, cysteic acid, cysteine, cystine, glutamic acid, glycine, histidine, isoleucine, leucine, lysine, methionine, norleucine, ornithine, phenylalanine, proline, serine, threonine, tryptophan, tyrosine, and valine (3983b).

The presence in cigarette MSS of numerous free amino acids and amino acid–derived compounds was demonstrated in the mid-1950s. This occurred soon after the publication of the results of several cigarette smoke–related epidemiological and biological studies led to a massive escalation in tobacco smoke composition studies; e.g., Buyske et al. (562) reported the identification of glutamic acid and its derivative glutamine (glutamic acid 5-amide) in tobacco smoke. Other amino acids identified in tobacco smoke include alanine, aspartic acid (and asparagine), cysteine, glycine, leucine, ornithine, phenylalanine, proline, serine, threonine, and valine [Ishiguro and Sugawara (1884)].

In the early 1960s, pyrocoll (dipyrrolo[*a,d*]pyrazine-5,10-dione) was identified in cigarette MSS by Mold et al. (2592) who proposed that the amino acid proline—either free or bound—was its precursor. During their study of the isolation and identification of *N*-heterocyclic components (the indoles and carbazoles) in cigarette MSS, Rodgman and Cook (3279) confirmed the presence of pyrocoll. Two decades earlier, Van Order and Linwall (4B01) had demonstrated that dry distillation of the amino acid tryptophan yielded indole and 3-methylindole (skatole), both of which were subsequently identified as tobacco smoke components by the isolation and identification of *N*-heterocyclic components (the indoles and carbazoles) in cigarette MSS, Rodgman and Cook (3279). Roberts [see citation in the isolation and identification of *N*-heterocyclic components (the indoles and carbazoles) in cigarette MSS, Rodgman and Cook (3279)] had also identified indole as a component of burley tobacco.

By means of pyrolysis studies (850°C, nitrogen atmosphere) with the amino acids lysine, leucine, and tryptophan, Patterson et al. (2902) demonstrated that each of the three amino acids yielded the *N*-heterocyclic compounds indole, quinoline, isoquinoline, several nitriles, and a series of PAHs ranging in complexity from bicyclic to tetracyclic (their findings are summarized in Table 4.4). In their study, B[*a*]P was found only in the pyrolysate from leucine. From their own findings and from a previous report by Jarboe and Rosene (1923a) that quinoline and isoquinoline were components of a nicotine pyrolysate, Patterson et al. (2902) suggested that the precursors in tobacco of the aza-arenes quinoline and isoquinoline in tobacco smoke might be nicotine and/or the amino acids. They also reported that tryptophan, on a per mole pyrolyzed basis, yielded a phenol fraction whose weight was more than 5 times that generated from lysine and about 30 times that from leucine.

In another series of experiments, Patterson et al. (2903) reported (1) the effect of the pyrolysis temperature on the composition of the pyrolysate from the amino acid phenylalanine with emphasis on the levels of PAHs generated and (2) the effect of other compounds (tryptophan or pyrrole) on the composition of the pyrolysate when mixtures of equimolar

TABLE 4.2
Tobacco and/or Tobacco Smoke Carboxylic Acids Used in Flavor Formulations

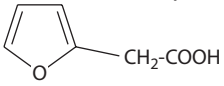
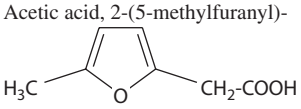
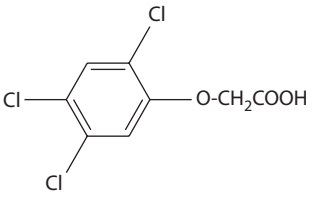
CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Identified in	
			Smoke	Tobacco
64-19-7	Acetic acid	Acetic acid	+	+
107-95-9	β-Alanine	β-Alanine	+	+
74-79-3	*L*-Arginine	*L*-Arginine	–	+
5794-13-8	*L*-Asparagine monohydrate	Asparagine	+	+
56-84-8	*L*-Aspartic acid	*l*-Aspartic acid	+	+
103-82-2	Benzeneacetic acid	Phenylacetic acid	+	+
65-85-0	Benzoic acid	Benzoic acid	+	+
147-71-7	Butanedioic acid, 2,3-dihydroxy-	Tartaric acid	–	+
6915-15-7	Butanedioic acid, hydroxy-	Malic acid	+	+
107-92-6	Butanoic acid	Butyric acid	+	+
116-53-0	Butanoic acid, 2-methyl-	2-Methylbutyric acid	+	+
503-74-2	Butanoic acid, 3-methyl-	Isovaleric acid	+	+
13201-46-2	2-Butenoic acid, 2-methyl-	Methyl-2-butenoic acid	+	+
52-90-4	*L*-Cysteine	*L*-Cysteine	+	+
334-48-5	Decanoic acid	Capric acid	+	+
143-07-7	Dodecanoic acid	Lauric acid	+	+
6899-05-4	*L*-Glutamic acid	*L*-Glutamic acid	+	+
6899-04-3	*L*-Glutamine	*L*-Glutamine	+	+
111-14-8	Heptanoic acid	Enanthic acid	+	+
57-10-3	Hexadecanoic acid	Palmitic acid	+	+
110-44-1	2,4-Hexadienoic acid[a]	Sorbic acid[a]	+	+
142-62-1	Hexanoic acid	Caproic acid	+	+
4536-23-6	Hexanoic acid, 2-methyl-	2-Methylhexanoic acid	+	+
1289-40-3	2-Hexenoic acid	2-Hexenoic acid	+	–
71-00-1	*L*-Histidine	*L*-Histidine	–	+
73-32-5	*DL*-Isoleucine	*DL*-Isoleucine	–	+
56-87-1	*L*-Lysine	*L*-Lysine	–	+
112-05-0	Nonanoic acid	Nonanoic acid	+	+
506-21-8	9,12-Octadecadienoic acid	Linoleic acid	+	+
463-40-1	9,12,15-Octadecatrienoic acid	Linolenic acid	+	+
112-80-1	9-Octadecenoic acid	Oleic acid	+	+
124-07-2	Octanoic acid	Caprylic acid	+	+
109-52-4	Pentanoic acid	Valeric acid	+	+
97-61-0	Pentanoic acid, 2-methyl-	2-Methylvaleric acid	+	+
105-43-1	Pentanoic acid, 3-methyl-	3-Methylpentanoic acid	+	+
646-07-1	Pentanoic acid, 4-methyl-	4-Methylpentanoic acid	+	+
123076-2	Pentanoic acid, 4-oxo-	Levulinic acid	+	+
591-80-0	4-Pentenoic acid	4-Pentenoic acid	+	+
63-91-2	*L*-Phenylalanine	*L*-Phenylalanine	+	+
147-85-3	*L*-Proline	*L*-Proline	+	+
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	Citric acid	+	+
79-09-4	Propanoic acid	Propionic acid	+	+
50-21-5	Propanoic acid, 2-hydroxy-	Lactic acid	+	+
79-31-2	Propanoic acid, 2-methyl-	Isobutyric acid	+	+
127-17-3	Propanoic acid, 2-oxo-	Pyruvic acid	+	+
501-52-0	Propanoic acid, 3-phenyl-	3-Phenylpropionic acid	+	+
499-12-7	1-Propene-1,2,3-tricarboxylic acid	Aconitic acid	+	+
621-82-9	2-Propenoic acid, 3-phenyl-	Cinnamic acid	+	+
544-63-8	Tetradecanoic acid	Myristic acid	+	+
72-19-5	*L*-Threonine	*L*-Threonine	+	+
60-18-4	*L*-Tyrosine	*L*-Tyrosine	–	+
7004-03-7	Valine	Valine	+	+

[a] 2,4-Hexadienoic acid (sorbic acid) is not included in the Doull et al. list (1053) but is included in flavor formulations used by cigarette manufacturers outside of the United States [see Table 7A in (3266)].

TABLE 4.3
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	64-19-7	Acetic acid CH_3-COOH	18, 126a, 126b, 167, 172, 237, 239, 424, 563, 565, 568b, 722, 916, 937, 938, 960, 966, 1023, 1063–1066, 1068–1074, 1099, 1132, 1140, 1232, 1263, 1348, 1350, 1354, 1360, 1364, 1365, 1375, 1375a, 1375b, 1377, 1388–1390, 1437, 1445, 1586, 1668, 1674, 1744, 1842, 1882, 1884, 1903, 1904, 1917, 2043, 2079, 2086, 2088, 2133, 2170, 2195, 2200, 2203, 2253, 2270, 2293, 2310, 2337, 2387, 2414, 2475, 2529, 2543, 2545, 2570, 2582, 2601a, 2619, 2623, 2628, 2702, 2765, 2767, 2777, 2799a, 2821, 2855, 2857, 2858, 2934, 2939, 3060, 3064, 3105, 3187, 3255, 3257, 3263, 3266, 3300, 3302, 3308, 3324, 3384, 3394, 3397, 3403, 3452, 3495, 3553, 3557, 3559, 3797, 3799, 3876, 3973, 3992, 4064, 4065, 4249, 4301, 4304, 4319, 4332, 4342, 4406, 4570a, 5079, 5189, 5359, 5512, 5811b, 5835	120, 212, 404, 565, 568b, 647, 937, 938, 1053, 1063, 1085, 1087, 1276, 1550, 1893b, 1705, 1982, 1999, 2014, 2079, 2154, 2270, 2283, 2293, 2337, 2338, 2339a, 2386, 2389, 2529, 2544, 2862a, 2917a, 2939, 3052, 3188, 3266, 3328, 3374, 3507, 3549, 3550, 3655b, 3787, 3797, 3905, 3973, 3974a, 3983a, 4064, 4249, 5079, 5114, 5165, 5189, 5381, 5419, 5478, 5695, 5708, 5709, 5712, 5735, 5811b, 5846, 5896	1228, 1354, 1360, 1375a, 1377, 2244, 2387, 3393, 3401, 3402, 3404, 3405
2.	13831-30-6	Acetic acid, (acetyloxy)- CH_3-COO-CH_2-COOH	568b, 1375a, 1377, 2387, 3553, 4249, 5811b	568b, 2336, 4249	1375a, 1377, 2387
3.	79-43-6	Acetic acid, dichloro- Cl_2CH-COOH		1948, 3821a, 4249	
4.	94-75-7	Acetic acid, 2,4-dichlorophenoxy- {2,4-D}		3633, 5015, 5521, 5811b	
5.	32833-96-8	Acetic acid, (dimethylamino)oxo- $(H_3C)_2$═N-CO-COOH		4249, 4647	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

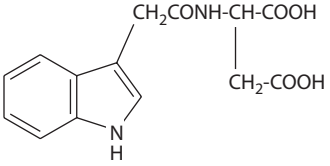
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
6.	123617-80-1	Acetic acid, 3-furanyl- 	91b, 5811b		
7.	79-14-1	Acetic acid, hydroxy-{glycolic acid} $HOCH_2$-COOH	237, 1099, 1371, 1375a, 1377, 1445, 1674, 1882, 2133, 2493, 2777, 2939, 3059, 3060, 3061, 3255, 3302, 3384, 3394, 3496, 3741, 3743, 4249, 5811b	3060, 3194, 3797, 3973, 3974a, 4249, 5811b	1375a, 1377, 3393, 3402, 3405
8.	625-45-6	Acetic acid, methoxy- H_3CO-CH_2-COOH		429b, 1948, 4249	
9.	72360-04-4	Acetic acid, 2-(5-methylfuranyl)- 	91b, 5811b		
10.	298-12-4	Acetic acid, oxo-{glyoxylic acid} O═CH-COOH	1310, 2939, 3059, 3302	120, 1310, 1312, 2939, 3797, 3973, 3974a, 5651, 5811b	
11.	13147-57-4	Acetic acid (phosphonoxy)-		4249	
12.	93-76-5	Acetic acid, 2,4,5-trichlorophenoxy-{2,4,5-T®} 		3633, 5015	
13.	6898-94-8	Alanine	1910, 1914, 2858, 2939, 3266, 3555, 3797	1053, 1086, 2079, 3266, 3555, 3797	
14.	62-57-7	Alanine, 2-methyl-		429b, 4249, 4580, 4626, 5777	
15.	13100-82-8	Alanine, 3-sulfo-		3983b	
16.	107-95-9	β-Alanine H_2N-$(CH_2)_2$-COOH	1083, 1351, 1910, 1914, 2858, 2939, 3224, 3266, 3302, 3491, 3797, 4249, 4319, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2270, 2337, 2338, 2359, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5603, 5785, 5811b, 5827, 5831, 5881, 5905	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
17.	79-83-4 137-08-8	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- {pantothenic acid} $HO\text{-}CH_2\text{-}C(CH_3)_2\text{-}CHOH\text{-}CO\text{-}NH\text{-}(CH_2)_2\text{-}COOH$		429b, 1941, 4249, 4758, 5079	
18.	10478-42-9	β-Alanine, *N*-methyl-*N*-nitroso- {NMPA} {propanoic acid}, 3-(methylnitrosamino)- $H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOH$	3256, 3300, 3943a, 3944–3946, 5811b	466, 485, 503, 982, 2852, 3943a, 3944–3946, 3971, 3973, 5811b	
19.	133201-38-4	β-Alanine, *N*-(nitrosomethyl)-	4249	4249	
20.	923-16-0	*D*-Alanine, *N*-*D*-alanyl-		1351, 2337, 2797, 3491, 4249, 5811b	
21.	56-41-7	*L*-α-Alanine $H_3C\text{-}CH(NH_2)\text{-}COOH$	1083, 1351, 1914, 2724, 3491, 5811b	120, 158, 622, 749, 752–754, 826a, 1223, 1305a, 1351, 1493, 1918, 1919, 2799a, 2270, 2337, 2338, 2394a, 2453, 2529, 2532, 2597a, 2795, 2911a, 2911c, 3491, 3499, 3780, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4398c, 5079, 5603, 5699, 5785, 5811b, 5881, 5905, 5907	
22.	16124-24-6 25127-16-6	*L*-Alanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1063–1066, 1068–1074, 1351, 2337, 3639, 3797, 3923, 4362, 5811b	
23.	19701-89-4	*DL*-Alanine, *N,N*-dimethyl-	2882, 4249		
24.	13752-83-5	Arabinonic acid $HO\text{-}CH_2\text{-}(CHOH)_3\text{-}COOH$		2362a	
25.	7004-12-8	Arginine $H_2N\text{-}C(=NH)\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		826a, 2911c, 2939, 3491, 3705, 3973, 3974b, 4224, 4226, 4244, 4398c, 5079, 5189, 5435, 5436, 5785, 5827	
26.	1069-09-6 34522-32-2	Arginine, N_2-(1-carboxyethyl)- $H_2N\text{-}C(=NH)\text{-}NH\text{-}(CH_2)_3\text{-}CH\text{-}[NH\text{-}CH(CH_3)\text{-}COOH]\text{-}COOH$		3427a, 3973, 4249, 4688	
27.	74-79-3	*L*-Arginine $H_2N\text{-}C(=NH)\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$	3797, 5811b	120, 158, 555a, 555b, 622, 749, 751–756, 1053, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 1918, 1919, 2079, 2270, 2283, 2337, 2338, 2394a, 2453, 2532, 2597a, 2722, 2795, 2911c, 2939, 3266, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4244, 4249, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
28.	7006-34-0	Asparagine H_2N-CO-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 1965, 2724, 3266, 4159, 4249, 5811b	120, 480, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1223, 1305a, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2532, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4244, 4249, 4398c, 5048, 5079, 5126, 5189, 5437, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
29.	70-47-3	*L*-Asparagine		429b, 2338, 5811b	
30.	5794-13-8	*L*-Asparagine monohydrate		3973	
31.	6899-03-2	Aspartic acid	3555	3555, 3705, 5699, 5785, 5831, 5905, 5907, 17B17	
32.	56-84-8	*L*-Aspartic acid HOOC-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3797, 4159, 4249	120, 158, 480, 555a, 555b, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4159, 4224, 4226, 4244, 4249, 4359, 4398b, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
33.	31105-02-9	*L*-Aspartic acid *N*-(1-deoxy-*D*-fructos-1-yl)-		5811	
34.	2456-73-7	*L*-Aspartic acid, *N*-(1*H*-indol-3-ylacetyl)-  		4249, 4659	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

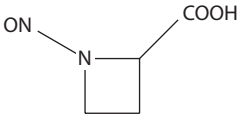
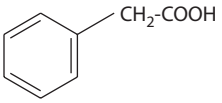
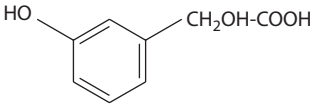
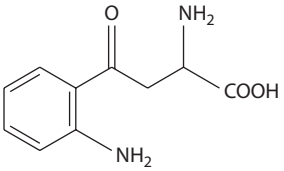
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
35.	34441-14-0	1-Azetidinebutanoic acid, α-[(3-amino-3-carboxypropyl) amino]-2-carboxy-, [2S-[1[αR*(R*)],2R*]]- {nicotianamine}		3491, 4249, 4855, 5811b	
36.	2517-04-6	2-Azetidinecarboxylic acid		3491, 4249, 5811b	
37.	55556-98-4	2-Azetidinecarboxylic acid, 1-nitroso- 		486, 4249, 5811b	
38.	103-82-2	Benzeneacetic acid {phenylacetic acid} 	172, 568b, 1132, 1063–1066, 1068–1074, 1099, 1165, 1359, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1587a, 1882, 1886, 2270, 2338, 2387, 2529, 2543, 2570, 2601a, 2641–2643, 2758, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3266, 3302, 3308, 3394, 3410, 3553, 3557, 4249, 5811b	120, 212, 172a, 174b, 404, 568b, 848, 908, 1053, 1165, 1587a, 1590a, 1620, 1999, 2014, 2270, 2283, 2338, 2386, 2389, 2529, 2544, 2758, 2862a, 2939, 3215, 3219, 3266, 3329, 3332, 3532, 3543, 3549, 3560, 3561, 3767a, 3973, 3974a, 3974b, 4249, 5708	1360, 1375a, 2387
39.		Benzeneacetic acid, labeled with ^{14}C {phenylacetic acid-^{14}C}	1359	1359	
40.	17119-15-2	Benzeneacetic acid, α,3-dihydroxy- 	3712, 3737, 3741, 3743, 4249, 5811b		
41.	1198-84-1	Benzeneacetic acid, α,4-dihydroxy-	3712, 3737, 3741, 3743		
42.		Benzeneacetic acid, α,?-dihydroxy-ethyl-	4249		
43.	4412-10-6	Benzeneacetic acid, α-ethylidene-		5811b	
44.	20432-26-2	Benzeneacetic acid, α-ethylidene-, (*E*)-		3767a	
45.	90-64-2	Benzeneacetic acid, α-hydroxy- {mandelic acid}		429b	
46.	492-37-5	Benzeneacetic acid, α-methyl- {hydratropic acid}	568b, 2873, 3308, 3797, 4249, 5811b		
47.	7782-24-3	Benzeneacetic acid, α-methyl-, (S)-(+)-	5811		
48.	7782-26-5	Benzeneacetic acid, α-methyl-, (R)-(-)-	5811		
49.	19988-45-5	Benzeneacetic acid, 2,3-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
50.	614-82-4	Benzeneacetic acid, 2,4-dihydroxy	5811a		
51.	451-13-8	Benzeneacetic acid, 2,5-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
52.	102-32-9	Benzeneacetic acid, 3,4-dihydroxy-	3712, 3737, 3741, 3743, 5811b	52, 970, 1248, 4249, 4677	
53.	4670-09-1	Benzeneacetic acid, 3,5-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
54.	96937-42-7	Benzeneacetic acid, ar,ar-dihydroxy-ar,ar-dimethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
55.	96937-37-0	Benzeneacetic acid, ar,α-dihydroxy-ar-ethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
56.	96937-48-3	Benzeneacetic acid, ar,ar-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
57.	96937-41-6	Benzeneacetic acid, 3,4-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
58.	614-75-5	Benzeneacetic acid, 2-hydroxy-	1626, 1884, 2722, 2939, 3302, 3712, 3797, 4163, 4249, 4377, 5811b	2939, 3797, 3973, 3974a, 4163, 4249, 4377, 5811b	
59.	621-37-4	Benzeneacetic acid, 3-hydroxy-	1626, 1884, 2722, 2939, 3302, 3712, 3737, 3741, 3743, 3797, 4113, 4163, 4249, 4377, 5811b	2939, 3797, 3973, 3974a, 4163, 4249, 4377, 5811b	3395
60.	156-38-7	Benzeneacetic acid, 4-hydroxy-	101, 1626, 1884, 1886, 2722, 2939, 3302, 3712, 3797, 4113, 4163, 4249, 4377, 5811b	120, 908, 2722, 2939, 3532, 3560, 3561, 3973, 3974a, 4163, 4249, 4377, 5811b	3393, 3395
61.	306-08-1	Benzeneacetic acid, 4-hydroxy-3-methoxy- {homovanillic acid}	3712, 3737, 3741, 3743, 4113, 4249, 5811b		
62.	343-65-7	Benzenebutanoic acid, α,2-diamino-γ-oxo- {kynurenine} 		4249	
63.	88-99-3	1,2-Benzenedicarboxylic acid {phthalic acid}	1886, 2939, 3053, 3061, 3302, 3308, 3496, 3737, 3741, 3743, 4249, 4319, 5811b	2356, 2386, 4249, 4677, 5811b	
64.	121-91-5	1,3-Benzenedicarboxylic acid {isophthalic acid}	1981, 4249		
65.	100-21-0	1,4-Benzenedicarboxylic acid {terephthalic acid}	2939, 5811b	120, 1221, 2079, 2270, 2283, 3797, 3973, 3974a, 5079, 5439, 5811b	
66.	501-52-0	Benzenepropanoic acid {3-phenylpropionic acid; hydrocinnamic acid}	568b, 1360, 1364, 1371, 1375a, 2543, 2761, 2762, 2765, 2766, 2773, 2775, 3266, 3308, 3410, 3506, 3553, 3555, 4249, 5811b	172a, 174b, 568b, 1053, 2092, 3266, 3555, 3973, 4249, 5811b	1360, 1375a
67.	156-05-8	Benzenepropanoic acid, α-hydroxy- {phenyllactic acid} C_6H_5-CH_2-CH_2OH-COOH		120, 2270, 2722, 3532, 3973, 3974a, 4249	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

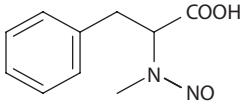
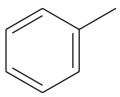
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
68.	7326-19-4	Benzenepropanoic acid, α-hydroxy-, (R)-		3560, 3561	
69.	4593-90-2	Benzenepropanoic acid, β-methyl-	4249, 5811b		
70.	156-06-9	Benzenepropanoic acid, α-oxo- {phenylpyruvic acid}		3797, 3973, 3974a, 4249	
71.	24696-05-7	Benzenepropanoic acid, 2-(β-*D*-glucopyranosyloxy)-		4249, 4915	
72.		Benzenepropanoic acid, dihydroxy-methoxy-	3737, 3741, 3743		
73.		Benzenepropanoic acid, 2-(methylnitrosamino)- 	1013	1008, 1009	
74.	3714-73-6	Benzenepropanoic acid, 2,3-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
75.	96937-38-1	Benzenepropanoic acid, 2,3-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
76.	5631-68-5	Benzenepropanoic acid, 2,4-dihydroxy-	5811a		
77.	10538-47-3	Benzenepropanoic acid, 2,5-dihydroxy-	101, 3712, 3737, 3741, 3743, 4249, 4897, 5811b	5811b	
78.	96937-34-7	Benzenepropanoic acid, 2,5-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
79.	98114-50-2	Benzenepropanoic acid, 2,6-dihydroxy-	5811a		
80.	495-78-3	Benzenepropanoic acid, 2-hydroxy-	3737, 3741, 3743, 4249, 4897, 5811b	1305b, 3973, 3974a, 4249, 5668	
81.	1078-61-1	Benzenepropanoic acid, 3,4-dihydroxy- {dihydrocaffeic acid}	101, 3712, 3737, 3741, 3743, 4113, 5811b	970, 3797, 3973, 3974a, 5811b	
82.	96961-47-6	Benzenepropanoic acid, 3,4-dihydroxy-2,5,6-trimethyl-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
83.	96937-33-6	Benzenepropanoic acid, 3,4-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
84.	621-54-5 33393-93-0	Benzenepropanoic acid, 3-hydroxy-	1884, 2939, 3302, 3712, 3737, 3741, 3743, 3797, 4249, 4377, 5811b	2939, 3973, 3974a, 4249, 4377, 4951	
85.	26539-01-5	Benzenepropanoic acid, 3,5-dihydroxy	5811a		
86.	501-97-3	Benzenepropanoic acid, 4-hydroxy-	1626, 2939, 3302, 3712, 3737, 3797, 3741, 3743, 4163, 4249, 4377, 5811b	2722, 2939, 3532, 3560, 3561, 4163, 4249, 4377, 4951, 5811b	
87.	156-39-8	Benzenepropanoic acid, 4-hydroxy-α-oxo-	1871a, 3712, 4249, 5811b		
88.	1135-23-5	Benzenepropanoic acid, 4-hydroxy-3-methoxy- {hydroferulic acid}	596, 3712, 3737, 3741, 3743, 4249		
89.	96937-36-9	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methoxy-	4249, 4897, 5811b		
90.	96937-35-8	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methyl-	4249, 4897, 5811b		

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

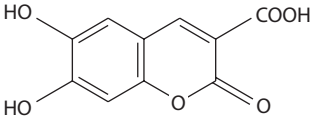
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
91.	65-85-0	Benzoic acid {benzenecarboxylic acid} 	126b, 172, 237, 395, 563, 565, 568b, 966, 1063–1066, 1068–1074, 1099, 1132, 1233, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1445, 1586, 1668, 1674, 1882, 1884, 1903, 1904, 2079, 2133, 2170, 2270, 2529, 2543, 2545, 2601a, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2873, 2939, 3059, 3255, 3266, 3302, 3308, 3394, 3410, 3496, 3553, 3555, 3557, 3559, 3876, 4202, 4249, 4304, 4319, 4342, 4354, 5034, 5079, 5207, 5811b	120, 565, 568b, 848, 908, 1053, 1590a, 1620, 1999, 2014, 2283, 2338, 2339a, 2356, 2386, 2389, 2529, 2544, 2862a, 2917a, 2939, 3194, 3217, 3219, 3266, 3329, 3332, 3543, 3547, 3549, 3555, 3560, 3561, 3767a, 3973, 3974a, 4249, 5708, 5709, 5811b	1360, 1375a, 1377, 3393, 3402
92.	96937-46-1	Benzoic acid, dihydroxy-dimethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
93.	96937-47-2	Benzoic acid, dihydroxy-ethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
94.	96937-44-9	Benzoic acid, dimethyl-hydroxy-	3737, 3741, 3743, 4249, 4897, 5811b		
95.	96937-43-8	Benzoic acid, ethyl-hydroxy-	3737, 3741, 3743, 4249, 4897, 5811b		
96.	87323-67-9	Benzoic acid, hydroxy-methoxy-	3737, 3741, 3743, 4249, 4897, 5811b		
97.	28965-86-8	Benzoic acid, hydroxy-methyl-	3737, 3741, 3743, 4249, 4897		
98.	25567-10-6	Benzoic acid, methyl- {toluic acid}	1371, 2543, 2773, 2775, 3410		
99.	50-78-2	Benzoic acid, 2-acetoxy-		5811, 5811b	
100.	118-92-3	Benzoic acid, 2-amino-		3797, 4249	
101.	612-19-1	Benzoic acid, 2-ethyl-	91b, 5811b		
102.	10366-91-3	Benzoic acid, 2-(β-*D*-glucopyranosyloxy)-		4249, 5811b	
103.	612-20-4	Benzoic acid, 2-(hydroxymethyl)-	4249		
104.	69-72-7	Benzoic acid, 2-hydroxy- {salicylic acid}	414, 568b, 1879, 1884, 1886, 1981, 3255, 3308, 3394, 3712, 3737, 3741, 3743, 3793, 3797, 4113, 4249, 5811b	120, 568b, 1620, 2092, 2270, 2356, 2389, 2544, 2954, 3748, 3749, 3751, 4249, 5811b	
105.	50-85-1	Benzoic acid, 2-hydroxy-4-methyl-	3712, 4113, 4249		

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
106.	579-75-9	Benzoic acid, 2-methoxy- {*o*-anisic acid}		2389, 2544, 4249	
107.	118-90-1	Benzoic acid, 2-methyl- {*o*-toluic acid}	568b, 1063–1066, 1068–1074, 1882, 5811b	568b, 1948, 2092, 4249, 5811b	
108.	303-38-8	Benzoic acid, 2,3-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b	3103	
109.	3934-81-4	Benzoic acid, 2,3-dihydroxy-4-methoxy-	3712, 4113, 4249		
110.	3929-89-3	Benzoic acid, 2,3-dihydroxy-4-methyl-	3712		
111.	603-79-2	Benzoic acid, 2,3-dimethyl-	91b, 5811b		
112.	610-02-6	Benzoic acid, 2,3,4-trihydroxy-	3712, 4113, 4249		
113.	89-86-1	Benzoic acid, 2,4-dihydroxy- {β-resorcylic acid}	3712, 4113, 4249		
114.	490-79-9	Benzoic acid, 2,5-dihydroxy- {gentisic acid}	3737, 3741, 3743, 4249, 5811b	3103, 3748, 3749, 3751, 4249, 4914	
115.	96937-49-4	Benzoic acid, 2,5-dihydroxy-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
116.	610-72-0	Benzoic acid, 2,5-dimethyl-	91b, 5811b		
117.	303-07-1	Benzoic acid, 2,6-dihydroxy-	3712, 3737, 3741, 3743, 4249, 5811b	3103, 5811b	
118.	619-20-5	Benzoic acid, 3-ethyl-	91b, 5811b		
119.	99-06-9	Benzoic acid, 3-hydroxy-	101, 568b, 1099, 1371, 1626, 1879, 1884, 1886, 2767, 2939, 3302, 3308, 3394, 3553, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	568b, 1234, 1980, 2939, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5811b	3393
120.	645-08-9	Benzoic acid, 3-hydroxy-4-methoxy- {isovanillic acid}	2042, 3308, 3394, 3712, 3793, 3797, 5811b		
121.	586-30-1	Benzoic acid, 3-hydroxy-4-methyl-	101, 3712, 3737, 3741, 3743, 4113, 4249, 5811b	3103	
122.	586-38-9	Benzoic acid, 3-methoxy-	91b, 5811b		
123.	99-04-7	Benzoic acid, 3-methyl- {*m*-toluic acid}	2873, 3308, 4249, 5811b	1886, 2389, 2544, 2917a, 4249, 5811b	3393
124.	99-50-3	Benzoic acid, 3,4-dihydroxy- {protocatechuic acid}	1626, 1884, 2939, 3302, 3308, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	120, 970, 1980, 2270, 2722, 2939, 3103, 3655a, 3655b, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5079, 5811b	
125.	96937-39-2	Benzoic acid, 3,4-dihydroxy-dimethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
126.	96937-40-5	Benzoic acid, 3,4-dihydroxy-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
127.		Benzoic acid, 3,4-dihydroxy-C_4-alkyl-methyl-	3737, 3741, 3743		

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
128.	93-07-2	Benzoic acid, 3,4-dimethoxy-		1971, 4249	
129.	619-04-5	Benzoic acid, 3,4-dimethyl-	91b, 5811b		
130.	149-91-7	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}	1373, 1842, 2195, 3219, 3265, 3308, 3712, 4249	3655b, 5079	
131.	99-10-5	Benzoic acid, 3,5-dihydroxy-	3712, 3737, 3741, 3743, 4113, 4249, 5811b		
132.	499-06-9	Benzoic acid, 3,5-dimethyl-	91b, 5811b	3608, 4249	
133.	1918-00-9	Benzoic acid, 3,6-dichloro-2-methoxy- {Dicamba®}	4857	3633, 3973, 4249, 4857, 5015, 5521, 5811b	
134.	619-64-7	Benzoic acid, 4-ethyl-	91b, 5811b		
135.	32142-31-7	Benzoic acid, 4-(β-*D*-glucopyranosyloxy)-3-methoxy-		429b, 4249, 4915	
136.	99-96-7	Benzoic acid, 4-hydroxy- {*p*-salicylic acid}	101, 414, 568b, 1626, 1879, 1884, 1886, 2042, 2043, 2939, 3302, 3308, 3394, 3553, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	568b, 908, 952, 2939, 3532, 3560, 3561, 3748, 3749, 3751, 3797, 3973, 3974a, 5811b	3393
137.	530-57-4	Benzoic acid, 4-hydroxy-3,5-dimethoxy- {syringic acid}	1626, 1884, 2939, 3302, 3308, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 4378, 5811b	3797, 3973, 3974a	
138.	121-34-6	Benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid}	568b, 1235, 1427, 1626, 1884, 1886, 2042–2044, 2046, 2939, 3219, 3302, 3308, 3553, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	120, 568b, 908, 952, 1248, 1620, 2270, 2939, 2954, 3103, 3219, 3329, 3532, 3560, 3561, 3748, 3749, 3751, 3797, 3973, 3974a, 4092, 4249, 4677, 5811b	
139.	96937-45-0	Benzoic acid, 4-hydroxy-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
140.	99-94-5	Benzoic acid, 4-methyl- {*p*-toluic acid}	1063–1066, 1068–1074, 2873, 3308, 5811b		3393
141.		2*H*-1-Benzopyran-3-carboxylic acid, 6,7-dihydroxy-2-oxo- 		4249, 4556	
142.	19484-74-3	2*H*-1-Benzopyran-3-carboxylic acid, 7,8-dihydroxy-2-oxo-		4249	
143.	19250-17-0	Bicyclo[3.1.1]hept-2-ene-2-carboxylic acid, 6,6-dimethyl-		5811, 5811b	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

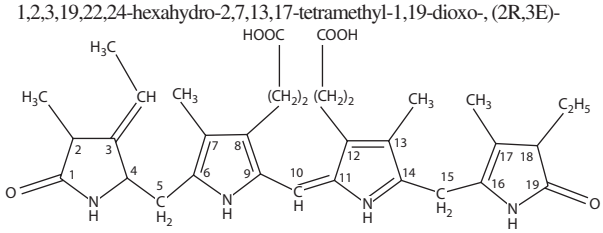
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
144.	20298-86-6	21*H*-Biline-8,12-dipropanoic acid, 18-ethyl-3-ethylidene-1,2,3,19,22,24-hexahydro-2,7,13,17-tetramethyl-1,19-dioxo-, (2R,3E)- 		4249	
145.	110-15-6	Butanedioic acid {succinic acid} HOOC-$(CH_2)_2$-COOH	101, 126b, 172, 237, 722, 1099, 1375a, 1377, 1445, 1674, 1882, 1886, 2079, 2133, 2170, 2939, 3053, 3060, 3061, 3255, 3302, 3308, 3324, 3394, 3496, 3555, 3741, 3743, 4249, 5079, 5359, 5811b	120, 836, 838, 839, 1305a, 1330, 1923, 1982, 2079, 2270, 2283, 2356, 2532, 2939, 3052, 3060, 3353, 3555, 3655b, 3656, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 5079, 5381, 5384, 5745, 5753, 5811b, 5896	1375a, 1377, 3393, 3405
146.	6915-15-7	Butanedioic acid, hydroxy- {malic acid} HOOC-CHOH-CH_2-COOH	565, 1371, 2939, 3059, 3061, 3224, 3266, 3302, 3308, 3496, 3555, 3741, 3743, 4249, 5811b	120, 172a, 256, 385, 543a, 555, 634, 677b, 722, 826a, 835, 836, 838–840, 963, 1053, 1063–1066, 1068–1074, 1279, 1289, 1305a, 1330, 1332, 1333, 1548 1923, 1933a, 1982, 2014, 2079, 2154, 2270, 2283, 2356, 2529, 2532, 2543, 2545, 2688, 2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3052, 3107, 3194, 3266, 3353, 3476, 3486, 3555, 3655b, 3656, 3667, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 3974b, 3976, 3984, 4103, 4131, 4249, 4275, 5079, 5109, 5126, 5189, 5244, 5342, 5381, 5384, 5389, 5419, 5430, 5477, 5478, 5745, 5749, 5753, 5811b, 5832, 5896, 17B17	3393
147.		Butanedioic acid, hydroxy-, labeled with ^{14}C {malic acid}-^{14}C	2763	2763	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
148.	71608-04-3	Butanedioic acid, (hydroxymethylene)-	1871a, 4249		
149.	498-21-5	Butanedioic acid, methyl-	1099, 1886, 3255, 3394, 3741, 3743, 4249, 5811b		3393
150.	636-60-2	Butanedioic acid, methyl-, (±)-	1099		
151.	97-65-4	Butanedioic acid, methylene-{itaconic acid} $HOOC-C(=CH_2)-CH_2-COOH$	3394, 5811b	3029, 5811b	3393
152.	2338-45-6	Butanedioic acid, (1-methylethyl)-		3797, 3974a	
153.	3878-55-5	Butanedioic acid, monomethyl ester $HOOC-(CH_2)_2-COO-CH_3$	568b, 1235, 3302, 3553, 4249, 5811b	5811b	
154.	328-42-7	Butanedioic acid, oxo-{oxalacetic acid} $HOOC-CO-CH_2-COOH$		120, 3797, 3973	
155.	3237-44-3	Butanedioic acid, 2-hydroxy-2-(1-methylethyl)-		1259, 2722, 4249	
156.	18734-79-7	Butanedioic acid, 2-methyl-3-phenyl-		4249	
157.	35392-77-9	Butanedioic acid, 2,3-diethyl-, (R^*,R^*)-(±)-{succinic acid, 2,3-diethyl-} $HOOC-CH(C_2H_5)-CH(C_2H_5)-COOH$		1980, 4249	
158.	526-83-0	Butanedioic acid, 2,3-dihydroxy-{tartaric acid} $HOOC-CHOH-CHOH-COOH$	1268, 1270, 3266, 3555, 4249	1053**,** 1268, 1270, 1982, 3266, 3555, 4249, 5529, 5764	
159.	147-71-7	Butanedioic acid, 2,3-dihydroxy- {*d*-tartaric acid}		172a, 1053, 3266	
160.	87-69-4	Butanedioic acid, 2,3-dihydroxy- {*l*-tartaric acid}		174c, 1053, 3266, 5811b	
161.	133-37-9	Butanedioic acid, 2,3-dihydroxy- {*dl*-tartaric acid}		1053, 3266	
162.	147-73-9	Butanedioic acid, 2,3-dihydroxy- {*meso*-tartaric acid}		1053, 3266	
163.	13545-04-5	Butanedioic acid, 2,3-dimethyl- {succinic acid, 2,3-dimethyl-} $HOOC-CH(CH_3)-CH(CH_3)-COOH$		2356, 3560, 3561, 4249	
164.	107-92-6	Butanoic acid {butyric acid} $H_3C-(CH_2)_2-COOH$	526, 563, 565, 568b, 960, 1063–1066, 1068–1074, 1132, 1140, 1360, 1364, 1365, 1371, 1375a, 1388–1390, 1586, 1587a, 1638, 1884, 1886, 1903, 1904, 1917, 2043, 2079, 2088, 2170, 2270, 2337, 2338, 2387, 2493, 2543, 2570, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3263, 3266, 3302, 3308, 3410, 3452, 3495, 3553, 3799, 3800, 3809, 3910, 3912, 4052, 4056, 4064, 4065, 4185, 4249, 4304, 4319, 4406, 5079, 5189, 5811b	172a, 174b, 404, 568b, 647, 848, 981a, 1053, 1085, 1087, 1276, 1587a, 1590a, 1982, 1999, 2014, 2092, 2337, 2338, 2570, 2649, 2722, 3266, 3328, 3370, 3507, 3655b, 3809, 3973, 3974a, 3974b, 4064, 4249, 5079, 5381, 5708, 5735, 5811b, 5846	1360, 1375a, 2387, 3393, 3401, 3402, 4052, 4056

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

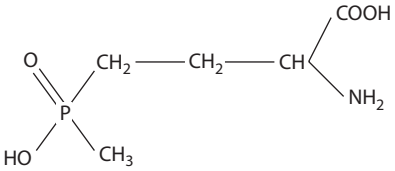
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
165.	80-60-4	Butanoic acid, 2-amino- $H_3C\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1580, 2939	480, 1329, 1351, 2337, 2597a, 2939, 3491, 3726, 3797, 3974a, 3978, 5785, 5811b, 5827, 5881, 5907	
166.	7004-04-8	Butanoic acid, 2-amino-3-hydroxy- $H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	429b	429b, 4249	
167.	1927-25-9	Butanoic acid, 2-amino-4-hydroxy-		5777, 5811, 5905	
168.	51276-47-2 53369-07-6	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®} 		5521	
169.	454-41-1	Butanoic acid, 2-amino-4-(methylsulfinyl)-		172, 429b, 4249	
170.	1118-85-0 3226-65-1	Butanoic acid, 2-amino-4-(methylsulfonyl)- {methionine sulfone; methionine S-oxide} $H_3C\text{-}SO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		120, 172, 1305a, 1351, 2337, 3491, 3729, 3797, 3974a, 4224, 4249	
171.	2338-03-6	Butanoic acid, 2-amino-4-oxo-, (S)-		4249	
172.	597-04-6	Butanoic acid, 2,2-dimethyl-3-oxo-		568b, 4249	
173.	14287-61-7	Butanoic acid, 2,3-dimethyl- $(H_3C)_2{=}CH\text{-}CH(CH_3)\text{-}COOH$	2092, 4249	2092, 3547, 4249, 5811b	
174.	88-09-5	Butanoic acid, 2-ethyl-{diethylacetic acid} $(H_3C\text{-}CH_2)_2{=}CH\text{-}COOH$	568b, 3452, 4249, 5811b	568b, 1982, 2917a, 3547, 4249, 5811b	
175.	565-70-8	Butanoic acid, 2-hydroxy- $H_3C\text{-}CH_2\text{-}CHOH\text{-}COOH$	568b, 1882, 3553, 4249, 4677, 5811b	568b, 1886, 2336, 2337a, 3553, 4249	3393
176.	3739-30-8	Butanoic acid, 2-hydroxy-2-methyl- $H_3C\text{-}CH_2\text{-}C(CH_3)(OH)\text{-}COOH$		1948, 4249	
177.	4026-18-0	Butanoic acid, 2-hydroxy-3-methyl- $H_3C\text{-}CH(CH_3)\text{-}CHOH\text{-}COOH$	1260	1085, 1260, 4249	
178.	116-53-0 600-07-7	Butanoic acid, 2-methyl- {2-methylbutyric acid} $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}COOH$	568b, 1140, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1587a, 1999, 2270, 2338, 2387, 2543, 2545, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2939, 3266, 3410, 3452, 3553, 3797, 4249, 5811b	120, 172a, 174b, 404, 568b, 848, 937, 938, 1053, 1587a, 1590a, 1999, 2014, 2283, 2288, 2291, 2338, 2339a, 2386, 2389, 2544, 2570, 2722, 2862, 2917a, 2939, 3219, 3266, 3329, 3370, 3537, 3547, 3550, 3560, 3561, 3973, 3974a, 4249, 5708, 5811b, 5831	1360, 1375a, 2387
179.	600-18-0	Butanoic acid, 2-oxo- $H_3C\text{-}CH_2\text{-}CO\text{-}COOH$	3302, 4249	1312	
180.	2835-82-7	Butanoic acid, 3-amino-		480	
181.	1070-83-3	Butanoic acid, 3,3-dimethyl- $(H_3C)_3{\equiv}C\text{-}CH_2\text{-}COOH$		404, 4092, 4249	
182.	300-85-6	Butanoic acid, 3-hydroxy- $H_3C\text{-}CHOH\text{-}CH_2\text{-}COOH$	3394, 5811b		3393
183.	625-08-1	Butanoic acid, 3-hydroxy-3-methyl- $H_3C\text{-}C(CH_3)(OH)\text{-}CH_2\text{-}COOH$	5811b	1948, 4249	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
184.	503-74-2	Butanoic acid, 3-methyl-{isovaleric acid} $(H_3C)_2$═CH-CH_2-COOH	563, 565, 775, 960, 1063–1066, 1068–1074, 1132, 1360, 1371, 1375, 1375a, 1375b, 1388–1390, 1418, 1586, 1587a, 1668, 1886, 1903, 1904, 2043, 2079, 2270, 2337, 2338, 2387, 2543, 2570, 2619, 2623, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 3224, 3266, 3302, 3308, 3410, 3452, 3553, 3557, 3794, 3799, 3800, 3809, 4249, 4319, 4997, 5811b	120, 172a, 174b, 404, 563, 565, 908, 909, 981a, 1053, 1085, 1221, 1587a, 1590a, 1982, 1999, 2014, 2079, 2283, 2291, 2337, 2338, 2339a, 2386, 2389, 2544, 2570, 2611, 2816, 2817, 2917a, 2939, 3215, 3219, 3266, 3507, 3537, 3545, 3547, 3550, 3560, 3561, 3809, 3973, 3974a, 3974b, 4249, 5079, 5180, 5708, 5735, 5811b, 5846	1360, 1375a, 2387, 3393
185.	541-50-4	Butanoic acid, 3-oxo- {acetoacetic acid} H_3C-CO-CH_2-COOH	3302, 4249	1312	
186.	56-12-2	Butanoic acid, 4-amino- H_2N-$(CH_2)_3$-COOH	1083, 1351, 1580, 1910, 1914, 2724, 2858, 2939, 3302, 3491, 3797, 4249, 5811b	120, 480, 555a, 555b, 622, 749, 752–754, 826a, 927, 1086, 1223, 1351, 2270, 2337, 2338, 2532, 2597a, 2795, 2911c, 2939, 3491, 3555, 3705, 3797, 3974a, 3978, 4224, 4244, 4249, 4398c, 5079, 5699, 5811b, 5905	
187.	61445-55-4 133201-39-5	Butanoic acid, 4-(methylnitrosoamino)-Butanoic acid, 4-[(nitrosomethyl)amino] (NMBA) CH_3-N(NO)-$(CH_2)_3$-COOH	466, 486, 982, 2852, 3256, 3300, 3943a, 3944–3946, 3973, 5811b	486, 982, 2852, 3943a, 3944–3946, 3947, 3948, 3973, 5001, 5811b	
188.	583-92-6	Butanoic acid, 4-(methylthio)-2-oxo-		429b, 4249, 4699	
189.	54344-76-2	Butanoic acid, 4-(2,6,6-trimethylcyclohexen-1-yl)-		2917a	
190.	462-10-2	Butanoic acid, 4,4′-dithiobis[2-amino- {homocystine} $[S-(CH_2)_2-CH(NH_2)-COOH]_2$		2337, 3491, 3729, 3797, 3974a, 4224, 4226, 4249	
191.	6915-18-0	2-Butenedioic acid HOOC-CH═CH-COOH		3001a	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

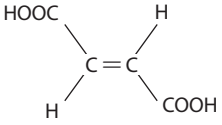
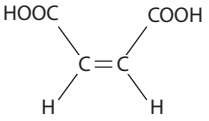
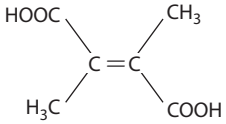
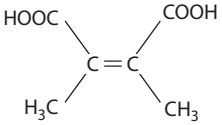
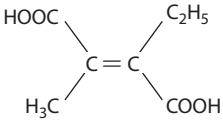
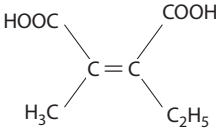
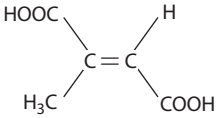
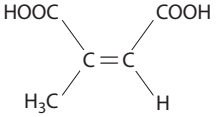
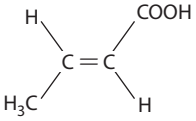
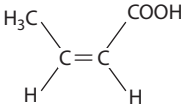
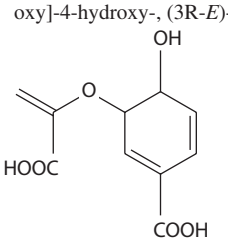
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
192.	110-17-8	2-Butenedioic acid (*E*)- {fumaric acid} 	101, 1235, 2079, 2170, 3302, 3324, 3394, 3555, 3741, 3743, 4249, 5079, 5359, 5811b	120, 836, 839, 1305a, 1923, 1982, 2079, 2270, 2283, 2532, 2939, 3353, 3486, 3555, 3655b, 3656, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5079, 5384, 5811b, 5896	3393
193.	110-16-7	2-Butenedioic acid (*Z*)- {maleic acid} 	1375a, 1377, 2584, 3394, 4249, 5811b	120, 702, 1305a, 1923, 2270, 2283, 2356, 2939, 3974a, 5896	1375a, 1377, 3393
194.	21788-49-8	2-Butenedioic acid, 2,3-dimethyl-, (*E*)- 		937, 4249	
195.	488-21-1	2-Butenedioic acid, 2,3-dimethyl-, (*Z*)- 		937, 4249	
196.	28098-80-8	2-Butenedioic acid, 2-ethyl-3-methyl-, (*E*)- 		937, 4249	
197.	41654-09-5	2-Butenedioic acid, 2-ethyl-3-methyl-, (*Z*)- 		937, 4249, 5811b	
198.	498-24-8	2-Butenedioic acid, 2-methyl-, (*E*)- {mesaconic acid} 	3741, 3743, 4249, 4897, 5811b		
199.	498-23-7	2-Butenedioic acid, 2-methyl-, (*Z*)- {citraconic acid} 	3029, 3393, 3741, 3743, 4249	3029	3393
200.	3724-65-0	2-Butenoic acid {crotonic acid} H_3C-CH═CH-COOH	1360, 1375, 1375a, 1375b, 1586, 1882, 2387, 2767, 3553, 3557, 5811b	120, 848, 1999, 2014, 2338, 2386, 2389, 2544, 2862a, 2939, 3974a, 5811b	1360, 1375a, 2387, 3393, 3402

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
201.	107-93-7	2-Butenoic acid, (*E*)- {*trans*-crotonic acid} 	568b, 1365, 2543, 2761, 2762, 2765, 2766, 2773, 3410, 4249	568b, 2939, 3549, 4249	
202.	503-64-0	2-Butenoic acid, (*Z*)- {*cis*-crotonic acid} 	2387		2387
203.	13201-46-2	2-Butenoic acid, 2-methyl-, (*Z*)- {angelic acid}	565, 568b, 1586, 1886, 2767, 2769, 3266, 3553, 3557, 4249, 5811b	120, 172a, 174b, 404, 568b, 937, 938, 1053, 2270, 2283, 2611, 2917a, 3266, 3153, 3547, 4249, 5811b	3393
204.	80-59-1	2-Butenoic acid, 2-methyl-, (*E*)- {tiglic acid}	565, 1586, 1886, 2767, 2769, 3266, 3553, 3557, 4249	120, 172a, 174b, 404, 937, 938, 1053, 2270, 2283, 2611, 2917a, 3266, 3153, 3547, 4249	3393
205.		2-Butenoic acid, 2-phenyl-		938, 4249	
206.	541-47-9	2-Butenoic acid, 3-methyl-	568b, 2767, 3266, 3553, 4249, 5811b	404, 568b, 1053, 2611, 3186, 3266, 3547, 3550, 4249	
207.	32040-41-8	2-Butenoic acid, 4-(formylamino)-4-oxo-, (*Z*)- O═CH-NH-CO-CH═CH-COOH		4249, 4918	
208.	625-38-7	3-Butenoic acid H_2C═CH-CH_2-COOH	568b, 1063–1066, 1068–1074, 1586, 2767, 3410, 3553, 3557, 4249, 5811b		
209.	1617-31-8	3-Butenoic acid, 3-methyl-	568b, 3553, 4249, 5811b	568b, 3547, 4249	
210.	2243-53-0	3-Butenoic acid, 4-phenyl- {styrylacetic acid}	3553, 4249	943, 2092, 4249, 5811b	
211.	594-07-0	Carbamodithioic acid		2574, 4249	
212.	617-12-9	1,5-Cyclohexadiene-1-carboxylic acid, 3-[(1-carboxyethenyl) oxy]-4-hydroxy-, (3R-*E*)- {chorismic acid} 		429b, 4249, 4476	
213.	34214-77-2	Cyclohexanecarboxylic acid, 3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]trihydroxy-, (1α,3α,4α,5β)-	3302, 3792, 4249	1309, 3797, 4249, 5811b	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

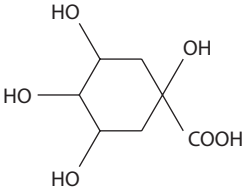
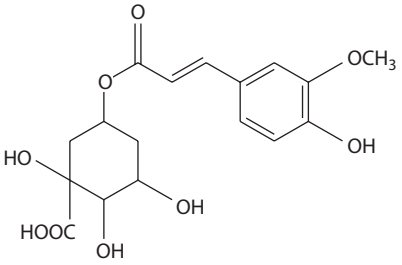
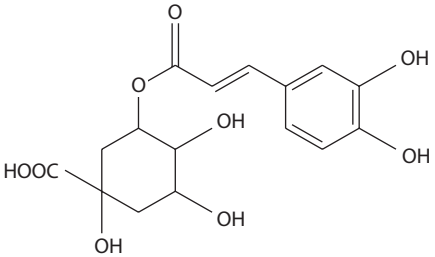
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
214.	77-95-2 562-73-2	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy- {quinic acid} 	1083, 2675, 3302	120, 1086, 2079, 2270, 2531, 2892c, 2939, 3059, 3655b, 3797, 3973, 3974a, 4249, 4999, 5079, 5189, 5383, 5389, 5698, 5713, 5722, 5779, 5784, 5786, 5811b, 5831	
215.	36413-60-2	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, (1α,3α,4α,5β)-		2892c, 2939, 3797, 4249	
216.	1899-30-5	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]-, [1S-(1α,3α,4α,5β)]- {*p*-coumaroylquinic acid}		3973, 3974a, 4402	
217.	1899-29-2 27044-07-1	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)- {3-*O*-feruloylquinic acid}  Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-		3797, 3973, 3974a, 4249, 4402, 4913, 5811b	
218.	2450-53-5	Cyclohexanecarboxylic acid, 3,5-bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4-dihydroxy-, [1R-(1α,3α,4α,5β)]- {isochlorogenic acid}		1309, 4249, 5705	
219.	15016-60-1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*Z*),4α,5α]]-	3302, 3792, 4249	3797, 4249	
220.	15076-00-3	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*E*),4α,5α]]-		4249	
221.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid; 3-*O*-caffeoylquinic acid} 	172, 602, 1884, 3257, 3302, 3792, 3797, 4249, 5811b	69, 72, 120, 254, 385, 486, 598, 602, 657, 665, 677b, 718, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1040, 1063–1066, 1068–1074, 1077b, 1309, 1329, 1333, 1352, 1485, 1625, 1626, 1923, 2014, 2056a, 2079, 2154, 2250a, 2270, 2283, 2313a, 2338, 2361, 2395, 2514, 2531, 2529, 2557a, 2810–2812, 2911c, 2911d, 2914, 2939, 2954, 3029, 3059, 3096, 3161, 3302, 3366a, 3367a, 3400, 3459–3462, 3551, 3616, 3628, 3631, 3641, 3646, 3655b, 3700, 3705, 3738, 3748,	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
222.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid; 3-*O*-caffeoylquinic acid} (cont.)	172, 602, 1884, 3257, 3302, 3792, 3797, 4249, 5811b	3749, 3751, 3754, 3792, 3794, 3797, 3806, 3973, 3974a, 3974b, 3984, 3999,4005–4007, 4156, 4221, 4249, 4275, 4279, 4372, 4402, 4403, 4421, 4999, 5079, 5189, 5200, 5246, 5353, 5389, 5576, 5592–5594, 5596, 5604, 5652, 5665, 5672, 5673, 5681, 5697. 5698, 5700, 5705, 5713, 5722, 5737, 5761, 5782, 5784, 5788, 5808–5810, 5811b, 5812, 5827, 5831, 5834, 5839, 5850, 5856, 5889, 3890, 5896, 5900, 5908	
223.	906-33-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-(1a,3a,4a,5b)]- {neochlorogenic acid; 5-*O*-caffeoylquinic acid} Also listed as cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxxy-	3302, 3792, 5811b	120, 602, 830a, 831, 834, 835, 838, 840, 890, 970, 1206a, 1626, 2557a, 2939, 3646, 3738, 3792, 3797, 3973, 3974a, 4249, 4402, 5705, 5811b, 5831	
224.	24321-18-4	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dioxo-1,5-cyclohexadien-1-yl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-		3633, 3973, 4271a, 5811b	
225.	70898-22-5	Cyclohexanecarboxylic acid, 3-[[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-		4249, 4785, 4984	
226.	17608-52-5	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy- {4-*O*-caffeoylquinic acid}		831, 834, 835, 838, 840, 890, 1206a, 3646, 3738, 3973, 3974a, 4249, 5705, 5811b, 5889	
227.	534-61-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4- dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-[1S-(1α,3β,4β,5 α)]-	5811, 5811b	5811b	
228.	905-99-7	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-, (1α,3α,4α,5β)-		4249, 5811b	
229.		Cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-5-phenyl-		5705, 5749	
230.	471-90-9	1-Cyclohexene-1-carboxylic acid, 2,6,6-trimethyl- {cyclogeranic acid}		2389, 2544, 2917a, 3218, 3547, 5811b	
231.	138-59-0	1-Cyclohexene-1-carboxylic acid, 3,4,5-trihydroxy-, [3R-(3α,4α,5β)]- {shikimic acid}		3059, 3797, 3973, 3974a, 4249, 5778, 5783, 5786	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

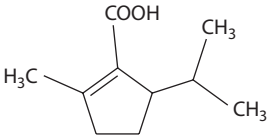
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
232.	6082-44-6	1-Cyclohexene-1-carboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-4,5-dihydroxy-, (3α,4α,5β)-		4249	
233.	38073-89-1	3-Cyclohexene-1-carboxylic acid, 6-(1-methylethyl)-, *cis*-		2407a, 3547, 4249	
234.	3400-45-1	Cyclopentanecarboxylic acid {cyclopentanoic acid}		120, 2263, 2270, 2283, 3353, 4249	
235.	38655-27-5	Cyclopentanecarboxylic acid, 1-methyl-3-(1-methylethenyl)-		938, 3767a, 4249, 5811b	
236.	66016-71-5	1,2-Cyclopentanedicarboxylic acid, 1-methyl-3-(1-methylethyl)-		734, 4101, 4249	
237.	56169-12-1	1-Cyclopentene-1-carboxylic acid, 2-methyl-5-(1-methylethyl)- 		735, 738, 1156, 1251, 3851, 4090, 4249	
238.	53109-18-5	1-Cyclopentene-1-pentanoicacid, δ-hydroxy-3,5-bis(1-methylpropyl)-β-oxo-		4249	
239.	22059-21-8	Cyclopropanecarboxylic acid, 1-amino-		4249, 5811b	
240.	17219-23-7	Cyclopropanecarboxylic acid, 2,3-dimethyl-		3547, 4249	
241.	498-40-8	Cysteic acid $HO\text{-}SO_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$		622, 1351, 2337, 3491, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079	
242.	52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto-(R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1274, 3265, 3266, 4249	120, 158, 172, 342, 722, 927, 1053, 1128b, 1305a, 1351, 1918, 2049, 2337, 2939, 3266, 3491, 3729, 3797, 3974a, 3978, 4224, 4249, 4398c, 5079, 5189, 5376, 5811b, 5874, 5881	
243.	636-58-8	*L*-Cysteine, *N*-*L*-γ-glutamyl-		4249	
244.	24645-67-8	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-} $\{S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH\}_2$		116, 120, 172, 622, 722, 749, 752–754, 1063–1066, 1068–1074, 1127b, 1329, 1330, 1332, 1351, 2049, 2079, 2270, 2337, 2453, 2597a, 2939, 3491, 3499, 3705, 3729, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079, 5189, 5376, 5603, 5881, 5907	
245.	56-89-3 13028-62-1	*L*-Cystine		5811, 5811b	
246.	63889-75-8	Decadienoic acid		731, 738, 3219, 4249	
247.	59286-28-1	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*Z,E*)- $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}CH[CH(CH_3)_2]\text{-}CH{=}CH\text{-}C(CH_3){=}CH\text{-}COOH$		2, 736, 1156, 4090, 4249	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
248.	58315-84-7	2,4-Decadienoicacid,3-methyl-6-(1-methylethyl)-9-oxo-,[S-(*E,E*)]-		2, 736, 1156, 4090, 4249	
249.	59262-52-1	2,7-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*E,E*)- H_3C-CO-CH═CH-CH[$CH(CH_3)_2$]-$(CH_2)_2$-$CH(CH_3)$═CH-COOH		2, 731, 738, 1156, 4090, 4249	
250.	158815-70-4	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-		736, 4249, 5811b	
251.	111-20-6	Decanedioic acid {sebacic acid}	2341, 2572, 4249	2341, 2210, 4249, 5811b	
252.	334-48-5	Decanoic acid {capric acid} H_3C-$(CH_2)_8$-COOH	60, 563, 565, 568b, 809, 1132, 1232, 1348, 1360, 1375, 1375a, 1375b, 1668, 1884, 1917, 2418, 2939, 3266, 3293, 3308, 3553, 3797, 4249, 4993, 5079, 5811b	60, 120, 172a, 174b, 404, 524, 568b, 848, 908, 565, 1053, 1893a, 1893b, 2270, 2356, 2283, 2389, 2544, 2592, 2611, 2917a, 3266, 3370, 3543, 3545, 3547, 3560, 3561, 3633, 3767a, 3974a, 4249, 4993, 5657, 5695, 5811b	1360, 1375a
253.		Decanoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-	2092, 4249	2092, 4249	
254.	5601-60-5	Decanoic acid, 8-methyl-		2092, 4249, 5811b	
255.	63892-04-6	2,7,9-Decatrienoic acid, 3,9-dimethyl-6-(1-methylethyl)-, (*E,E*)-		731, 738, 1156, 4090, 4249	
256.	26446-27-5 72881-27-7	Decenoic acid {three isomers detected}	2092, 4249	2092, 4249, 5811, 5811b	
257.	60924-66-5	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-		737, 4249	
258.	129777-23-7	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-, [R-[R*,S*-(*E*)]]-		737, 4249, 5811b	
259.	5894-59-7	Digalacturonic acid		5811, 5811b	
260.	29564-66-7	Docosadienoic acid, (*Z,Z*)-		4249, 4753	
261.	112-85-6	Docosanoic acid {behenic acid} H_3C-$(CH_2)_{20}$-COOH	60, 101, 172, 257, 258, 1348, 1586, 1785, 2570, 2767, 3302, 3557, 5811b	60, 101, 1785, 2286, 2593, 3974a, 4280, 5811b	
262.	36332-95-3	Docosanoic acid, 20-methyl- H_3C-CH_2 $CH(CH_3)$-$(CH_2)_{18}$-COOH		3974a, 4249, 4719, 4964	
263.	59708-74-6	Docosanoic acid, 21-methyl- $(H_3C)_2$═CH-$(CH_2)_{19}$-COOH		3974a, 4249, 4719	
264.	112-86-7	13-Docosenoic acid, (*Z*)-		3737, 4249	
265.	65596-29-4	3,6-Dodecadienedioic acid, 10-hydroxy-4,9-dimethyl- HOOC-CH_2-CHOH-$CH(CH_3)$-CH_2-CH═CH-CH_2-$C(CH_3)$═CH-CH_2-COOH		739, 1156, 4090, 4249	
266.		2,4-Dodecadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-		9	
267.	693-23-2	Dodecanedioic acid	2572, 4249		
268.	143-07-7	Dodecanoic acid {lauric acid} H_3C-$(CH_2)_{10}$-COOH	60, 172, 257, 258, 568b, 765, 809, 1132, 1232, 1375, 1586, 1785, 1906, 1917, 2418, 2529, 2570, 2767, 2939, 3266, 3293, 3302, 3308, 3557, 4030, 4249, 4319, 4993, 5079, 5811b	60, 101, 120, 172a, 174b, 404, 568b, 908, 1053, 1785, 1893a, 1893b, 2092, 2093, 2270, 2283, 2339a, 2356, 2529, 2862, 2917a, 3194, 3266, 3370, 3547, 3633, 3973, 3974a, 4249, 4280, 4993, 5695	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
269.	7416-57-1	Dodecanoic acid, 10-methyl- H_3C-CH_2 $CH(CH_3)$-$(CH_2)_8$-COOH		4249, 4964	
270.	7548-13-2	2,6,10-Dodecatrienoic acid, 3,7,11-trimethyl-		2917a	
271.	1289-45-8	Dodecenoic acid	809, 3293		
272.	4412-16-2	2-Dodecenoic acid		3547	
273.	3625-52-3	Dotriacontanoic acid H_3C-$(CH_2)_{30}$-COOH	101, 3263, 3327a, 5811b		
274.	25448-01-5	Eicosadienoic acid		4249, 4753	
275.	506-30-9	Eicosanoic acid {arachidic acid} H_3C-$(CH_2)_{18}$-COOH	60, 101, 172, 257, 258, 765, 1348, 1586, 1785, 2570, 2767, 2939, 3302, 3308, 3557, 4030, 4249, 4280, 4719, 5811b	60, 101, 908, 1785, 2389, 2544, 2593, 2939, 3974a, 4249, 4280, 5811b	
276.	36332-93-1	Eicosanoic acid, 18-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{16}$-COOH	2570, 4249, 4964	2769, 3974a, 4249	
277.	59708-73-5	Eicosanoic acid, 19-methyl- $(H_3C)_2$═CH-$(CH_2)_{17}$-COOH		3974a, 4249, 4719	
278.	506-32-1	5,8,11,14-Eicosatetraenoic acid, (all-*Z*)- {arachidonic acid}	3797	2939, 3974a, 4249	
279.	26764-41-0	Eicosenoic acid	60, 4249	60, 4249	
280.	144-62-7	Ethanedioic acid {oxalic acid} HOOC-COOH	765, 1375a, 1377, 1886, 2210, 2939, 3053, 3060, 3061, 3302, 3308, 3496, 3555, 4249, 4304, 4319, 5079, 5467, 5811b	120, 256, 385, 555, 634, 677b, 826a, 835, 836, 838, 839, 963, 1063–1066, 1068–1074, 1289, 1330, 1332, 1333, 1548, 1923, 1933a, 1982, 2014, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2529, 2532, 2543, 2545, 2688, 2761–2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3053, 3060, 3107, 3194, 3555, 3655b, 3701a, 3797, 3974a, 3976, 3984, 3973, 3974b, 4131, 4249, 5079, 5108, 5109, 5126, 5244, 5381, 5389, 5419, 5477, 5745, 5749, 5753, 5764, 5832, 5896	1375a, 1377, 2210
281.	43058-40-8	Ethanedioic acid, labeled with ^{14}C {oxalic acid-^{14}C}	2763, 4249	2763, 4249	
282.	6276-03-5	9*H*-Fluorene-1-carboxylic acid	396, 2939, 3302, 4249	3974a	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
283.	64-18-6	Formic acid H-COOH	126a, 126b, 172, 237, 424, 563, 565, 722, 765, 916, 960, 1023, 1063–1066, 1068–1074, 1099, 1140, 1263, 1388–1390, 1445, 1668, 1674, 1744, 1842, 1882, 1886, 1917, 2079, 2086, 2088, 2133, 2170, 2195, 2253, 2265, 2270, 2293, 2310, 2338, 2414, 2475, 2529, 2543, 2570, 2583, 2619, 2623, 2702, 2765, 2777, 2782, 2804, 2821, 2939, 3060, 3105, 3251, 3255, 3257, 3263, 3300, 3302, 3308, 3394, 3403, 3452, 3495, 3797, 3904, 3963, 4064, 4065, 4135, 4249, 4301, 4304, 4305, 4319, 4330, 4342, 5079, 5189, 5207, 5512, 5811b, 5835	120, 212, 565, 937, 1085, 1893b, 1923, 1982, 1999, 2014, 2079, 2154, 2283, 2293, 2337, 2338, 2702, 2862a, 2939, 3052, 3476, 3507, 3655b, 3656, 3797, 3803, 3973, 3974a, 3974b, 4064, 4249, 5079, 5165, 5381, 5384, 5393, 5695, 5708, 5709, 5712, 5735, 5811b, 5846, 5896	1228, 3393
284.	2745-26-8	2-Furanacetic acid	568b, 1063–1066, 1068–1074, 1375a, 1377, 3553, 4249, 5811b		1375a, 1377
285.	26447-28-9	Furancarboxylic acid	689b, 5811b	3430, 5708	
286.	88-14-2	2-Furancarboxylic acid {furoic acid}	568b, 1132, 1063–1066, 1068–1074, 1099, 1235, 1365, 1375, 1375a, 1375b, 1377, 1882, 2337, 2761, 2762, 2765–2767, 2777, 2939, 3053, 3059, 3060, 3061, 3255, 3302, 3308, 3394, 3410, 3496, 3553, 3557, 4159, 4249, 5811b	120, 568b, 965, 1999, 2014, 2337, 2338, 2337a, 2389, 2544, 2722, 2862a, 2863, 2939, 3053, 3060, 3973, 3974a, 4249, 5811b	1375a, 1377, 3393, 3402, 3404
287.	71278-16-5	2-Furancarboxylic acid, 3-hydroxy-	1375a, 1377	1883, 4249	1375a, 1377
288.	6338-41-6	2-Furancarboxylic acid, 5-(hydroxymethyl)-	1089a, 1886m, 1887a, 2524a, 3741, 3743, 4249, 5811b		3393

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

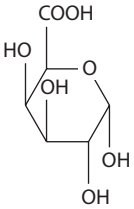
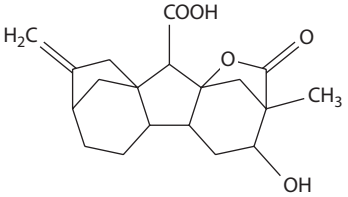
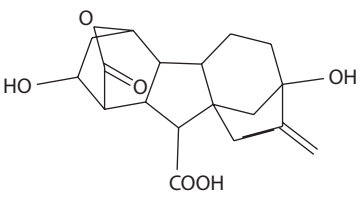
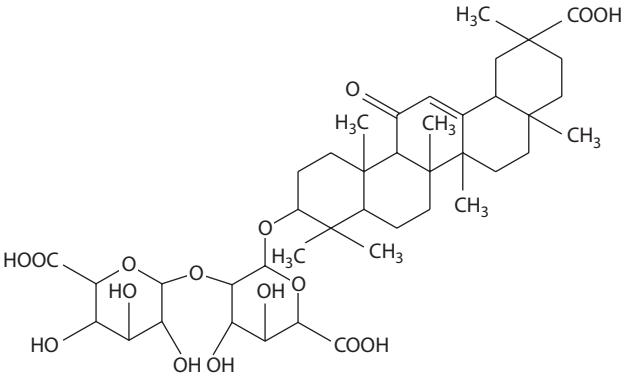
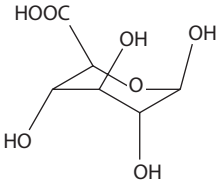
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
289.	1917-15-3	2-Furancarboxylic acid, 5-methyl-	568b, 1075, 1882, 3394, 3553, 4249, 5811b		3393
290.	488-93-7	3-Furancarboxylic acid	568b, 3553, 4249, 5811b		
291.	636-44-2	3-Furancarboxylic acid, 2,5-dimethyl-	91b, 5811b		
292.	6947-94-0	3-Furancarboxylic acid, 2-methyl-	91b, 5811b		
293.	4412-96-8	3-Furancarboxylic acid, 3-methyl-	3327a, 5811b		
294.	21984-93-0	3-Furancarboxylic acid, 5-methyl-	91b, 568b, 2767, 2777, 3553, 4249, 5811b		
295.	526-99-8	Galactaric acid HOOC-$(CHOH)_4$-COOH		1263, 1971, 4249, 5079	
296.	14982-50-4	Galacturonic acid 	2321, 4249	120, 344a, 722, 1263, 2079, 2939, 3107, 3555, 3797, 3973, 3974a, 4249, 5079, 5114, 5189, 5306	
297.	25990-10-7	Galacturonic acid, homopolymer		1051a, 1971, 4249, 5079, 5114	
298.	685-73-4	*D*-Galacturonic acid	2321, 4249	344a, 722, 2070, 2270, 2939, 3797, 4249, 5811b	
299.	34150-36-2	*D*-Galacturonic acid, anhydro-		4249, 4933	
300.	25249-06-3	*D*-Galacturonic acid, homopolymer		1051a, 1334e, 1971, 4249	
301.	19147-78-5	Gibbane-1,10-dicarboxylic acid, 2,3-epoxy-4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,3β,4aα,4bβ,10β)-		4249, 4635	
302.	545-97-1	Gibbane-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		429b, 4249, 4831	
303.	468-44-0	Gibbane-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)- 		2260a, 4249, 4635	
304.	561-56-8	Gibb-2-ene-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,4aα,4bβ,10β)-		429b, 4635	
305.	77-06-5	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)- {gibberellic acid} 		527a, 683a, 5804, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
306.	510-75-8	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		429b, 683a	
307.	1405-86-3	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid; glycyrrhizin} 		74e, 242, 743, 1356, 1361, 1671, 2313a, 3390, 3555, 4623, 5019, 5811b	
308.	53596-04-0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated 3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated; glycyrrhizin ammoniated}		172a, 174b, 1053, 3266	
309.	576-37-4	Glucuronic acid 	312, 4249	120, 2070, 2939, 3973, 4249, 4360a, 5079, 5478, 5708, 5785	
310.	6556-12-3	*D*-Glucuronic acid		5811	
311.	6899-05-4	Glutamic acid HOOC-$(CH_2)_2$-CH(NH_2)-COOH	562, 563, 1083, 1351, 1910, 1914, 2079, 2724, 2858, 2939, 3059, 3061, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 563, 622, 749, 751–756, 826a, 927, 966, 1033, 1034, 1053, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2026, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 4422, 5079, 5699, 5785, 5827, 5896, 5905, 5907	
312.	56-86-0	*L*-Glutamic acid	5811b	1053, 3266, 3973, 5811b	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
313.	997-68-2	*L*-Glutamic acid, *N*-(5-amino-5-carboxypentyl)-, (S)-		429b, 4249, 4698	
314.	58-05-9	*L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-		429b	
315.	1116-22-9	*L*-Glutamic acid, *N*-*L*-γ-glutamyl-		1351, 2027, 2337	
316.	3929-61-1	*L*-Glutamic acid, *N*-*L*-α-glutamyl-		2027, 2337, 3491	
317.	6899-04-3	Glutamine H_2N-CO-$(CH_2)_2$-CH(NH_2)-COOH		3705	
318.	56-85-9	*L*-Glutamine	480, 562, 563, 1351, 1668, 1910, 1914, 1965, 2079, 2724, 2858, 2939, 3059, 3266, 3302, 3491, 3797, 4159, 4249	120, 480, 563, 622, 749, 751–756, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2529, 2532, 2939, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 5079, 5189, 5434, 5437, 5699, 5785, 5811b, 5827, 5831, 5881, 5905, 5907	
319.	56-40-6	Glycine H_2N-CH_2-COOH	1083, 1351, 1914, 2724, 2939, 3302, 3491, 3797, 4249, 5811b	120, 158, 480, 622, 722, 749, 751–756, 826a, 927, 1063–1066, 1068–1074, 1086, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5905, 17B59	
320.	18875-39-3	Glycine, labeled with ^{14}C {glycine-^{14}C}		2099b	
321.	4429-05-4	Glycine, *N*-(1-deoxy-D-fructos-1-yl)-		3639	
322.	88476-94-2	Glycine, *N*-(1-nitroso-*L*-prolyl)-		3951, 4249	
323.	70-18-8	Glycine, *N*-(*N*-L-γ-glutamyl-L-cysteinyl)- {glutathione}		120, 1351, 1668, 2337, 2939, 3491, 3797, 3974a, 4249, 5079, 5220, 5572, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
324.	1071-83-6	Glycine, *N*-(phosphonomethyl)-		1121a	
325.	1118-68-9	Glycine, *N,N*-dimethyl- $(H_3C)_2$═N-CH_2-COOH		4249, 4528	
326.	73360-07-3	Glycine, *N*-[2-(2-aminoethoxy)ethenyl]-		4249	
327.	19246-18-5	Glycine, *N*-*L*-cysteinyl-		429b	
328.	20661-60-3	Glycine, *N*-methyl-*N*-nitro-		992	
329.	13256-22-9	Glycine, *N*-methyl-*N*-nitroso- {NSAR} H_3C-N(NO)-CH_2-COOH	1058, 2442, 3256	466, 485, 486, 498, 2442, 3947, 3948, 5001, 5811b	
330.	2363-71-5	Heneicosanoic acid H_3C-$(CH_2)_{19}$-COOH	60, 172, 257, 258, 1785, 2767, 3302, 3557, 4249, 5811b	60, 1785, 2286, 2593, 3973, 3974a, 4249, 4280	
331.	36332-94-2	Heneicosanoic acid, 19-methyl- H_3C-CH_2-CH(CH_3)-$(CH_2)_{17}$-COOH	60, 1586, 2570, 2767, 3302	60, 3973, 3974a	
332.	6704-01-4	Heneicosanoic acid, 20-methyl- $(H_3C)_2$═CH-$(CH_2)_{18}$-COOH	60, 1586, 2570, 3302, 3557, 4249	60, 3973, 3974a, 4249, 4964	
333.	28984-67-0	Heneicosenoic acid	60, 4249	60, 4249	
334.	66288-40-2	Heneicosenoic acid, 19-methyl-	2767, 2769, 4249		
335.	66288-41-3	Heneicosenoic acid, 20-methyl-	2769, 3226, 4249		
336.	38282-01-8	Hentriacontanoic acid H_3C-$(CH_2)_{29}$-COOH	101, 3327a		
337.	7138-40-1	Heptacosanoic acid H_3C-$(CH_2)_{25}$-COOH	101, 5811b	3649, 4249	
338.	506-12-7	Heptadecanoic acid H_3C-$(CH_2)_{15}$-COOH	60, 101, 172, 259, 809, 1348, 1364, 1365, 1586, 2418, 2570, 2767, 3293, 3308, 3557, 4030, 4249, 4280, 4570a, 5811b	60, 259, 2092, 2356, 2389, 2544, 2593, 2917a, 3974a, 4131, 4249, 5811b	
339.	29709-08-8	Heptadecanoic acid, 15-methyl- H_3C-CH_2-CH(CH_3)-$(CH_2)_{13}$-COOH	36, 1586, 2769, 4249	3557, 3974a	
340.	2724-58-5	Heptadecanoic acid, 16-methyl- $(H_3C)_2$═CH-$(CH_2)_{14}$-COOH	809, 2767, 2873, 3293, 3557, 4249, 5811b	3557, 3973, 3974a, 4249	
341.	26265-99-6	Heptadecenoic acid H-$(CH_2)_{14-n}$-CH═CH-$(CH_2)_n$-COOH	60, 259, 1586, 2767, 3557, 4249	60, 259, 2092, 2917a, 4249, 5811b	
342.	72693-11-9	2,5-Heptadienoic acid, 2,3-dimethyl-		1375, 4249	
343.	54557-55-0	4,6-Heptadienoic acid, 6-methyl-3-(1-methylethyl)-, (*E*)-		568b, 732, 943, 1156, 3547, 4090, 4249	
344.	111-16-0	Heptanedioic acid {pimelic acid} HOOC-$(CH_2)_5$-COOH	1063–1066, 1068–1074, 2572, 2584, 3741, 3743, 4249	731, 738, 4249	
345.	535-24-0	Heptanedioic acid, 2,6-diamino-3-hydroxy- HOOC-CH(NH_2)-$(CH_2)_2$-CHOH-CH(NH_2)-COOH		4249, 4602	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
346.	111-14-8	Heptanoic acid {enanthic acid} $H_3C\text{-}(CH_2)_5\text{-}COOH$	172, 526, 563, 565, 568b, 1132, 1360, 1364, 1365, 1371, 1375a, 1917, 2079, 2271, 2543, 2545, 2761, 2762, 2765, 2766, 2777, 2939, 3263, 3266, 3302, 3308, 3555, 3797, 3799, 3800, 4249, 4319, 4993, 5079, 5811b	172a, 174b, 568b, 848, 1053, 1085, 1590a, 1982, 1999, 2014, 2094, 2271, 2338, 2339a, 2356, 2389, 2544, 2570, 2722, 2917a, 3266, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3767a, 3797, 3973, 3974a, 3974b, 4131, 4249, 4993, 5811b, 5846	1360, 1375a, 3393
347.	97259-93-3	Heptanoic acid, dimethyl-		5811, 5811b	
348.	3274-29-1	Heptanoic acid, 2-ethyl-		3545	
349.	1188-02-9	Heptanoic acid, 2-methyl-		1053, 3266	
350.	59262-53-2	Heptanoic acid, 3-(1-methylethyl)-6-oxo-, (S)-		731, 738, 1156, 3858, 4090, 4249	
351.	1070-68-4	Heptanoic acid, 5-methyl-		3266	
352.	42330-36-9	Heptanoic acid, 5-methyl-, (S)-		4092, 4249	
353.	929-10-2	Heptanoic acid, 6-methyl-		4249	
354.	3128-07-2	Heptanoic acid, 6-oxo-	3410, 3553, 4249		
355.	34098-52-7	*D*-xylo-Hept-2-enaric acid, 2,6-anhydro-3-deoxy-{2*H*-pyran-2,4-dicarboxylic acid, 3,4-dihydro-3,4-dihydroxy-}		4249	
356.	25377-46-2	Heptenoic acid	2092, 4249	738, 4249	
357.	18999-28-5	2-Heptenoic acid $H_3C\text{-}(CH_2)_3\text{-}CH{=}CH\text{-}COOH$	2092, 4249	848, 937, 2092, 3547, 4249, 5811b	3393
358.	10352-88-2	2-Heptenoic acid, (*E*)-		5811, 5811b	
359.	499-84-3	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo- $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}C[CH(CH_3)_2]{=}CH\text{-}COOH$		731, 736, 738, 930, 936, 1156, 1256a, 2092, 4090, 4249	
360.	41654-06-2	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)-		736, 1156, 2092, 4090, 4249, 5811b	
361.	63892-03-5	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*Z*)-		736, 1156, 2092, 4090, 4249	
362.	35194-37-7	4-Heptenoic acid $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}(CH_2)_2\text{-}COOH$	2092, 4249	2092, 4249	
363.	41653-95-6	4-Heptenoic acid, (*Z*)-		2092, 5811b	
364.	105728-84-5	4-Heptenoic acid, 6-hydroxy-		2917a	
365.	41654-07-3	4-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)- $H_3C\text{-}CO\text{-}CH{=}CH\text{-}CH[CH(CH_3)_2]\text{-}CH_2\text{-}COOH$	2092	731, 736, 1156, 2092, 4090, 4249, 5811b	
366.	1119-60-4	6-Heptenoic acid $H_2C{=}CH\text{-}(CH_2)_4\text{-}COOH$		848, 4249	
367.		6-Heptenoic acid, 5-methyl- $H_2C{=}CH\text{-}CH(CH_3)\text{-}(CH_2)_3\text{-}COOH$		3547, 4249	
368.	506-46-7	Hexacosanoic acid {cerotinic acid} $H_3C\text{-}(CH_2)_{24}\text{-}COOH$	101, 644, 765, 1785, 1971, 2939, 3302, 3308, 5811b	327, 613, 675, 1785, 4249, 4280	
369.		Hexacosanoic acid, 24-methyl-	4249, 4719, 4964		
370.	25377-52-0	Hexadecadienoic acid {palmitolenic acid}	1586	2092, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
371.	505-54-4	Hexadecanedioic acid		101	
372.	57-10-3	Hexadecanoic acid {palmitic acid} $H_3C\text{-}(CH_2)_{14}\text{-}COOH$	60, 101, 172, 239, 257, 258, 568b, 722, 723, 765, 809, 966, 1132, 1063–1066, 1068–1074, 1231, 1329, 1330, 1332, 1333, 1348, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1377, 1388–1390, 1437, 1448, 1449, 1582, 1586, 1651, 1744, 1785, 1944, 2387, 2418, 2529, 2543, 2545, 2570, 2601a, 2683, 2761, 2762, 2766, 2767, 2773, 2775, 2777, 2799a, 2857, 2939, 3265, 3266, 3293, 3302, 3308, 3384, 3410, 3447, 3454, 3457, 3496, 3553, 3555, 3557, 3608, 3876, 4005–4007, 4030, 4249, 4280, 4319, 4354, 4570a, 5512, 5552, 5811b	60, 101, 120, 172a, 174b, 404, 568b, 634, 637, 722, 835, 836, 838, 891, 908, 1053, 1329, 1330, 1332, 1333, 1388–1390, 1590a, 1651, 1785, 1848, 1893a, 1893b, 1982, 2079, 2270, 2283, 2338, 2339a, 2356, 2386, 2389, 2529, 2544, 2570, 2593, 2862, 2917a, 2939, 3155, 3194, 3219, 3266, 3328, 3329, 3332, 3349, 3430, 3511, 3543, 3545, 3547, 3549, 3550, 3555, 3560, 3561, 3608, 3755, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 5079, 5189, 5367, 5380, 5388, 5695, 5811b	1330, (0) 1332 (0), 1375a, 1377, 2387
373.	3233-90-7	Hexadecanoic acid, 10,16-dihydroxy-		3973, 3974a, 4249, 4822	
374.	506-13-8	Hexadecanoic acid, 16-hydroxy- $HOCH_2\text{-}(CH_2)_{14}\text{-}COOH$		2326a, 4249, 4774	
375.	28801-93-6	Hexadecanoic acid, methyl-	1371, 2543, 2731, 2735, 3410	908, 3547, 3550, 4098s	
376.	27147-71-3	Hexadecanoic acid, 2-methyl- $H_3C\text{-}(CH_2)_{13}\text{-}CH(CH_3)\text{-}COOH$		2092, 5811b	
377.	42172-35-0	Hexadecanoic acid, 3-methyl- $H_3C\text{-}(CH_2)_{12}\text{-}CH(CH_3)\text{-}CH_2\text{-}COOH$		4249	
378.	5918-29-6	Hexadecanoic acid, 14-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{12}\text{-}COOH$	60, 809, 2767, 3293, 3308, 3557, 4249	60, 2092, 2389, 2544, 3973, 3974a, 4249, 4964	
379.	1603-03-8	Hexadecanoic acid, 15-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{13}\text{-}COOH$	60, 2570, 2767, 3308, 3557, 4249	60, 2092, 2389, 2544, 3973, 3974a, 4249	
380.	25377-56-4	Hexadecatrienoic acid	3226, 4249	101, 5811b	
381.	32839-24-0	Hexadecatrienoic acid, (*Z,Z,Z*)-		4249, 4570, 5811b	
382.	25447-95-4	Hexadecenoic acid	60, 259, 809, 3293, 3308, 4280	60, 101, 259, 5811b	
383.	28039-99-8	Hexadecenoic acid, (*Z*)-		2339a, 4249, 4570, 5811b	
384.	1686-10-8	3-Hexadecenoic acid, (*E*)-		568c, 4249, 4570, 5811b	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
385.	373-49-9	9-Hexadecenoic acid, (*Z*)- {palmitoleic acid $H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_5\text{-}COOH$	60, 257, 258, 765, 1586, 1785, 1944, 2767, 2939, 3122, 3557, 4115, 4249, 4280, 5811b	80, 1785, 2092, 2339a, 4249, 4280, 5811b	
386.	10030-73-6 2091-29-4	9-Hexadecenoic acid, (*E*)- {palmitelaidic acid} $H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_5\text{-}COOH$	1944, 3122, 4115, 4249	2339a, 2917a	
387.	110-44-1 22500-92-1	2,4-Hexadienoic acid, (*E,E*)- {sorbic acid} $H_3C\text{-}(CH{=}CH)_2\text{-}COOH$	1371, 1886, 2543, 2773, 2873, 3308, 4249, 5811b	454, 742, 1547, 2092, 3266, 3547, 3767a, 4249, 5018, 5811b	3393
388.	90-65-3	2,5-Hexadienoic acid, 3-methoxy-5-methyl-4-oxo-	3760, 4249	3760, 4249, 5811b	
389.	124-04-9	Hexanedioic acid {adipic acid}	1063–1066, 1068–1074, 1360, 1375a, 1377, 1971, 2939, 3061, 3302, 3308, 3496, 3741, 3743, 4249, 5811b	731, 4249	1360, 1375a, 1377, 3393
390.	542-32-5	Hexanedioic acid, 2-amino-		2337, 2597a, 3491, 3797, 3974a, 4224, 4226	
391.	3184-35-8	Hexanedioic acid, 2-oxo-	3302, 4249	1312	
392.	142-62-1	Hexanoic acid {caproic acid} $H_3C\text{-}(CH_2)_4\text{-}COOH$	172, 526, 563, 565, 568b, 960, 1132, 1140, 1232, 1360, 1364, 1365, 1371, 1375a, 1586, 1587a, 1668, 1903, 1917, 2079, 2088, 2170, 2271, 2338, 2543, 2545, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3263, 3266, 3308, 3410, 3555, 3557, 3797, 3799, 3800, 3809, 4064, 4065, 4249, 4319, 4993, 5079, 5811, 5811b	120, 172a, 174b, 404, 563, 568b, 848, 908, 1053, 1085, 1587a, 1590a, 1982, 1999, 2014, 2079, 2271, 2283, 2338, 2356, 2386, 2389, 2544, 2570, 2611, 2722, 2862a, 2917a, 2939, 3219, 3266, 3329, 3370, 3507, 3545, 3547, 3549, 3555, 3560, 3561, 3633, 3767a, 3797, 3973, 3974b, 4131, 4249, 4993, 5695, 5708, 5811, 5811b, 5846	1360, 1375a, 3393
393.	60308-81-8	Hexanoic acid, 4,5-dimethyl-		3547, 4249, 4993	
394.		Hexanoic acid, 2,6-di-(methylnitrosamino)- $R\text{-}(CH_2)_4\text{-}CH(R)\text{-}COOH$ where $R = CH_3N(NO)\text{-}$	1008, 1009, 1012, 3256, 3300	1008, 1009	
395.	149-57-5	Hexanoic acid, 2-ethyl-	270, 568b, 2543, 2773, 4249, 5811b	568b, 2389, 2544, 2917a, 3560, 3561, 4249	
396.		Hexanoic acid, hydroxy-	3741, 3743		
397.	6064-63-7	Hexanoic acid, 2-hydroxy-		4101, 4249	
398.	1191-25-9	Hexanoic acid, 6-hydroxy-	4249, 4897, 5811b		
399.	40309-49-7	Hexanoic acid, 3-hydroxy-5-methyl-		4101, 4249	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
400.	4536-23-6	Hexanoic acid, 2-methyl-{2-methylhexanoic acid}	568b, 1132, 1884, 3266, 3302, 3553, 3557, 3797, 4249	568b, 1053, 2337a, 2389, 2544, 3266, 3370, 4249, 5811b	
401.	3780-58-3	Hexanoic acid, 3-methyl-		4092, 4249, 5811b	
402.	1561-11-1	Hexanoic acid, 4-methyl-	5811b	731, 738, 937, 1248, 2917a, 4249, 5811b	
403.	6818-07-1	Hexanoic acid, 4-methyl-5-oxo-	568b, 4249		
404.	628-46-6	Hexanoic acid, 5-methyl-		568b, 2092, 2917a, 3547, 4249, 5811b	
405.	41654-04-0	Hexanoic acid, 5-methyl-4-oxo-	2092, 4249	2092, 4249, 5811b	
406.	2543-54-6	Hexanoic acid, 2-(1-methylethyl)-5-oxo-		9, 936, 940, 1156, 1257, 2092, 2389, 2544, 3767a, 4090, 4249, 5811b	
407.	16825-90-4	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, (S)-	568b, 3559, 4249	5811b	
408.	1117-74-4	Hexanoic acid, 4-oxo-	568b, 3553, 4249, 5811b	568b, 1980, 4249	
409.	3128-06-1	Hexanoic acid, 5-oxo-	568b, 3553, 4249, 5811b		
410.	1289-40-3	Hexenoic acid	2092, 4249	2092	
411.	1191-04-4	2-Hexenoic acid $H_3C\text{-}(CH_2)_2\text{-}CH{=}CH\text{-}COOH$	5811b	848, 2092, 3266, 3547, 424	3393
412.	13419-69-7	2-Hexenoic acid, (*E*)-		172a, 174b, 1053, 3266, 3370, 5811, 5811b	
413.	5309-52-4	2-Hexenoic acid, 2-ethyl-		1871, 3219, 4249	
414.	41653-96-7	2-Hexenoic acid, 5-methyl- $(H_3C)_2{=}CH\text{-}CH_2\text{-}CH{=}CH\text{-}COOH$		2092, 2389, 2544, 3547, 3767a, 4249, 5811b	
415.	51424-01-2	2-Hexenoic acid, 5-methyl-, (*E*)-		568b, 937, 4249, 5811b	
416.	4219-24-3	3-Hexenoic acid {hydrosorbic acid} $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}CH_2\text{-}COOH$	60, 1586, 2663, 2767, 3266, 3557, 4249	172a, 174b, 1053, 2092, 3186, 3188, 3266, 3547, 4249	
417.	1775-43-5	3-Hexenoic acid, (*Z*)-		172a, 174b, 1053, 3266, 5811b	
418.	35194-36-6	4-Hexenoic acid $H_3C\text{-}CH{=}CH\text{-}(CH_2)_2\text{-}COOH$	60, 1586, 2767, 3557	2092, 5811b	
419.	1577-20-4	4-Hexenoic acid, (*E*)-	1586, 2767, 3557, 4249	2092, 3557, 4249	
420.	5636-65-7	4-Hexenoic acid, 5-methyl-		3547	
421.	1577-22-6	5-Hexenoic acid		948, 4092, 4249	
422.	62446-36-0	Hexuronic acid		120, 2153a, 3665a, 4249, 4793	
423.	7006-35-1	Histidine		429b, 3797, 4249, 5699, 5785, 5831,	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

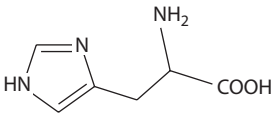
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
424.	71-00-1	*L*-Histidine 		120, 158, 553, 622, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5478, 5699, 5785, 5831	
425.	332-80-9	*L*-Histidine, 1-methyl-	1083	1086, 1351, 2337, 2597a, 3491, 3797, 3974a, 3972, 4249	
426.	368-16-1	*L*-Histidine, 3-methyl-	1083	1086, 2597a	
427.	62504-27-2	*L*-Histidine, *N*-(1-carboxyethyl)-, (R)-		3565, 4249	
428.	454-29-5	*DL*-Homocysteine HS-$(CH_2)_2$-CH(NH_2)-COOH		172	
429.	498-19-1 672-15-1	Homoserine {2-amino-4-hydroxybutanoic acid} HO-$(CH_2)_2$-CH(NH_2)-COOH	3557	1351, 2337, 2939, 3491, 3797, 3974a	
430.	1415-93-6	Humic acids		2665a	
431.	120293-52-9	1*H*-Imidazo[4,5-*c*]pyridine-4-propanoic acid, 4,6-dicarboxy-4,5,6,7-tetrahydro-, (4R-*cis*)-		4249	
432.	32536-43-9	1*H*-Indoleacetic acid		120, 2058b, 2409a, 2722, 2939, 3797, 3973, 3974a, 4249, 5743, 5854	
433.	87-51-4	1*H*-Indole-3-acetic acid	5811b	2058b, 3973, 4249, 5743, 5811b, 5854	
434.	133-32-4	1*H*-Indole-3-butanoic acid		3580a, 4249, 4487	
435.	771-50-6	1*H*-Indole-3-carboxylic acid		1948, 4249	
436.	830-96-6	1*H*-Indole-3-propanoic acid		429b, 4249, 4457	
437.	35656-49-6	1*H*-Indolepropanoic acid, α-oxo-		4249	
438.	392-12-1	1*H*-Indole-3-propanoic acid, α-oxo-		429b, 4249, 4943	
439.	7004-09-3	Isoleucine		3555, 3705, 3797, 3973, 4249, 4398c, 5079, 5413, 5699, 5785, 5827, 5831, 5905	
440.	1509-34-8	Isoleucine, allo-		3974b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
441.	73-32-5	*L*-Isoleucine H_3C-CH_2-CH(CH_3)-CH(NH_2)-COOH		120, 158, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 5811b	
442.	139681-66-6	*L*-Isoleucine,*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-valyl)-*L*-phenylalanyl]-*L*-leucyl]-		4249	
443.	27836-87-9	Isopentadecanoic acid		2028, 4249	
444.	7005-03-0	Leucine $(H_3C)_2$═CH-CH_2-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5699, 5785, 5827, 5831, 5881, 5905	
445.	61-90-5	*L*-Leucine	5811b	424a, 2338, 3973, 5811b	
446.	139681-65-5	*L*-Leucine,*N*-[*N*-[*N*-[*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-phenylalanyl)-*L*-seryl]-*L*-leucyl]-*L*-leucyl]-*L*-methionyl]-*L*-valyl]-*L*-valyl]-		4249	
447.	6899-06-5	Lysine		429b, 2911c, 3973, 4398c, 5079, 5623, 5785, 17B59	
448.	1190-94-9 28902-93-4	Lysine, hydroxy-		726, 749, 752–754, 4249	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
449.	56-87-1	*L*-Lysine H_2N-$(CH_2)_4$-CH(NH_2)-COOH		120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 5811b	
450.	7005-18-7	Methionine		116, 120, 3705, 4249, 5907	
451.	63-68-3	*L*-Methionine H_3C-S-$(CH_2)_2$-CH(NH_2)-COOH		116, 120, 158, 172, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1127b, 1305a, 1329, 1330, 1332, 1351, 1493, 2049, 2270, 2337, 2359, 2532, 2597a, 2795, 2939, 3186, 3188, 3266, 3491, 3499, 3705, 3729, 3797, 3973, 3974a, 3978, 4226, 4249, 4398c, 5079, 5376, 5811b, 5907	
452.	20236-97-9	*D*-Methionine, *N*-(carboxyacetyl)-		4249, 4699	
453.	86-87-3	1-Naphthaleneacetic acid		3973	
454.	31519-22-9	2-Naphthalenecarboxylic acid, 1,4-dihydroxy-		3748, 3749, 3751	
455.	1338-24-5	Naphthenic acid		4249, 4517	
456.	4250-38-8	Nonacosanoic acid H_3C-$(CH_2)_{27}$-COOH	101, 5811b	3649, 4249	
457.	646-30-0	Nonadecanoic acid H_3C-$(CH_2)_{17}$-COOH	60, 172, 2570, 2767, 3308, 3557, 4030, 4249, 4280, 5811b	60, 2389, 2544, 2593, 3974a, 4249, 5811b	
458.	53254-53-8	Nonadecanoic acid, 17-methyl- H_3C-CH_2-CH(CH_3)-$(CH_2)_{15}$-COOH	1586, 2767, 2769, 3557, 4249	3974a	
459.	6250-72-2	Nonadecanoic acid, 18-methyl- $(H_3C)_2$═CH-$(CH_2)_{16}$-COOH	2570, 2769, 4249, 4964	3974a, 4249, 5811b	
460.	51109-34-3	Nonadienoic acid		2092, 4249, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
461.		2,4-Nonadienoic acid, 2,3-dimethyl-		3547, 4249	
462.	60026-10-0	2,6-Nonadienoic acid	5811b	2389, 2544, 3547, 3767a, 4249, 4573, 5811b	
463.	23605-13-2	2,6-Nonadienoic acid, (*E,Z*)-		568b, 2389, 2544, 4249, 5811b	
464.	70898-29-2	2,7-Nonadienoic acid, (*E,Z*)-		731, 2389, 2544, 4249	
465.		4,6-Nonadienoic acid		3543	
466.	123-99-9	Nonanedioic acid {azelaic acid}	1364, 1371, 3741, 3743, 5811b	120, 1620, 2270, 2283, 2722, 3219, 3329, 3532, 3557, 3560, 3561, 3974a, 5811b	
467.	112-05-0	Nonanoic acid {pelargonic acid} $H_3C\text{-}(CH_2)_7\text{-}COOH$	172, 563, 565, 568b, 809, 1132, 1348, 1364, 1371, 1886, 1917, 1999, 2079, 2545, 2939, 3266, 3293, 3302, 3555, 3797, 4249, 4993, 5079, 5811b	172a, 174b, 404, 568b, 848, 908, 1053, 1590a, 1999, 2014, 2338, 2339a, 2356, 2389, 2544, 2722, 2917a, 3219, 3266, 3370, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3767a, 3974b, 3973, 3974a, 4131, 4249, 4993, 5811b	
468.	41653-89-8	Nonanoic acid, 7-methyl-		2092, 4249, 5811b	
469.	6064-52-4	Nonanoic acid, 4-oxo-		568b, 908, 2092, 2389, 2544, 3219, 3331, 3767a, 4249, 5811b	
470.	3760-11-0	2-Nonenoic acid	5811b	731, 3545, 3560, 3561, 3767a, 4249	
471.	14812-03-4	2-Nonenoic acid, (*E*)-		938, 1084, 4249, 5811b	
472.	4124-88-3	3-Nonenoic acid		2917a, 3767a	
473.	41653-98-9	3-Nonenoic acid, (*Z*)-		908, 1084, 2092, 3219, 4249, 5811b	
474.	41653-99-0	6-Nonenoic acid, (*Z*)-		2092, 4249, 5811b	
475.	31642-67-8	8-Nonenoic acid		404, 4249, 4573	
476.	327-57-1 5157-09-5	Norleucine {2-aminohexanoic acid} $H_3C\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		1351, 2337, 2597a, 3491, 3797, 3974a, 3978, 4249	
477.	506-48-9	Octacosanoic acid $H_3C\text{-}(CH_2)_{26}\text{-}COOH$	101, 5811b	3649, 4249	
478.	26764-25-0	Octadecadienoic acid	4115, 4249	5811b	
479.	28984-77-2	Octadecadienoic acid, (*Z,Z*)-		4249, 5811b	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
480.	60-33-3	9,12-Octadecadienoic acid, (*Z,Z*)- {linoleic acid}	60, 1785, 2601a, 3122, 4249, 4280, 5811b	60, 1785, 2338, 2917a, 3747, 4249, 4280, 5811b	
481.	506-21-8	9,12-Octadecadienoic acid, (*E,E*)- {linoleic acid} H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COOH	60, 101, 257, 258, 723, 765, 966, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1448, 1582, 1586, 1651, 1744, 1842, 1944, 2529, 2543, 2570, 2683, 2767, 2777, 2939, 3122, 3266, 3302, 3308, 3384, 3454, 3457, 3557, 3608, 3876, 4005–4007, 4115, 4249, 4280, 4570a, 5512, 5552	60, 101, 120, 634, 722, 836, 838, 891, 908, 966, 981a, 1053, 1329, 1330, 1332, 1333, 1651, 1731, 1893a, 1893b, 1982, 2079, 2270, 2283, 2338, 2389, 2529, 2544, 2570, 2593, 2939, 3155, 3219, 3266, 3329, 3435, 3461, 3543, 3549, 3608, 3755, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 5079, 5189, 5367, 5388	1330, 1332, 1360, 1375a
482.	4546-59-2	9,12-Octadecadienoic acid, 18-hydroxy-, (*Z,Z*)-		4249, 4774, 5811b	
483.	57-11-4	Octadecanoic acid {stearic acid} H_3C-$(CH_2)_{16}$-COOH	60, 101, 172, 257, 258, 722, 765, 809, 966, 1063–1066, 1068–1074, 1132, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1388–1390, 1448, 1582, 1586, 1651, 1744, 1785, 1842, 1944, 2418, 2529, 2570, 2601a, 2683, 2767, 2777, 2939, 3265, 3293, 3302, 3308, 3384, 3447, 3457, 3557, 3608, 3876, 4005–4007, 4030, 4249, 4280, 4319, 5512, 5552, 5811b	60, 101, 120, 404, 634, 835, 836, 838, 908, 1329, 1330, 1332, 1333, 1388–1390, 1472, 1651, 1785, 2092, 2270, 2283, 2338, 2339a, 2356, 2389, 2529, 2544, 2570, 2593, 2649, 2917a, 2939, 3155, 3219, 3329, 3332, 3349, 3461, 3511, 3545, 3547, 3560, 3561, 3608, 3755, 3812, 3876, 3974a, 4131, 4042c, 4249, 4280, 5079, 5189, 5367, 5811b	1330, 1332, 1360, 1375a
484.	1330-70-7	Octadecanoic acid, hydroxy-		2283, 3974a, 4249	
485.	3155-42-8	Octadecanoic acid, 18-hydroxy- $HOCH_2$-$(CH_2)_{16}$-COOH		3974a, 4249, 4774	
486.	17001-28-4	Octadecanoic acid, 16-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{14}$-COOH	2570, 2769	3973, 3974a, 4249, 4964, 5811b	
487.	2724-59-6	Octadecanoic acid, 17-methyl- $(H_3C)_2$═CH-$(CH_2)_{15}$-COOH		3973, 3974a, 4249, 4719	
488.	51592-59-7	3,6,9,12,15-Octadecapentaenoic acid, (all-*Z*)-		613, 4249	
489.	25448-06-0	Octadecatetraenoic acid		603, 3093a, 4249	
490.	25448-03-7	Octadecatrienoic acid		4249, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

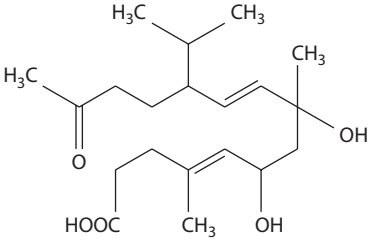
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
491.	27213-43-0	Octadecatrienoic acid, (*Z,Z,Z*)-		339a, 5811b	
492.	13296-76-9	9,11,13-Octadecatrienoic acid	2092, 4249		
493.	463-40-1	9,12,15-Octadecatrienoic acid, (*Z,Z,Z*)- {linolenic acid} $H_3C\text{-}(CH_2CH{=}CH)_3\text{-}(CH_2)_7\text{-}COOH$	101, 257, 258, 723, 765, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1448, 1582, 1586, 1651, 1744, 1785, 1842, 2529, 2543, 2570, 2601a, 2683, 2767, 2799a, 2939, 3204, 3122, 3266, 3302, 3308, 3384, 3454, 3457, 3557, 3608, 3797, 4005–4007, 4031, 4249, 4280, 4570a, 5079, 5512, 5811b	101, 120, 404, 634, 835, 836, 838, 891, 908, 1053, 1329, 1330, 1332, 1333, 1651, 1785, 2092, 2270, 2283, 2338, 2389, 2529, 2544, 2570, 2593, 2917a, 2939, 3266, 3329, 3435, 3461, 3608, 3755, 3797, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 4774, 5079, 5380, 5695, 5811b	1330, 1332, 1360, 1375a
494.	51327-73-2	9,12,15-Octadecatrienoic acid, 18-hydroxy-, (*Z,Z,Z*)- $HOCH_2\text{-}(CH_2CH{=}CH)_3\text{-}(CH_2)_7\text{-}COOH$		4249, 4774	
495.	26764-26-1	Octadecenoic acid {oleic acid}	60, 101, 257, 258, 723, 765, 966, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1448, 1582, 1586, 1651, 1744, 1785, 1842, 2529, 2543, 2570, 2683, 2767, 2939, 2773, 2777, 3122, 3266, 3302, 3308, 3384, 3454, 3457, 3557, 3608, 3876, 4030, 4280, 4354, 4570a, 5512, 5552	60, 101, 120, 297, 634, 722, 835, 836, 838, 891, 981a, 1053, 1329, 1330, 1332, 1333, 1651, 1785, 1893b, 2079, 2270, 2283, 2338, 2339a, 2389, 2529, 2544, 2552, 2570, 2593, 2649, 2917a, 2939, 3155, 3266, 3435, 3461, 3543, 3545, 3608, 3755, 3812, 3973, 3974a, 4131, 4249, 4280, 5811b	1330, 1332, 1360, 1375a
496.	112-79-8	Octadecenoic acid, (*E*)- {elaidic acid}	3122	2917a	
497.	27104-13-8	Octadecenoic acid, (*Z*)-		2339a, 4249, 4570, 5811b	
498.	112-80-1	9-Octadecenoic acid (*Z*)- {oleic acid} $H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}COOH$	60, 257, 258, 568b, 765, 966, 1329, 1330, 1332, 1333, 1360, 1373, 1375, 1375a, 1375b, 1744, 1785, 1944, 2601a, 2683, 2939, 3302, 3384, 3555, 3557, 3876, 4005–4007, 4030, 4249, 4280, 4354, 4570a, 5079, 5512, 5811b	60, 297, 568b, 634, 908, 1329, 1330, 1332, 1333, 1785, 2356, 2389, 2544, 2552, 3555, 4042c, 4249, 4280, 5079, 5189, 5367, 5388, 5695	1360, 1375a
499.	24753-52-4	9-Octadecenoic acid, 18-hydroxy-, (*Z*)-		4249, 4774, 5811b	
500.	459-80-3	2,6-Octadienoic acid, 3,7-dimethyl- {geranic acid}		1156, 2092, 2389, 2544, 2611, 3547, 3767a, 4090, 4249, 5811b	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
501.	4698-08-2	2,6-Octadienoic acid, 3,7-dimethyl-, (*E*)-		2092, 3547, 4101, 4249, 5811b	
502.	4613-38-1	2,6-Octadienoic acid, 3,7-dimethyl-, (*Z*)-		3547, 4101, 4249	
503.	64090-50-2	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-		404, 732, 1156, 3547, 4090, 4249	
504.	54557-54-9	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-, (*E*)-		404, 651	
505.	505-48-6	Octanedioic acid {suberic acid}	2572, 3741, 3743, 4249, 5811b	4249, 4677	
506.	124-07-2	Octanoic acid {caprylic acid} $H_3C\text{-}(CH_2)_6\text{-}COOH$	172, 563, 565, 568b, 722, 809, 1132, 1232, 1348, 1364, 1371, 1587a, 1668, 1917, 1971, 2079, 2338, 2543, 2545, 2765, 2773, 2775, 2939, 3266, 3293, 3302, 3308, 3410, 3555, 3797, 4064, 4065, 4249, 4319, 4993, 5079, 5811b	120, 172a, 174b, 404, 568b, 848, 908, 1053, 1085, 1221, 1587a, 1590a, 1893a, 1893b, 1982, 1999, 2014, 2079, 2270, 2283, 2338, 2356, 2389, 2544, 2570, 2611, 2649, 2722, 2917a, 3219, 3266, 3370, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3633, 3767a, 3797, 3973, 3974a, 3974b, 4131, 4249, 4993, 5079, 5180, 5363, 5695, 5811b, 5846	
507.	14352-59-1	Octanoic acid, 3,3-dimethyl-		4092, 4249	
508.	16493-80-4	Octanoic acid, 4-ethyl-		4249	
509.	3004-93-1	Octanoic acid, 2-methyl-		2092, 2917a, 4249, 5811b	
510.	6061-10-5	Octanoic acid, 3-methyl-		5811, 5811b	
511.	504-99-4	Octanoic acid, 6-methyl-		5811, 5811b	
512.	693-19-6	Octanoic acid, 7-methyl-		4093, 4249, 5811b	
513.	96937-51-8	Octanoic acid, oxo-	3741, 3743, 4249, 4897, 5811b		
514.	28962-27-8	Octenoic acid	2092, 4249		
515.	1470-50-4	2-Octenoic acid		2389, 2544, 3547, 4249, 5811b	
516.		2-Octenoic acid, 4-(1-methylethyl)-7-oxo-		731, 738, 1156, 4090, 4249	
517.	41654-08-4	4-Octenoic acid, 6-ethyl-3-hydroxy-3,7-dimethyl-		4249, 5811b	
518.		4-Octenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-		1156, 2092, 3547, 4090, 4249	
519.	63892-00-2	5-Octenoic acid		2092, 4249	
520.	41653-97-8	5-Octenoic acid, (*Z*)-		2092, 4249, 5811b	
521.	502-47-6	6-Octenoic acid, 3,7-dimethyl-		172a, 174b, 1053, 3266, 3370	
522.	18719-24-9	7-Octenoic acid		404, 2092, 5811b	
523.	508-02-1	Olean-12-en-28-oic acid, 3-hydroxy-, (3β)-		4249	
524.	471-53-4	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-	3390, 4249		

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
525.	7006-33-9	Ornithine {2,3-diaminopentanoic acid} $H_2N\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 2858, 2939, 3302, 3491, 3797, 4249	555a, 622, 749, 752–754, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 2597a, 2795, 3491, 3705, 3797, 3973, 3974a, 3978, 4249, 5827, 17B34	
526.	70-26-8	*L*-Ornithine	429b	429b, 5811b	
527.	20197-09-5	*L*-Ornithine, *N*2-(1-carboxyethyl)-, (R)-		3565, 4249	
528.	372-75-8	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline} $H_2N\text{-}CO\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		120, 622, 1305a, 1329, 1330, 1332, 1351, 2337, 2939, 3491, 3797, 3973, 3974a, 3978, 4249, 4398c, 5079	
529.	9046-40-6	Pectic acid	—	120, 925, 2270, 2947c, 3492, 3973, 4249, 5079, 5114, 5189, 5306, 5419	
530.		Pectic acid, labeled with ^{14}C {pectic acid-^{14}C}		2764	
531.	9047-18-1	Pectinic acid		120, 344a, 925, 1263, 2270, 2337, 2338, 3702, 3973, 3974b, 5079	
532.	506-38-7	Pentacosanoic acid $H_3C\text{-}(CH_2)_{23}\text{-}COOH$	101, 990, 1785, 4249, 5811b	996, 1785, 2286, 4249, 4280	
533.		Pentacosanoic acid, 23-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{21}\text{-}COOH$		3973, 3974a, 4249, 4719	
534.		Pentacosanoic acid, 24-methyl		4249, 4719, 4964	
535.	102734-47-4	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4, 8-dimethyl-11-(1-methylethyl)-14-oxo-		5811b	
536.	70898-33-8 102734-49-6	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-{isomer} 	2722	943, 2098, 2722, 4089, 4249, 5811, 5811b	
537.	1460-18-0	Pentadecanedioic acid $HOOC\text{-}(CH_2)_{13}\text{-}COOH$	2584, 4249		

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

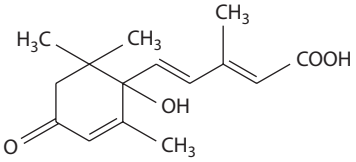
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
538.	1002-84-2	Pentadecanoic acid H_3C-$(CH_2)_{13}$-COOH	60, 101, 172, 259, 809, 1348, 1360, 1364, 1375a, 1586, 1646, 2418, 2570, 2761, 2762, 2765–2767, 2777, 2939, 3293, 3302, 3308, 3557, 4030, 4280, 5811b	60, 101, 259, 404, 1785, 2092, 2339a, 2356, 2389, 2544, 2917a, 3547, 3973, 3974a, 4280, 5811b	1360, 1375a
539.		Pentadecanoic acid, 13-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COOH	1586, 3557	3973, 3974a	
540.	4669-02-7	Pentadecanoic acid, 14-methyl- $(H_3C)_2$═CH-$(CH_2)_{12}$-COOH	1586, 2570, 2767, 4249	958, 3973, 3974a, 4249, 4964	
541.	26444-04-2	Pentadecenoic acid	60, 257–260, 1586, 2570, 2767, 3302, 3557, 4249	60, 259, 3984, 4249	
542.	17351-34-7	14-Pentadecenoic acid		404, 2917a	
543.	21293-29-8 14375-45-2	2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-, [S-(*Z,E*)]- {abscisic acid} 		1156, 1206a,, 2864a, 3216, 3218, 3973, 4090, 5811b	
544.	110-94-1	Pentanedioic acid {glutaric acid} HOOC-$(CH_2)_3$-COOH	1099, 1886, 3053, 3061, 3255, 3302, 3496, 3741, 3743, 4249, 5811b	738, 1310, 4249, 5811b	3393
545.	63892-02-4	Pentanedioic acid, 2-(1-methylethyl)-, (S)- HOOC-$(CH_2)_2$-$CH[CH(CH_3)_2]$-COOH		731, 738, 4249	
546.	617-62-9	Pentanedioic acid, 2-methyl- HOOC-$(CH_2)_2$-$CH(CH_3)$-COOH		1948, 4249	
547.	328-50-7	Pentanedioic acid, 2-oxo-{α-ketoglutaric acid} HOOC-$(CH_2)_2$-CO-COOH	1238, 1310, 2939, 3059, 3302, 4249	120, 1310, 1312, 2939, 3797, 3973, 3974a, 4249, 5651	
548.	626-51-7	Pentanedioic acid, 3-methyl- HOOC-CH_2-$CH(CH_3)$-CH_2-COOH	2601a, 3741, 3743, 5811b		
549.		Pentanedioic acid, 2,3,4-trihydroxy- HOOC-$(CHOH)_3$-COOH		1971, 4249	
550.	109-52-4	Pentanoic acid {valeric acid} H_3C-$(CH_2)_3$-COOH	526, 563, 565, 568b, 960, 1132, 1063–1066, 1068–1074, 1140, 1263, 1364, 1371, 1375, 1375b, 1586, 1587a, 1646, 1668, 1886, 1917, 2043, 2079, 2088, 2170, 2270, 2271, 2338, 2543, 2570, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2858, 2939, 3061, 3263, 3266, 3308, 3393, 3410, 3553, 3557, 3799, 3800, 3809, 4064, 4065, 4079, 4249, 4319, 4993, 5079, 5811b	120, 172a, 174b, 404, 568b, 848, 908, 981a, 1053, 1085, 1087, 1263, 1587a, 1590a, 1893b, 1982, 1999, 2014, 2092, 2270, 2271, 2283, 2338, 2389, 2544, 2570, 2611, 2917a, 2939, 3219, 3266, 3328, 3329, 3370, 3507, 3547, 3717, 3809, 3973, 3974a, 3974b, 4064, 4249, 4993, 5079, 5364, 5695, 5708, 5811b, 5846	3393

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

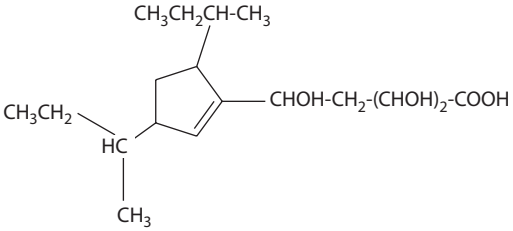
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
551.	96937-52-9	Pentanoic acid, hydroxy-methyl-	3741, 3743, 4249, 4897, 5811b		
552.	27936-41-0	Pentanoic acid, methyl-		908, 4249	
553.	96937-54-1	Pentanoic acid, methyl-oxo-	3741, 3743, 4249, 4897, 5811b		
554.	96937-53-0	Pentanoic acid, oxo-	3741, 3743, 4249, 4897, 5811b		
555.	6600-40-4	Pentanoic acid, 2-amino-		5777	
556.	1185-39-3	Pentanoic acid, 2,2-dimethyl-		2917a	
557.	20225-24-5	Pentanoic acid, 2-ethyl-		4092, 4249	
558.	617-31-2	Pentanoic acid, 2-hydroxy-		2337a, 2796, 3797, 3973, 3974a, 4249	
559.	488-15-3	Pentanoic acid, 2-hydroxy-3-methyl-		2092, 2796, 3973, 3974a, 4249, 5811b	
560.	498-36-2	Pentanoic acid, 2-hydroxy-4-methyl-		2337a, 2796, 3797, 3973, 3974a, 4249	
561.	54031-97-9	Pentanoic acid, 2-hydroxy-4-oxo-		4249, 4845	
562.	97-61-0	Pentanoic acid, 2-methyl- {2-methylvaleric acid}	565, 568b, 2761, 2858, 3266, 3393, 3405, 4249, 5811b	172a, 174b, 174b, 568b, 848, 1053, 3266, 3370, 3560, 3561, 3974b, 4249, 5811b	
563.	6641-83-4	Pentanoic acid, 2-methyl-4-oxo-	568b, 3553, 4249, 5811b		
564.		Pentanoic acid, 2,5-di-(methylnitrosoamino)- R-$(CH_2)_3$-CH(R)-COOH where R = CH_3-N(NO)-	1008, 1009, 1013, 3256, 3300	1008, 1009	
565.	150-96-9	Pentanoic acid, 3-hydroxy-3-methyl-		3797, 3973, 3974a, 4249	
566.	5980-21-2	Pentanoic acid, 3-hydroxy-4-methyl-		3797, 3973, 3974a, 4249	
567.	105-43-1	Pentanoic acid, 3-methyl- {β-methylvaleric acid; 3-methylpentanoic acid}	172, 526, 565, 568b, 775, 1063–1066, 1068–1074, 1099, 1132, 1140, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1587a, 1881, 1884, 1886, 1903, 1904, 1999, 2092, 2270, 2338, 2387, 2493, 2543, 2545, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2816, 2817, 2858, 2939, 3224, 3255, 3266, 3302, 3308, 3015, 3410, 3529, 3553, 3557, 3795, 3799, 3800, 3809, 3827, 4249, 4319, 5811b	51, 120, 172a, 174b, 404, 568b, 848, 908, 981a, 1053, 1087, 1587a, 1590a, 1982, 1999, 2014, 2270, 2283, 2288, 2291, 2338, 2339a, 2386, 2389, 2544, 2570, 2611, 2862a, 2863, 2917a, 2939, 3215, 3219, 3266, 3328, 3329, 3507, 3537, 3543, 3545, 3547, 3549, 3809, 3973, 3974a, 3974b, 4575, 4997, 5079, 5364, 5708, 5811b, 5846	1360, 1375a, 2387, 3393
568.	6628-79-1	Pentanoic acid, 3-methyl-4-oxo-	568b, 3553, 4249, 4897		
569.	10191-25-0	Pentanoic acid, 3-oxo-	3553, 4249	2389, 2544, 4249	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
570.	150-97-0	Pentanoic acid, 3,5-dihydroxy-5-methyl- {mevalonic acid}		3973	
571.	41654-03-9	Pentanoic acid, 4-hydroxy-3-methyl-		2092, 4249, 5811b	
572.	646-07-1	Pentanoic acid, 4-methyl- {isocaproic acid}	568b, 1132, 1364, 1371, 1879, 1881–1884, 2543, 2765, 3266, 3302, 3308, 3410, 3553, 3797, 3799, 3800, 3809, 4249, 5811b	404, 568b, 848, 1053, 1085, 1087, 2092, 2270, 2570, 2722, 2917a, 3266, 3547, 3809, 3973, 3974a, 4249, 5846	3393
573.	123-76-2	Pentanoic acid, 4-oxo- {levulinic acid} $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}COOH$	565, 568b, 741, 1099, 1103, 1237, 1238, 1360, 1375, 1375a, 1375b, 1586, 1882, 2088, 2570, 2761, 2762, 2765–2767, 2939, 3059, 3060, 3061, 3224, 3255, 3266, 3302, 3308, 3394, 3496, 3553, 3557, 4249, 4319, 4897, 5811b	307, 568b, 569, 570, 833, 1053, 1103, 1312, 3060, 3266, 4249, 5811b	1360, 1375a, 3393, 3402, 3404, 3405
574.	67920-51-8	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (±)-		2796, 4249, 4817a	
575.	63316-30-3	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (R)-		2796, 4249, 4817a, 5811b	
576.	63316-29-0	Pentanoic acid, 5-amino-2-hydroxy-, (R)-		5811, 5811b	
577.	16814-81-6	Pentanoic acid, 5-amino-2-hydroxy-, (S)-		2796, 4249	
578.	63316-28-9	Pentanoic acid, 5-amino-3-hydroxy-		2796, 4249	
579.	106-60-5	Pentanoic acid, 5-amino-4-oxo-		2024a, 4249, 4869	
580.		Pentanoic acid, 5-hydroxy-3-(1-methylethyl)-		2033	
581.	526-91-0 D 4172-43-4 4172-44-5 L 17828-56-7 DL	Pentanoic acid, 2,3,4,5-tetrahydroxy- $HOCH_2\text{-}(CHOH)_3\text{-}COOH$		926, 4249	
582.	488-31-3	Pentaric acid		4249	
583.	320-77-4	Pentaric acid, 3-carboxy-2,3-dideoxy-		4249	
584.	1724-02-3	2-Pentenedioic acid {glutaconic acid} $HOOC\text{-}CH_2\text{-}CH{=}CH\text{-}COOH$		2356, 4249	
585.	27516-53-6	Pentenoic acid	1646, 3226, 4249		
586.	626-98-2	2-Pentenoic acid $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}COOH$	1063–1066, 1068–1074, 1360, 1375a, 1886, 3553, 4249, 5811b	848, 2092, 3547, 4249	1360, 1375a, 3393
587.	3142-72-1	2-Pentenoic acid, 2-methyl- $H_3C\text{-}CH_2\text{-}CH{=}C(CH_3)\text{-}COOH$	568b, 1063–1066, 1068–1074, 4249	568b, 3547, 4249	
588.	3675-21-6	2-Pentenoic acid, 3-methyl- $H_3C\text{-}CH_2\text{-}C(CH_3){=}CH\text{-}COOH$		3547, 4249	
589.		2-Pentenoic acid, 3-methyl-5-(2,6,6-trimethyl-1-cyclohexenyl)-		2917a	
590.	10321-71-8	2-Pentenoic acid, 4-methyl- $H_3C\text{-}CH(CH_3)\text{-}CH{=}CH\text{-}COOH$		3547, 4249	
591.	1617-32-9	3-Pentenoic acid, (*E*)-	1063–1066, 1068–1074, 1365, 3553, 4249, 5811b		

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
592.	33698-87-2	3-Pentenoic acid, (*Z*)-	568b, 1365, 3553, 4249, 5811b		
593.	16313-37-4	3-Pentenoic acid, 3-methyl-		2092, 4249	
594.	41653-93-4	3-Pentenoic acid, 3-methyl-, (*E*)-		2092, 4249, 5811b	
595.	41653-94-5	3-Pentenoic acid, 3-methyl-, (*Z*)-		5811, 5811b	
596.	504-85-8	3-Pentenoic acid, 4-methyl-		2917a, 3547, 4249	
597.	591-80-0	4-Pentenoic acid	2761, 3266, 4249	848, 1053, 3266, 4092, 4093, 4249	
598.	16386-93-9	4-Pentenoic acid, 2,2-dimethyl-		3547, 4249	
599.	1575-74-2	4-Pentenoic acid, 2-methyl-		3547, 4249	
600.	491-14-5	Pentonicacid, 5-C-[3, 5-bis(1-methylpropyl)-1-cyclopenten-1-yl]-4-deoxy- 	4249	4249	
601.	63-91-2	*L*-Phenylalanine C_6H_5-CH_2-$CH(NH_2)$-$COOH$	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3797, 4159, 4249, 5811b	120, 158, 622, 722, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1102, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 02359, 2394a, 2453, 2532, 2597a, 2795, 2903, 2905, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3829, 3973, 3974a, 3975, 3978, 4098a, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5831, 5905, 5907	
602.	31105-03-0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
603.	51064-37-0	Phenylalanine, ar,ar-dihydroxy-		4249	
604.	15664-29-6	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, [3S-(3α,4β,21β)]- {pheophorbide A}		4249, 4445, 5517	
605.	13406-98-9	1-Piperidinecarboxylic acid		2566, 4249, 4511	
606.		2-Piperidineacetic acid, 1-nitroso- {NPIPAC}		486	
607.	535-75-1	2-Piperidinecarboxylic acid {pipecolic acid}	5048	1351, 2337, 2722, 3491, 3797, 3974a, 4249, 4398c, 4475, 5079, 5873	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

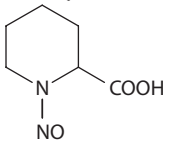
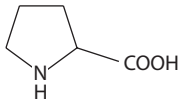
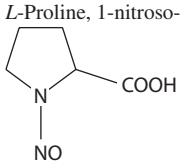
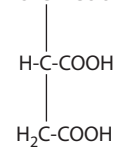
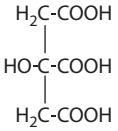
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
608.	4515-18-8 30310-81-7	2-Piperidinecarboxylic acid, 1-nitroso- {*N*-nitrosopipecolic acid: NPIC} 	3256, 3300, 3943a, 3944–3946, 4249, 5811b	486, 992, 3943a, 3944–3946, 3947, 3948, 5811, 5811a, 5811b	
609.	65445-62-7	3-Piperidinecarboxylic acid, 1-nitroso-	3951	3300**,** 4249	
610.	6238-69-3	4-Piperidinecarboxylic acid, 1-nitroso-		3300, 4249	
611.	644-00-8	21*H*,23*H*-Porphine-2-propanoicacid,8,13-diethyl-3,7,12,17-tetramethyl-		3491, 4249	
612.	1976-85-8	21*H*,23*H*-Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetrakis(carboxymethyl)-5,10,15,20,22,24-hexahydro-		4249, 4538	
613.		Proline, hydroxy-		5907	
614.	147-85-3	*L*-Proline 	1351, 1910, 1914, 1933, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249, 4319, 5048	120, 158, 480, 486, 749, 751–756, 826a, 927, 1033, 1053, 1063–1066, 1068–1074, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1933a, 1971, 2133, 2270, 2337, 2394a, 2395, 2453, 2529, 2532, 2592, 2597a, 2795, 2858, 2911c, 2914, 2939, 3059, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4226, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5881, 5896, 5905, 5907	
615.		*L*-Proline, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
616.	18610-59-8	*L*-Proline, 1-hydroxy-		1063–1066, 1068–1074, 1351, 2337, 2394a, 2597a, 3491, 3797, 3973, 3974a, 4224, 4226, 4249	
617.	147427-29-0	*L*-Proline, 1-[1-[1-(1-*L*-seryl-*L*-prolyl)-*L*-prolyl]-*L*-prolyl]-		4249	
618.	51-35-4	*L*-Proline, 4-hydroxy-, *trans*-		120, 1305a, 5811b	
619.	30310-80-6	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}		486, 3947, 3948, 5811b	
620.	7519-36-0	*L*-Proline, 1-nitroso- {NPRO} 	204–206, 486, 499, 509, 1058, 1673, 1695, 1719, 1870, 1871, 3256, 3260, 3300, 3943a, 3944–3946, 3951, 4249	466, 468, 485, 486, 498, 499, 511, 992, 1870, 1871, 3256, 3566, 3943a, 3944–3946, 3947, 3948, 3973, 4130, 4249, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
621.	62137-28-4	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-		4249, 4429	
622.	62137-29-5	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-L-ar abinofuranosyl)oxy]-, *trans*-		4249, 4429	
623.	141-82-2	Propanedioic acid {malonic acid} $H_2C{=}(COOH)_2$	722, 1375a, 1377, 2939, 3060, 3061, 3302, 3555, 4249, 5811b	120, 266, 836, 838, 839, 1330, 1923, 1982, 2014, 2270, 2338, 2356, 2529, 2532, 2939, 3052, 3060, 3353, 3555, 3701, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5079, 5447, 5811b, 5896	1375a, 1377, 3393
624.	80-69-3	Propanedioic acid, hydroxy- $HO\text{-}CH{=}(COOH)_2$		4249, 4950a	
625.	516-05-2	Propanedioic acid, methyl- $H_3C\text{-}CH{=}(COOH)_2$	3741, 3743	2917a	
626.	99-14-3	Propanetricarboxylic acid		4543; 5777	
627.	30810-51-6	1,2,3-Propanetricarboxylic acid, 1-hydroxy- {isocitric acid} 		120, 3973, 5811b	
628.	77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid} 	2079, 3029, 3302, 3324, 3555, 5079, 5447, 5811b	69, 120, 172a, 256, 305, 385, 543a, 555, 634, 677b, 826a, 835, 836, 838, 839, 963, 840, 1053, 1063–1066, 1068–1074, 1289, 1305a, 1330, 1332, 1333, 1548, 1923, 1933a, 1982, 2014, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2374, 2529, 2532, 2688, 2761–2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3052, 3107, 3194, 3266, 3353, 3370, 3476, 3486, 3555, 3660, 3655b, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 3974b, 3976, 4249, 4275, 5079, 5108, 5109, 5126, 5244, 5381, 5389, 5419, 5477, 5478, 5745, 5749, 5753, 5764, 5811b, 5832, 5896, 5909	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
629.	58308-53-5	1,2,3-Propanetricarboxylic-1,3-$^{14}C_2$ acid, 2-hydroxy-	2763, 4249	2763, 4249	
630.	79-09-4	Propanoic acid {propionic acid} H_3C-CH_2-COOH	563, 565, 568b, 916, 960, 1023, 1063–1066, 1068–1074, 1132, 1140, 1232, 1263, 1360, 1364, 1365, 1371, 1375a, 1388–1390, 1586, 1587a, 1668, 1744, 1842, 1882, 1903, 1904, 1917, 2043, 2079, 2088, 2265, 2270, 2337, 2338, 2339b, 2387, 2493, 2529, 2543, 2545, 2570, 2619, 2623, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3060, 3105, 3255, 3263, 3266, 3300, 3302, 3308, 3410, 3495, 3553, 3555, 3557, 3799, 3973, 4064, 4065, 4249, 4304, 4319, 5079, 5512, 5811b	120, 172a, 174b, 404, 563, 565, 568b, 647, 848, 937, 1053, 1085, 1087, 1263, 1587a, 1590a, 1923, 1999, 2014, 2092, 2283, 2337, 2338, 2339, 2386, 2389, 2544, 2570, 2862a, 2939, 3266, 3507, 3549, 3555, 3655b, 3973, 3973, 3974a, 3974b, 4249, 5079, 5381, 5708, 5735, 5811b, 5846, 5896	1360, 1375a, 2387, 3393, 3401, 3404
631.	75-98-9	Propanoic acid, 2,2-dimethyl-{pivalic acid} $(H_3C)_3{\equiv}C$-COOH	1871a, 4249, 5811b	404, 2917a, 4092, 4249	
632.	473-81-4	Propanoic acid, 2,3-dihydroxy-{glyceric acid} $HOCH_2$-CHOH-COOH	1882, 1886, 4249, 5811b	120, 2892b, 2939, 3797, 3974a, 4249, 5811b	
633.	6000-40-4	Propanoic acid, 2,3-dihydroxy-, (R)-		4249	
634.	82546-67-6	Propanoic acid, 3-(ethoxycarbonyl)-3-(1-cyclohexenenyl)-	2601a		
635.	50-21-5 598-82-3	Propanoic acid, 2-hydroxy- {lactic acid} H_3C-CHOH-COOH	126b, 172, 237, 568b, 1099, 1235, 1364, 1445, 1674, 1744, 1842, 1882, 2133, 2493, 2582, 2767, 2939, 3053, 3059, 3060, 3061, 3255, 3266, 3302, 3308, 3384, 3394, 3496, 3553, 3557, 3559, 4249, 5512, 5811b	120, 172a, 174b, 568b, 722, 1053, 1279, 2079, 2917a, 2939, 3052, 3053, 3060, 3266, 3486, 3797, 3973, 3974a, 4131, 4249, 5079, 5447, 5811b	3393, 3402, 3405
636.	594-61-6	Propanoic acid, 2-hydroxy-2-methyl- $(H_3C)_2{=}$COH-COOH		1948, 2337a, 4249	
637.	820-11-1	Propanoic acid, 2-hydroxy-3-(phosphonooxy)-		429b, 4249, 4634, 5811b	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
638.	79-31-2	Propanoic acid, 2-methyl- {isobutyric acid} $(H_3C)_2$═CH-COOH	563, 565, 568b, 775, 960, 1063–1066, 1068–1074, 1132, 1140, 1360, 1371, 1375a, 1388–1390, 1668, 1886, 2079, 2088, 2529, 2543, 2570, 2619, 2623, 2761, 2762, 2765, 2766, 2777, 2939, 3224, 3266, 3302, 3308, 3410, 3452, 3553, 3799, 3800, 4249, 4319, 5811b	120, 172a, 174b, 404, 563, 565, 568b, 848, 908, 981a, 1053, 1085, 1087, 1999, 2014, 2079, 2270, 2283, 2338, 2339a, 2389, 2544, 2570, 2862a, 2917a, 2939, 3266, 3370, 3507, 3547, 3549, 3560, 3561, 3973, 3974a, 3974b, 4249, 5708, 5811b, 5846	1360, 1375a, 3393
639.	127-17-3	Propanoic acid, 2-oxo- {pyruvic acid} H_3C-CO-COOH	563, 568b, 1310, 2088, 2939, 3059, 3224, 3302, 3308, 3553, 4249, 5811b	69, 120, 172a, 174b, 563, 568b, 1053, 1305a, 1310, 1312, 1923, 2389, 2544, 2939, 3266, 3370, 3797, 3973, 3974a, 4249, 5811b, 5896	
640.	3913-50-6	Propanoic acid, 2-oxo-3-(phosphonooxy)-		429b, 4249, 4634	
641.	4272-12-2	Propanoic acid, 3-(acetyloxy)- H_3C-COO-$(CH_2)_2$-COOH	1075, 2775, 3553, 4249, 5811b		
642.	935-13-7	Propanoic acid, 3-(2-furanyl)-	91b, 5811b		
643.	503-66-2	Propanoic acid, 3-hydroxy- HO-$(CH_2)_2$-COOH	568b, 1364, 1371, 1882, 3255, 3394, 3553, 4249	120, 568b, 3974a, 4249	3393
644.	4835-90-9	Propanoic acid, 3-hydroxy-,2,2-dimethyl- {hydroxypivalic acid} HOH_2C-$C(CH_3)_2$-COOH		2917a	
645.	2553-59-5	Propanoic acid, 3-hydroxy-2-(phosphonooxy)-		429b, 4634	
646.	1113-60-6	Propanoic acid, 3-hydroxy-2-oxo- HOH_2C-CO-COOH		1971, 2939, 3797, 4634, 5777, 5811	
647.		Propanoic acid, 3-hydroxyphenyl-	1626, 3797		
648.	2544-06-1	Propanoic acid, 3-methoxy-		1948, 4249	
649.		Propanoic acid, 3-methylbutyl ester		2339a	
650.	1456-08-2	Propanoic acid, 3-(5-methyl-2-furanyl)-	91b, 5811b		
651.	10478-42-9	Propanoic acid, 3-(methylnitrosoamino)- {NMPA} CH_3-N(NO)-$(CH_2)_2$-COOH		992, 2852, 3300, 3973, 5001	
652.	499-12-7	1-Propene-1,2,3-tricarboxylic acid {aconitic acid}	2572, 3255, 3257, 3265, 4249	1053, 3266, 3370	
653.	79-10-7	2-Propenoic acid {acrylic acid} H_2C═CH-COOH	568b, 1365, 2767, 3410, 3553, 3557, 4249, 5811b, 5869a	5811b	
654.	138-08-9	2-Propenoic acid, 2-(phosphonooxy)-		429b, 568b, 4249, 4750	
655.	79-41-4	2-Propenoic acid, 2-methyl- {methacrylic acid}	568b, 1063–1066, 1068–1074, 1586, 1882, 1886, 2767, 3553, 3557, 4249, 5811b	568b, 4093, 4249	3393

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

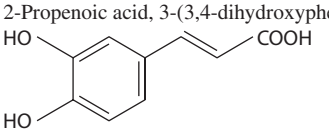
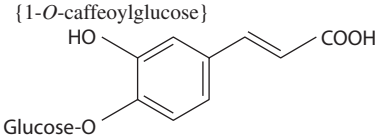
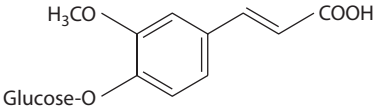
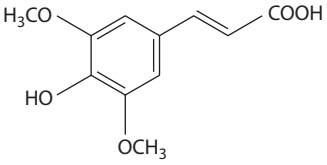
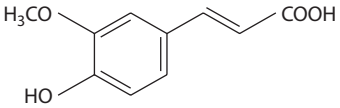
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
656.	539-47-9	2-Propenoic acid, 3-(2-furanyl)-	91b, 5811b		
657.	31082-90-3	2-Propenoic acid, 3-(2,3-dihydroxyphenyl)-	3712, 3741, 3743, 4249, 4897, 5811b		
658.	331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid} 	1626, 1743, 1744, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3300, 3308, 3712, 3714, 3797, 4036, 4113, 4163, 4249, 4376, 5079, 5389, 5512, 5811b, 4A01	72, 120, 722, 835, 890, 1102, 1626, 1981, 2154, 2216, 2270, 2514, 2939, 2954, 3029, 3103, 3161, 3462, 3476, 3655b, 3660, 3700, 3748, 3749, 3751, 3973, 3974a, 4249, 4999, 5079, 5126, 5385, 5389, 5591, 5652, 5672. 5673, 5705, 5713, 5722, 5809, 5810, 5811b, 5830, 5831, 5900, 5908, 4A01	
659.	501-16-6	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*E*)- {*cis*-caffeic acid}	1626, 3302, 3308, 3712, 3741, 3743, 4163, 4376, 4377, 5811b	1626, 3748, 3749, 3751, 3797, 4249	
660.	4361-87-9	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*Z*)- {*trans*-caffeic acid}	1626, 2939, 3302, 3308, 3712, 3741, 3743, 4163, 4249, 4376, 4377, 5811b	1309, 1626, 2939, 3748, 3749, 3751, 3797, 4249	
661.	2316-26-9	2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-		2389, 2544, 5811b	
662.	17093-82-2	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]- {1-*O*-caffeoylglucose} 		3797, 3974a, 4402	
663.	7196-71-6 14364-12-6	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-methoxyphenyl]- {1-*O*-feruloylglucose} 		3797, 3974a, 4249, 4402, 5811, 5811b	
664.	14364-05-7	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)phenyl]-		2023	
665.	7361-90-2	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*Z*)- {*cis*-sinapic acid}	1626	1102, 3748, 3749, 3751, 4249, 4624	
666.	7362-37-0	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*E*)- {*trans*-sinapic acid} 	1626, 1884, 3302, 3712, 3797, 4249, 4377	1102, 3748, 3749, 3751, 4249	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
667.	537-73-5	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-	3712, 4113, 4249		
668.	25522-33-2	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-, (*E*)-	3712, 5811b		
669.	1782-55-4	2-Propenoic acid, 3-(4,5-dihydroxy-3-methoxyphenyl)- {5-hydroxyferulic acid}		1102	
670.	1135-24-6	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-{cinnamic acid, 3-hydroxy-4-methoxy-; ferulic acid}	3712, 5811b	5811b	
671.	530-59-6	2-Propenoic acid, 3-(4-hydroxy-3,5-dimethoxyphenyl)-	5811, 5811b		
672.	537-98-4	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid} 	1626, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3555, 3749, 3797, 4249, 4377, 5811b	404, 1102, 1626, 1884, 2216, 2389, 2544, 2939, 2954, 3103, 3161, 3555, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 4377	
673.	1014-83-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid}	1626, 1842, 2216, 2939, 3255, 3257, 3302, 3712, 3741, 3743, 3749, 4249, 4377	1102, 1626, 2216, 2389, 2544, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3797, 3973, 3974a, 4249	
674.	25429-38-3	2-Propenoic acid, 3-(hydroxyphenyl)-	3712, 4249, 4553a		
675.	583-17-5 614-60-8	2-Propenoic acid, 3-(2-hydroxyphenyl)- {*o*-coumaric acid}	3265, 3741, 3743, 4113, 4249, 5811b	3109, 4249, 5811b	
676.	588-30-7	2-Propenoic acid, 3-(3-hydroxyphenyl)-		3748, 3749, 3751	
677.	14755-02-3	2-Propenoic acid, 3-(3-hydroxyphenyl)-, (*E*)-		3748, 3749, 3751, 4249	
678.	7400-08-0	2-Propenoic acid, 3-(4-hydroxyphenyl)- {coumaric acid}	101, 1626, 1842, 2543, 2939, 3302, 3308, 3712, 4113, 4163, 4377, 5811b	120, 908, 1102, 1626, 2386, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3973, 3974a, 4163, 4377, 4677	
679.	501-98-4	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*E*)- {*cis*-coumaric acid}	1626, 1842, 2775, 3302, 3741, 3743, 3939, 4163, 4377, 5811b	1626, 2270, 3748, 3749, 3751, 4163, 4377	
680.	4501-31-9	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*Z*)- {*trans*-coumaric acid}	1626, 1842, 2775, 3302, 3410, 3712, 3741, 3743, 4163, 4377, 5811b	1626, 3748, 3749, 3751, 4163, 4377	
681.	17570-26-2	2-Propenoic acid, 3-(3-methoxyphenyl)-, (*E*)-	2388, 4249	3561, 3797	
682.	14779-25-0	2-Propenoic acid, 3-(5-methyl-2-furanyl)-	91b, 5811b		
683.	621-82-9	2-Propenoic acid, 3-phenyl-{cinnamic acid}	2767, 3265, 3266, 3557, 4159, 4249, 5811b	172a, 174b, 722, 1053, 1102, 1983, 2389, 2544, 2914, 3266, 3370, 3973, 4249, 5811b	
684.	140-10-3	2-Propenoic acid, 3-phenyl-, (*E*)- {*trans*-cinnamic acid}	568b, 3266, 3553, 4249	568b, 1053, 2092, 2389, 2544, 3266, 4249	
685.	102-94-3	2-Propenoic acid, 3-phenyl-, (*Z*)- {*cis*-cinnamic acid}	3266, 3553, 3557, 4249	1053, 2092, 2389, 2544, 3266, 4249	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

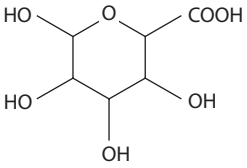
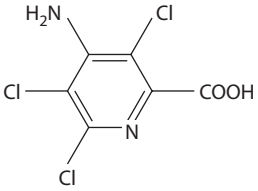
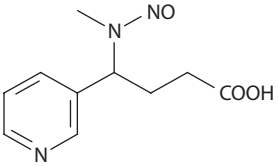
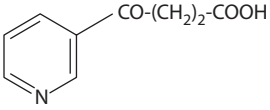
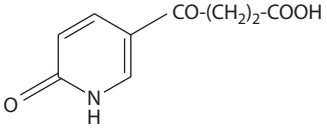
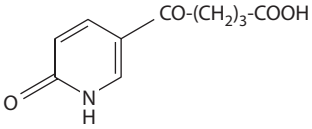
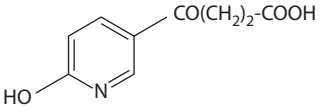
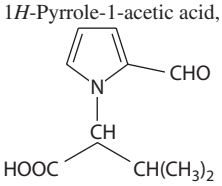
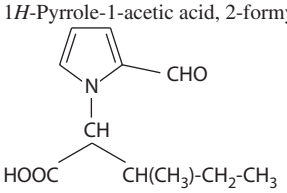
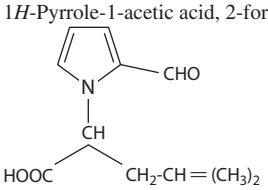
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
686.	90-50-6	2-Propenoic acid, 3-(3,4,5-trimethoxyphenyl)-		2389, 2544, 5811b	
687.	9046-38-2	2-Pyrancarboxylic acid, 3,4,5,6-tetrahydroxytetrahydro-{oxane-2-carboxylic acid, 3,4,5,6-tetrahydroxy-; *D*-galacturonan} 		5811, 5811b	
688.	499-78-5	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-	1375a (0), 1377 (0)		1375a, 1377
689.	1918-02-1	2-Pyridinecarboxylic acid, 4-amino-3,5,6-trichloro- {Picloram®} 		3973, 4249	
690.	17270-48-3	3-Pyridinebutanoic acid, γ-(methylamino)-, (±)-		4249, 4779	
691.	152720-16-6	3-Pyridinebutanoic acid, γ-(methylnitroamino)-		3444, 4249	
692.	123743-84-0 133201-36-2	3-Pyridinebutanoic acid, γ-(methylnitrosoamino)- {iso-NNAC} 	59, 486, 1008, 1009, 1012, 1013, 1584, 1702, 1751, 3256, 3300, 4249, 5811, 5811a, 5811b	465, 486, 992, 993, 995, 1008, 1009, 1012, 1013, 1584, 1702, 1750, 3973, 4236, 4249, 5811, 5811a, 5811b	
693.	4192-31-8	3-Pyridinebutanoic acid, γ-oxo- 		1101, 2226, 3444, 4236, 4249, 5508	
694.	15873-27-5	3-Pyridinebutanoic acid, 1,6-dihydro-γ,6-dioxo- 	4249	1110, 4249, 4709	
695.	59-67-6	3-Pyridinecarboxylic acid {nicotinic acid}	43, 562, 563, 1224, 1668, 1568, 1890, 1891, 2079, 2224, 2349, 2724, 2767, 2939, 3059, 3302, 3309, 3444, 3491, 3505, 4080, 4249, 5079, 5811b, 25A84	120, 555a, 555b, 1222, 1224, 1225, 1226, 1568, 2270, 2283, 2724, 2794, 2914, 2939, 3444, 3491, 3797, 3974, 3973, 3974a, 3983a, 4249, 5079, 5390a, 5145, 5445, 5811b, 17B07, 17B08, 17B33, 17B34, 17B37, 17B48	
696.	5006-66-6	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-		4249	
697.	89-00-9	2,3-Pyridinedicarboxylic acid {quinolinic acid}		555b, 4249, 5531	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
698.	71608-01-0	3-Pyridinepentanoic acid, 1,6-dihydro-δ,6-dioxo- 		1101, 4249, 4945	
699.		2-Pyridinol-5-butanoic acid, γ-oxo- 		1101, 4249	
700.		2-Pyridinol-5-pentanoic acid, δ-oxo-		1101, 4249	
701.	42438-90-4	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydo-, (*S*)-	2447a		
702.	40678-46-4	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydo-1-methyl-, (1*S*-*cis*)-	2447a		
703.	84499-92-3	1*H*-Pyrrole-1-acetic acid, 2-(ethoxymethyl)-5-formyl-		4249, 4573a, 5811b	
704.	61837-43-2	1*H*-Pyrrole-1-acetic acid, 2-ethyl-5-formyl-α-(2-methylpropyl)-		4249, 4573a	
705.	60026-07-5	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylethyl)- 		965, 2544, 4249	
706.	60026-08-6	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylpropyl)- 		965, 2544, 4249	
707.	60026-09-7	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(2-methylpropyl)- 		965, 2544, 4249	
708.		1*H*-Pyrrole-1-acetic acid, 2-formyl-5-hydroxymethyl-α-(2-methylpropyl)-	2337, 4249		
709.	61837-42-1	1*H*-Pyrrole-1-acetic acid, 2-formyl-α,5-dimethyl-		4249, 4573a	
710.	61837-35-2	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-hexyl-		4249, 4573a	
711.	60026-30-4	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-methyl-		4249, 4573a	
712.	61837-38-5	1*H*-Pyrrole-1-butanoic acid, 2-formyl-		4249, 4573a	
713.	61837-39-6	1*H*-Pyrrole-1-butanoic acid, 2-formyl-γ-methyl-		4249, 4573a	
714.	61837-44-3	1*H*-Pyrrole-1-butanoic acid, 2-formyl-5-methyl-		4249, 4573a	
715.	61837-40-9	1*H*-Pyrrole-1-hexanoic acid, 2-formyl-		4249, 4573a	
716.	61837-41-0	1*H*-Pyrrole-1-octanoic acid, 2-formyl-		4249, 4573a	
717.	70898-32-7	1*H*-Pyrrole-1-octanoic acid, 2-formyl-5-methyl-		4249, 4573a	
718.	61837-37-4	1*H*-Pyrrole-1-propanoic acid, β-ethyl-2-formyl-		4249, 4573a	
719.	61837-36-3	1*H*-Pyrrole-1-propanoic acid, 2-formyl-β-methyl-		4249, 4573a	
720.	634-97-9	1*H*-Pyrrole-2-carboxylic acid	568b, 1360, 1375a, 3553, 4249, 5811b		1360, 1375a

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

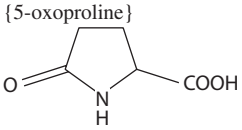
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
721.	3220-74-4	1*H*-Pyrrole-2-carboxylic acid, 2,5-dihydro-		3797, 4249	
722.	3757-53-7	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-	2767, 4249		
723.	487-90-1	1*H*-Pyrrole-3-propanoicacid,5-(aminomethyl)-4-(carboxymethyl)-		4249, 4870	
724.	28882-68-0	Pyrrolidinecarboxylic acid	2767, 4249		
725.	32389-40-5	Pyrrolidinecarboxylic acid, oxo-, (S)-		4249, 4543	
726.	56879-46-0	2-Pyrrolidineacetic acid		1351, 2337, 2722, 3491, 3797, 3974a, 4249, 5873	
727.		2-Pyrrolidineacetic acid, 1-nitroso-		486, 4249	
728.	98-79-3	5-Pyrrolidinone-2-carboxylic acid {5-oxoproline} 		2597a, 3052, 4249	
729.	3778-29-8	2-Quinolinecarboxylic acid, 4,6-dihydroxy-{6-hydroxykynurenic acid}		3491, 4249	
730.	492-27-3	2-Quinolinecarboxylic acid, 4-hydroxy-	5811, 5811a, 5811b		
731.	643-38-9	2,3-Quinolinedicarboxylic acid		3973	
732.	106777-19-9	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-		429b, 4249	
733.	27442-42-8	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-, 5-(dihydrogen phosphate)		429b, 4249	
734.	6898-95-9	Serine $HO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 2858, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1063–1066, 1068–1074, 1223, 1305a, 1351, 1493, 1918, 1919, 2048, 2270, 2337, 2338, 2339b, 2445a, 2453, 2532, 2597a, 2795, 2911a, 2911c, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c 5079, 5699, 5827, 5831, 5881, 5896, 5905, 5907	
735.	35688-48-3	*D*-Serine, *N*-(carboxyacetyl)-		2048, 4249, 4728	
736.	56-45-1	*L*-Serine		3973, 5811b	
737.	5147-00-2	*L*-Serine, acetate (ester) $CH_3\text{-}COO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$		429b, 4249, 4895	
738.	5692-15-9	*L*-Serine, labeled with ^{14}C {*L*-serine-^{14}C}		4249, 4940	
739.	142785-07-7	*L*-Serine,*L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		4249	
740.	146440-48-4	*L*-Serine,*L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		4249	

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
741.	71010-48-5	α-Tabacenic acid		2079, 3660, 4249, 5079, 5189, 5381, 5441	
742.	71010-46-3	β-Tabacenic acid		2079, 3660, 4249, 5079, 5189, 5381, 5441	
743.	71010-47-4	γ-Tabacenic acid		2079, 3660, 4249, 5079, 5189, 5381, 5441	
744.	1401-55-4	Tannins {tannic acid}		120, 1053, 2270, 2154, 2939, 2947c, 3266, 3708, 3973, 4249, 5079, 5126, 5381	
745.	557-59-5	Tetracosanoic acid {lignoceric acid} H_3C-$(CH_2)_{22}$-COOH	101, 1586, 1785, 2570, 2767, 3308, 3553, 3557, 3797, 4249, 5811b	613, 1785, 2286, 4249, 4280	
746.	36378-43-5	Tetracosanoic acid, 22-methyl-		3973, 3974a, 4249, 4984	
747.		Tetracosanoic acid, 23-methyl-		3973, 3974a, 4249, 4719	
748.	14490-79-0	15-Tetracosenoic acid {nervonic acid}	2767, 2769, 3557, 4249		
749.	506-37-6	15-Tetracosenoic acid, (Z)-	2767, 4249	3812, 4249	
750.	821-38-5	Tetradecanedioic acid HOOC-$(CH_2)_{12}$-COOH	2584, 4249		
751.	544-63-8	Tetradecanoic acid {myristic acid} H_3C-$(CH_2)_{12}$-COOH	60, 101, 172, 257, 258, 568b, 765, 809, 1132, 1348, 1360, 1364, 1375, 1375a, 1375b, 1586, 1646, 1651, 1785, 1884, 2389, 2418, 2529, 2544, 2570, 2601a, 2761, 2762, 2765–2767, 2777, 2876, 2939, 3219, 3266, 3293, 3302, 3308, 3547, 3557, 3797, 4030, 4249, 4280, 4319, 4993, 5552, 5811b	60, 101, 120, 404, 568b, 634, 647, 835, 836, 838, 891, 908, 1053, 1330, 1651, 1785, 1893a, 1893b, 2079, 2270, 2283, 2338, 2339a, 2356, 2389, 2529, 2544, 2570, 2862, 2917a, 2939, 3194, 3219, 3266, 3328, 3332, 3547, 3549, 3797, 3842, 3973, 3974a, 4042c, 4249, 4280, 4397, 4993, 5079, 5695, 5811b	1360, 1375a
752.	1961-72-4	Tetradecanoic acid, 3-hydroxy- H_3C-$(CH_2)_{10}$-CHOH-CH_2-COOH		3547, 4249	
753.	5502-94-3 5746-58-7	Tetradecanoic acid, 12-methyl- H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COOH	809, 2570, 3293, 3557, 4249	404, 732, 2389, 2544, 2917a, 3561, 3973, 3974a, 4249, 5811b	
754.	2485-71-4	Tetradecanoic acid, 13-methyl- $(H_3C)_2$═CH-$(CH_2)_{11}$-COOH		958, 3973, 3974a, 4249	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

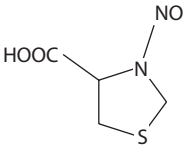
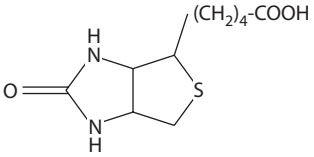
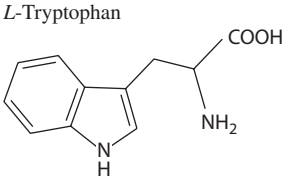
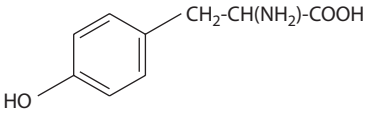
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
755.	30790-23-9	Tetradecatrienoic acid		1248, 4249, 5811b	
756.	26444-03-1	Tetradecenoic acid	60, 809, 3293, 4249	60, 4249	
757.	38232-04-1	Tetratriacontanoic acid $H_3C\text{-}(CH_2)_{32}\text{-}COOH$	101, 3263, 5811b		
758.	88381-44-6	4-Thiazolidinecarboxylic acid, 3-nitroso- {*N*-nitrosothioproline} 		486, 3300, 5811b	
759.	58-85-5	1*H*-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3aS-(3aα,4β,6aα)]- 		2408a, 4249, 4789	
760.	72-19-5	*L*-Threonine $H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3555, 3797, 4249, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1305a, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079 5811b, 5827, 5831, 5881	
761.	32190-57-1	*L*-Threonine,*N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]-		3819a, 4249	
762.		*L*-Threonine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337	
763.	506-50-3	Triacontanoic acid $H_3C\text{-}(CH_2)_{28}\text{-}COOH$	101, 3263, 5811b		
764.	2433-96-7	Tricosanoic acid $H_3C\text{-}(CH_2)_{21}\text{-}COOH$	101, 1785, 2767, 2769, 3557, 4249, 5811b	327, 613, 1785, 2286, 3973, 3974a, 4249, 4280, 5811b	
765.	36332-96-4	Tricosanoic acid, 21-methyl- $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{19}\text{-}COOH$	3251, 3294, 3302, 4249, 4719	3251, 3294, 3973, 3974a, 4249	
766.	4730-63-6	Tricosanoic acid, 22-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_{20}\text{-}COOH$	1586, 2767, 2769, 4249	1042, 3973, 3974a, 4249, 5811b	
767.	30326-99-9	Tricosenoic acid	2767, 4249		
768.	505-52-2	Tridecanedioic acid $HOOC\text{-}(CH_2)_{11}\text{-}COOH$	2572, 4249		

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
769.	638-53-9	Tridecanoic acid H_3C-$(CH_2)_{11}$-COOH	60, 172, 809, 1646, 2418, 2570, 2767, 3293, 3308, 3557, 4030, 4249, 4993, 5811b	60, 2092, 2356, 2917a, 3547, 4249, 4993, 5811b	
770.	2724-57-4	Tridecanoic acid, 12-methyl- $(H_3C)2{=}CH$-$(CH_2)_{10}$-COOH	809, 2570, 3219, 3293, 3308		
771.	41678-34-6	Tridecatrienoic acid		2092, 4249, 5811b	
772.		Tridecenoic acid	1586		
773.	38232-03-0	Tritriacontanoic acid H_3C-$(CH_2)_{31}$-COOH	101, 3263, 5811b		
774.	6912-86-3	Tryptophan		3705	
775.	73-22-3	*L*-Tryptophan 		120, 480, 622, 722, 749, 751–756, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 2079, 2270, 2337, 2338, 2359, 2510, 2532, 2597a, 2795, 2902, 2903, 2911c, 2939, 3491, 3705, 3797, 3829, 3973, 3974a, 3978, 4103, 4224, 4244, 4249, 4286b, 4398c, 5079, 5603, 5785, 5811b, 5831, 5881, 5905	
776.	60738-11-6	*L*-Tryptophan, labeled with ^{14}C {*L*-tryptophan-^{14}C}		2562a, 4249, 4876	
777.	55520-40-6	Tyrosine		3705	
778.	587-45-1	Tyrosine, 3-hydroxy-		429b	
779.	60-18-4	*L*-Tyrosine 		120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1965, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4398c, 5079, 5785, 5811b, 5827, 5905, 5907	

(*continued*)

TABLE 4.3 (continued)
Carboxylic Acids in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
780.	34393-22-1	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
781.	1852-04-6	Undecanedioic acid HOOC-$(CH_2)_9$-COOH	2584, 4249	731, 738, 2659a, 4249	
782.	112-37-8	Undecanoic acid H_3C-$(CH_2)_9$-COOH	172, 568b, 809, 1646, 1917, 2418, 2570, 2584, 3263, 3293, 4249, 4993, 5079, 5811b	568b, 2092, 2356, 2389, 2544, 2917a, 3973, 3974a, 4249, 4993, 5811b	
783.	112-38-9	10-Undecenoic acid		5811	
784.	94414-19-4	Urs-12-en-28-oic acid, 3,23-dihydroxy-, (3β,4α)-		4249	
785.	77-52-1	Urs-12-en-28-oic acid, 3-hydroxy-, (3β)-		429b	
786.	7004-03-7	Valine $(H_3C)_2$═CH-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4249, 4359, 4398c, 5079, 5493, 5785, 5827, 5831, 5881, 5905, 5907	
787.	72-18-4	*L*-Valine	5811b	424a, 429b, 2338, 5811b	
788.		*L*-Valine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

quantities of tryptophan and phenylalanine or pyrrole and phenylalanine were pyrolyzed. The results from this study are summarized in Table 4.5. The difference between the pyrogenesis of PAHs from phenylalanine and the mixture of equimolar quantities of phenylalanine and the amino acid tryptophan prompted Patterson et al. (2903) to propose the addition of amino acids to tobacco as a possible means to control the PAH content of the CSC:

> These results suggest the possibility that aromatic hydrocarbon content of tobacco "tar" may be affected by the amino acid composition of the tobacco and that it might be possible to affect deliberately the amount of aromatics and bases formed by adding suitable additives, such as amino acids, to the tobacco.

Of course, in 1971 when Patterson et al. offered this suggestion, the presence in amino acid pyrolysates of the so-called cooked food mutagens and the inordinately high mutagenicity of several of them were unknown.

Higman et al. (1647) also reported the generation of PAHs, phenols, pyridines, indole, quinoline, and other aromatic bases during the pyrolysis of amino acids and proteins from tobacco [cf. review on pyrogenesis of smoke components

TABLE 4.4
Components in Pyrolysates from the Amino Acids Lysine, Leucine, and Tryptophan (2902)

	Yield, mg/mol, of Amino Acid Pyrolyzed		
Pyrolysate Component	**Lysine[a]**	**Leucine**	**Tryptophan**
Nitrogen compounds			
Hydrogen cyanide	+	+	+
Aniline	60	5	–
Quinoline	160	8	17.7
Isoquinoline	80	6	2.4
Benzonitrile	470	40	1370
o-Tolunitrile	30	+	610
m-Tolunitrile	30	30	+
p-Tolunitrile	20	+	+
Phenylacetonitrile	6	–	400
Indole	20	+	610
1-Naphthonitrile	10	30	350
2-Naphthonitrile	–	–	170
Cyclic hydrocarbons			
Styrene	5	20	–
Biphenyl	10	30	+
Bibenzyl	2	–	+
Indene	40	70	–
Naphthalene	210	620	1100
Naphthalene, 1-methyl-	10	40	+
Naphthalene, 2-methyl-	10	50	–
Acenaphthene	20	–	–
Acenaphthylene	30	19	3
Fluorene	10	80	140
Anthracene/phenanthrene	30	250	7900
Fluoranthene	10	90	210
Pyrene	10	110	270
Pyrene, methyl-	2	20	–
Benzofluorene	10	30	150
Chrysene	10	50	110
Triphenylene	+	+	+
Benz[*a*]anthracene	+	+	+
Benzopyrene	–	30	–

+ indicates the presence of compound; – indicates the absence of the compound.

[a] Pyrolyzed as lysine monohydrochloride.

by Chortyk and Schlotzhauer (722)]. The pyrolysis results reported by Higman et al. are summarized in Table 4.6.

Tryptophan was also found to be the precursor in tobacco of two other *N*-heterocyclic compounds, namely, harman (1-methyl-9*H*-pyrido[3,4-*b*]indole) and norharman (9*H*-pyrido[3,4-*b*]indole), both present in tobacco smoke. These compounds were originally identified in tobacco and tobacco smoke by Philip Morris R&D personnel in 1961 and 1962 [Poindexter and Carpenter (2972)] and in 1963 [Poindexter et al. (2972)]. That tryptophan was indeed a precursor in tobacco of the two harmans in smoke was demonstrated by addition of radiolabeled tryptophan to cigarette tobacco and identification of radiolabeled harman and norharman in the MSS.

In the mid-1970s, pyrolysis studies with several amino acids led to the isolation and identification of several additional polycyclic *N*-heterocyclic compounds, which are reported not only to be tumorigenic to mouse skin but also to show inordinately high mutagenicity when tested in the Ames bioassay with *Salmonella typhimurium*. The impetus for these particular amino acid pyrolysis studies was not the attempt to define the relationship between tobacco leaf precursors and tobacco smoke components but the observation that the extracts of broiled, fried, or roasted foodstuffs (meat, fish, poultry, etc.) were highly mutagenic in the Ames bioassay (*S. typhimurium*). These *N*-heterocyclic compounds, all amines, derived from the amino acids and/or proteins in heated foodstuffs, were often described as "cooked food" mutagens. Eventually they were defined as *N*-heterocyclic amines. In a later chapter, the *N*-heterocyclic amines will be discussed in greater detail than in this chapter.

The studies in the 1970s on the tumorigenicity and mutagenicity of extracts of cooked foodstuffs were reminiscent of the studies in the 1920s by Kennaway (2074–2076, 2080) who reported the tumorigenicity of extracts of heated foodstuffs or pyrolysates from heated organic compounds such as cholesterol and by Roffo (4A03–4A05) who reported the tumorigenicity of pyrolyzed cholesterol. Subsequently it was shown that many of the foodstuff pyrolysates and the cholesterol pyrolysates contained a spectrum of PAHs, including B[*a*]P. Identification of the highly mutagenic *N*-heterocyclic compounds in amino acid pyrolysates was followed by identification of some of them not only in the broiled/roasted meats but also in mainstream CSC.

In 1977, Sugimura et al. (3829) reported the identification of the potent mutagens 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (coded Trp-P-2) and 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (coded Trp-P-1) in pyrolysates from tryptophan. The next year, Yamamota et al. (4365a) identified two additional highly mutagenic compounds in pyrolysates from glutamic acid: 2-aminodipyrido[1,2-*a*:3′,2′-d]imidazole (coded Glu-P-2) and 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (coded Glu-P-1).

Table 4.7 lists several polynuclear *N*-heterocyclic amines which exhibit extremely high mutagenicity levels in the Ames bioassay, are amino acid pyrolysis products, and have been identified in various broiled, fried, or roasted foodstuffs as well as in CSC [Sugimura (3828c)]. On a per microgram basis, B[*a*]P in the Ames bioassay with *S. typhimurium* (Strain TA 98) shows about 200 revertants/μg. Several of the amino acid-derived compounds in Table 4.7 exceed the B[*a*]P effect with the TA 98 strain by factors ranging from about 10 to over 2100.

Yoshida and Matsumoto (4388) reported the identification of two α-carbolines in CSC: 2-amino-9*H*-pyrido[2,3-*b*]indole (coded AαC) and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (coded MeAαC). These and several other such compounds were reported in CSC by Yamashita et al. (4367, 4368). The quantitative levels of the possibly amino acid-derived, mutagenic *N*-heterocyclics in CSC are shown in Table 4.7. In their studies, they emphasized in particular the identification and quantitation of 2-amino-3-methylimidazo[4,5-*f*]quinoline (coded IQ) because of its inordinately high mutagenicity (found

TABLE 4.5
Pyrolysis of Phenylalanine: Effect of Pyrolysis Temperature and Effect of Equimolar Addition of Tryptophan or Pyrrole (2903)

	Phenylalanine (Phe) Pyrolyzed at				Material Pyrolyzed		
					Phe	Phe + Try[b]	Phe + Pyr[c]
Pyrolysate Component[a]	450°C	650°C	850°C	950°C	850°C	850°C	850°C
Monocyclic aromatic hydrocarbons							
Biphenyl	–	1,270	10,300	4,360	10,300	2,980	2,240
Bibenzyl	10,300	12,000	2,550	+	2,550	–	345
Polycyclic aromatic hydrocarbons							
Indene	–	0.36	2.73	–	2.73	–	0.17
Naphthalene	0.12	1.45	3.50	1.27	3.50	3.52	5.60
Naphthalene, 1-methyl-	–	+	–	–	–	–	0.73
Naphthalene, 2-methyl-	–	–	–	–	–	2.98	0.34
Acenaphthene	–	0.48	1.94	<0.18	1.94	0.054	0.086
Acenaphthylene	–	1.70	2.55	0.73	2.55	0.40	0.99
Fluorene	0.42	1.33	4.50	0.85	4.50	0.78	0.65
Phenanthrene/anthracene	4.12	9.70	20.00	7.90	20.00	1.44	2.41
Benzofluorene	–	0.48	1.94	2.60	1.94	0.22	0.39
Fluoranthene	–	0.48	1.27	0.60	1.27	0.16	0.04
Pyrene	–	3.50	3.20	1.20	3.20	0.30	0.39
Pyrene, methyl-	–	–	3.20	<0.60	3.20	0.22	+
Chrysenes	–	0.48	2.55	1.58	2.55	0.16	0.30
N-containing compounds							
Benzonitrile	1.27	0.85	7.88	1.27	7.88	3.80	1.46
o-Tolunitrile	–	0.36	2.85	0.06	2.85	0.68	0.26
m-Tolunitrile	–	0.06	–	0.06	–	1.38	0.26
p-Tolunitrile	–	0.18	0.18	–	0.18	0.38	0.26
Phenylacetonitrile	–	1.40	–	–	–	0.22	0.13
1-Naphthonitrile	–	1.40	–	–	–	1.14	1.00
Indole	–	2.30	0.72	–	0.72	17.35	0.86
Quinoline	–	1.80	12.00	0.30	12.00	25.75	1.30
Isoquinoline	–	3.00	10.90	0.18	10.90	1.10	0.43

[a] Yield of pyrolysis component in mg/g of compound or mixture pyrolyzed.
[b] Pyrolysis involved equimolar quantities of phenylalanine and tryptophan (total mol. wt. = 369).
[c] Pyrolysis involved equimolar quantities of phenylalanine and pyrrole (total mol. wt. = 232).

to be 433,000 and 490,000 revertant/μg in several determinations) in the Ames bioassay with *S. typhimurium* strain TA98.

Demonstration of the mutagenicity of the compounds listed in Table 4.7 was followed by demonstration of their tumorigenicity in various laboratory animals. Ohgaki et al. (2849b) demonstrated the tumorigenicity of 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ) in mice. Takayama et al. (3862c) and Tanaka et al. (3865c) reported its tumorigenicity in rats. 3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) were reported to be tumorigenic in mice by Matsukura et al. (2491a) and in rats by Hosaka et al. (1835a) and Takayama et al. (3862d).

Ohgaki et al. (2849b) reported that 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1), 2-aminodipyrido[1,2-*a*:3′,2′-*d*]-imidazole (Glu-P-2), 2-amino-9*H*-pyrido[2,3-*b*]indole (AαC), and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC) were tumorigenic in mice, and Takayama et al. (3862d) reported Glu-P-1 and Glu-P-2 to be tumorigenic in rats.

In a 1989 manuscript which was subsequently published, Hoffmann and Hecht (1727) discussed amino acid–derived aromatic amines in cigarette MSS as follows:

> Of the known carcinogenic pyrolysis products of the amino acids, so far only 2-amino-3-methylimidazo(4,5-*f*)quinoline has been detected in trace amounts of 0.26 ng in the smoke of a Japanese filter cigarette [Yamashita et al. (4368)].

Apparently, Hoffmann and Hecht had overlooked not only the reports of the identification in CSC of several other known "carcinogenic" pyrolysis products of amino acids, e.g., 2-amino-9*H*-pyrido[2,3-*b*]indole (A*a*C) and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]-indole (MeA*a*C) (4388) or 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) (4367),

TABLE 4.6
Components in Pyrolysates from Amino Acids (Proline and Glycine) and Proteins (Casein and Collagen) (1647)

	Amino Acid or Protein			
Pyrolysate Component[a]	**Casein**	**Collagen**	**Proline**	**Glycine**
Nitrogen compounds				
Hydrogen cyanide	+	+	+	+
Pyridine	+	+	+	+
Pyridine, 2-methyl-	+	+	+	+
Pyridine, 3-methyl-	+	+	+	+
Pyridine, 4-methyl-	+	+	+	+
Pyridine, 3-vinyl-	+	+	–	–
Aniline	+	+	+	–
Pyrrole	+	+	+	+
Quinoline	+	+	+	–
Isoquinoline	+	+	+	–
Indole	+	+	+	–
Benzonitrile	+	+	–	+
o-Tolunitrile	+	+	+	–
m-Tolunitrile	+	+	+	–
Cyclic hydrocarbons				
Benzene	+	+	+	–
Toluene	+	+	+	+
Styrene	+	+	–	+
Xylenes	+	+	–	+
Indene	+	+	–	+
Naphthalene	+	+	–	–
Fluorene	+	+	–	–
Phenols				
Phenol	+	+	–	–
o-Cresol	+	–	–	–
m-Cresol	+	+	–	–
p-Cresol	+	+	–	–
Phenol, ethyl-	+	+	–	–
Xylenol	+	+	–	–

+ indicates the presence of compound; – indicates the absence of the compound.
[a] In the publication by Higman et al., actual pyrolysis yield data are listed for each compound.

TABLE 4.7
Amino Acid–Derived *N*-Heterocyclic Amines

Compound		Mutagenicity[a], rev/µg		
Code	**Name**	**TA 98**	**TA 100**	**Level in CSC, ng/cig[b]**
IQ	Imidazo[4,5-*f*]quinoline, 2-amino-3-methyl-	433,000 490,000	7000	0.26
Trp-P-1	5*H*-Pyrido[4,3-*b*]indole, 3-amino-1,4-dimethyl-	39,000	1700	0.29–0.48
Trp-P-2	5*H*-Pyrido[4,3-*b*]indole, 3-amino-1-methyl-	104,200	1800	0.82–1.1
Glu-P-1	Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-6-methyl-	49,000	3200	0.37–0.89
Glu-P-2	Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-	1900	1200	0.25–0.88
A*a*C	9*H*-Pyrido[2,3-*b*]indole, 2-amino-	300	20	25–260
MeA*a*C	9*H*-Pyrido[2,3-*b*]indole, 2-amino-3-methyl-	200	120	2–37

[a] *S. typhimurium*, strain TA 98 or TA 100, with S-9 mix.
[b] See Hoffmann and Hoffmann (1740, 1741).

TABLE 4.8
Summary of Lists of Tumorigenic *N*-Heterocyclic Amines in Tobacco Smoke

Component	Hoffmann and Hecht (1727)	OSHA (2825)	Hoffmann and Hoffmann (1740, 1741)	MSS Level wt/cig, ng	IARC (1870) Evaluation of Evidence Re Tumorigenicity in	
					Laboratory Animals	Humans
Glu-P-1	–	–	+	0.37–0.89	Sufficient	–
Glu-P-2	–	–	+	0.25–0.88	Sufficient	–
Trp-P-1	–	–	+	0.29–0.48	Sufficient	–
Trp-P-2	–	–	+	0.82–1.1	Sufficient	–
A*a*C	–	–	+	25–260	Sufficient	–
MeA*a*C	–	–	+	2–37	Sufficient	–
IQ	–	–	+	0.26	Sufficient	Probable
PhIP	–	–	+	11–23	Sufficient	Possible
IQ	–	–	+	0.26	Sufficient	Probable

but also the reports on the tumorigenicity of several other *N*-heterocyclic amines in different laboratory animals (1835a, 2491a, 2849, 2849a, 2849b, 3862b, 3862c, 3865c).

Table 4.8 summarizes the reported MSS levels of the *N*-heterocyclic amines considered to be significant tumorigens by Hoffman and Hoffmann (1740, 1741) plus the assessment of the IARC (1870) on their tumorigenicity in laboratory animals and humans.

During tobacco growth, curing, aging, and/or the smoking process, the amino acids in tobacco may react with ammonia and/or amino acids to yield Amadori compounds which, when heated during the smoking process, will generate a variety of pyrazines [Green et al. (1376)]. Many of the pyrazines found in tobacco smoke are highly flavorful and contribute uniquely to the aroma and taste not only of tobacco smoke but also of a variety of consumer food products [Maga and Sizer (1973)] such as coffee, tea, cocoa, roasted peanuts, and roasted, broiled, or fried meats, poultry, and fish.

Table 4.9 lists the tobacco and/or smoke amino acids that, according to the Doull et al. listing (1073), are or have been used recently as components in flavor formulations for tobacco. In their tabulation of possible flavorants for tobacco smoking products, Leffingwell et al. (2341) listed the contributions to tobacco smoke taste and aroma of 23 amino acids added individually to cigarette tobacco filler.

Table 4.10 lists the amino acids and related compounds identified in tobacco, tobacco smoke, and tobacco substitute smoke. In Table 4.10, a total of 117 such components are listed of which 36 have been identified in smoke, 117 in tobacco, and 36 in both smoke and tobacco.

TABLE 4.9
Tobacco and/or Tobacco Smoke Amino Acids Used in Flavor Formulations

CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Identified in	
			Smoke	Tobacco
107-95-9	β-Alanine	β-Alanine	+	+
74-79-3	*L*-Arginine	*L*-Arginine	–	+
5794-13-8	*L*-Asparagine monohydrate	Asparagine	+	+
56-84-8	*L*-Aspartic acid	*l*-Aspartic acid	+	+
52-90-4	*L*-Cysteine	*L*-Cysteine	+	+
6899-05-4	*L*-Glutamic acid	*L*-Glutamic acid	+	+
6899-04-3	*L*-Glutamine	*L*-Glutamine	+	+
71-00-1	*L*-Histidine	*L*-Histidine	–	+
73-32-5	*DL*-Isoleucine	*DL*-Isoleucine	–	+
56-87-1	*L*-Lysine	*L*-Lysine	–	+
63-91-2	*L*-Phenylalanine	*L*-Phenylalanine	+	+
147-85-3	*L*-Proline	*L*-Proline	+	+
72-19-5	*L*-Threonine	*L*-Threonine	+	+
60-18-4	*L*-Tyrosine	*L*-Tyrosine	–	+
7004-03-7	Valine	Valine	+	+

TABLE 4.10
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	6898-94-8	Alanine	1910, 1914, 2858, 2939, 3266, 3555, 3797	1053, 1086, 2079, 3266, 3555, 3797	
2.	62-57-7	Alanine, 2-methyl-		429b, 4249, 4580, 4626, 5777	
3.	13100-82-8	Alanine, 3-sulfo-		3983b	
4.	107-95-9	β-Alanine H_2N-$(CH_2)_2$-COOH	1083, 1351, 1910, 1914, 2858, 2939, 3224, 3266, 3302, 3491, 3797, 4249, 4319, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2270, 2337, 2338, 2359, 2532, 2597a, 2795, 2911a, 2939, 3266, 3491, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 5079, 5603, 5785, 5811b, 5827, 5831, 5881, 5905	
5.	79-83-4 137-08-8	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- {pantothenic acid} HO-CH_2-$C(CH_3)_2$-CHOH-CO-NH-$(CH_2)_2$-COOH		429b, 1941, 4249, 4758, 5079	
6.	10478-42-9	β-Alanine, *N*-methyl-*N*-nitroso- {NMPA} {propanoic acid, 3-(methylnitrosamino)- H_3C-N(NO)-$(CH_2)_2$-COOH	3256, 3300, 3943a, 3944–3946, 5811b	466, 485, 503, 982, 2852, 3943a, 3944–3946, 3971, 3973, 5811b	
7.	133201-38-4	β-Alanine, *N*-(nitrosomethyl)-	4249	4249	
8.		β-Alanine, *N*-methyl-*N*-nitroso-, methyl ester H_3C-N(NO)-$(CH_2)_2$-$COOCH_3$	4249	4249	
9.	923-16-0	*D*-Alanine, *N*-*D*-alanyl-		1351, 2337, 2797, 3491, 4249	
10.	56-41-7	*L*-α-Alanine H_3C-$CH(NH_2)$-COOH	1083, 1351, 1914, 2724, 3491, 5811b	120, 158, 622, 749, 752–754, 826a, 1223, 1305a, 1351, 1493, 1918, 1919, 2799a, 2270, 2337, 2338, 2394a, 2453, 2529, 2532, 2597a, 2795, 2911a, 2911c, 3491, 3499, 3780, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4398c, 5079, 5603, 5699, 5785, 5811b, 5881, 5905, 5907	
11.	16124-24-6 25127-16-6	*L*-Alanine, *N*-(1-deoxy-D-fructos-1-yl)-		1063–1066, 1068–1074, 1351, 2337, 3639, 3797, 3923, 4362, 5811b	
12.	19701-89-4	*DL*-Alanine, *N,N*-dimethyl-	2882, 4249		
13.	7004-12-8	Arginine H_2N-C(=NH)-NH-$(CH_2)_3$-$CH(NH_2)$-COOH		826a, 2911c, 2939, 3491, 3705, 3973, 3974b, 4224, 4226, 4244, 4398c,, 5079, 5189, 5435, 5436, 5785, 5827	
14.	1069-09-6 34522-32-2	Arginine, *N*2-(1-carboxyethyl)- H_2N-C(=NH)-NH-$(CH_2)_3$-CH-[NH-$CH(CH_3)$-COOH]-COOH		3427a, 3973, 4249, 4688	

(*continued*)

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

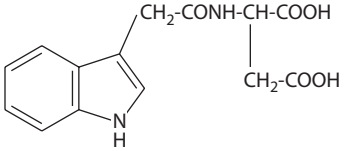
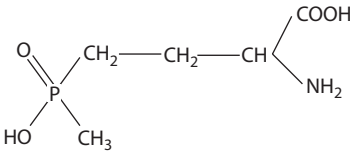
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
15.	74-79-3	*L*-Arginine H_2N-C(=NH)-NH-$(CH_2)_3$-CH(NH_2)-COOH	3797	120, 158, 555a, 555b, 622, 749, 751–756, 1053, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 1918, 1919, 2079, 2270, 2283, 2337, 2338, 2394a, 2453, 2532, 2597a, 2722, 2795, 2911c, 2939, 3266, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4244, 4249, 5811b	
16.	7006-34-0	Asparagine H_2N-CO-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 1965, 2724, 3266, 4159, 4249, 5811b	120, 480, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1223, 1305a, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2532, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4244, 4249, 4398c, 5048, 5079, 5126, 5189, 5437, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
17.	70-47-3	*L*-Asparagine		429b, 2338	
18.	5794-13-8	*L*-Asparagine monohydrate		3973	
19.	6899-03-2	Aspartic acid	3555	3555, 3705	
20.	56-84-8	*L*-Aspartic acid HOOC-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3797, 4159, 4249	120, 158, 480, 555a, 555b, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4159, 4224, 4226, 4244, 4249, 4359, 4398b, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
21.	31105-02-9	*L*-Aspartic acid *N*-(1-deoxy-*D*-fructos-1-yl)-		5811	
22.	2456-73-7	*L*-Aspartic acid, *N*-(1*H*-indol-3-ylacetyl)-  		4249, 4659	

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

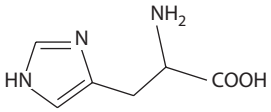
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
23.	80-60-4	Butanoic acid, 2-amino- $H_3C\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1580, 2939	480, 1329, 1351, 2337, 2597a, 2939, 3491, 3726, 3797, 3974a, 3978, 5785, 5811b, 5827, 5881, 5907	
24.	7004-04-8	Butanoic acid, 2-amino-3-hydroxy- $H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	429b	429b, 4249	
25.	1927-25-9	Butanoic acid, 2-amino-4-hydroxy-		5777, 5811, 5905	
26.	51276-47-2 53369-07-6	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®} 		5521	
27.	454-41-1	Butanoic acid, 2-amino-4-(methylsulfinyl)-		172, 429b, 4249	
28.	1118-85-0 3226-65-1	Butanoic acid, 2-amino-4-(methylsulfonyl)- {methionine sulfone; methionine S-oxide} $H_3C\text{-}SO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		120, 172, 1305a, 1351, 2337, 3491, 3729, 3797, 3974a, 4224, 4249, 5811b	
29.	2338-03-6	Butanoic acid, 2-amino-4-oxo-, (S)-		4249	
30.		Butanoic acid, 3-amino-		480	
31.	56-12-2	Butanoic acid, 4-amino- $H_2N\text{-}(CH_2)_3\text{-}COOH$	1083, 1351, 1580, 1910, 1914, 2724, 2858, 2939, 3302, 3491, 3797, 4249, 5811b	120, 480, 555a, 555b, 622, 749, 752–754, 826a, 927, 1086, 1223, 1351, 2270, 2337, 2338, 2532, 2597a, 2795, 2911c, 2939, 3491, 3555, 3705, 3797, 3974a, 3978, 4224, 4244, 4249, 4398c, 5079, 5699, 5811b, 5905	
32.	61445-55-4 133201-39-5	Butanoic acid, 4-(methylnitrosoamino)-Butanoic acid, 4-[(nitrosomethyl)amino] (NMBA) $CH_3\text{-}N(NO)\text{-}(CH_2)_3\text{-}COOH$	466, 486, 982, 2852, 3256, 3300, 3943a, 3944–3946, 3973, 5811b	486, 982, 2852, 3943a, 3944–3946, 3947, 3948, 3973, 5001, 5811b	
33.	462-10-2	Butanoic acid, 4,4′-dithiobis[2-amino- {homocystine} $[S\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH]_2$		2337, 3491, 3729, 3797, 3974a, 4224, 4226, 4249	
34.	498-40-8	Cysteic acid $HO\text{-}SO_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$		622, 1351, 2337, 3491, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079	
35.	52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto- (R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1274, 3265, 3266, 4249	120, 158, 172, 342, 722, 927, 1053, 1128b, 1305a, 1351, 1918, 2049, 2337, 2939, 3266, 3491, 3729, 3797, 3974a, 3978, 4224, 4249, 4398c, 5079, 5189, 5376, 5811b, 5874, 5881	
36.	636-58-8	*L*-Cysteine, *N*-*L*-γ-glutamyl-		4249	

(*continued*)

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
37.	24645-67-8	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-} $\{S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH\}_2$		116, 120, 172, 622, 722, 749, 752–754, 1063–1066, 1068–1074, 1127b, 1329, 1330, 1332, 1351, 2049, 2079, 2270, 2337, 2453, 2597a, 2939, 3491, 3499, 3705, 3729, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079, 5189, 5376, 5603, 5881, 5907	
38.	56-89-3 13028-62-1	*L*-Cystine		5811, 5811b	
39.	6899-05-4	Glutamic acid $HOOC\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	562, 563, 1083, 1351, 1910, 1914, 2079, 2724, 2858, 2939, 3059, 3061, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 563, 622, 749, 751–756, 826a, 927, 966, 1033, 1034, 1053, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2026, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4422, 5079, 5699, 5785, 5827, 5896, 5905, 5907	
40.	56-86-0	*L*-Glutamic acid	5811b	1053, 3266, 3973, 5811b	
41.	997-68-2	*L*-Glutamic acid, *N*-(5-amino-5-carboxypentyl)-, (S)-		429b, 4249, 4698	
42.	58-05-9	*L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-		429b	
43.	1116-22-9	*L*-Glutamic acid, *N*-*L*-γ-glutamyl-		1351, 2027, 2337	
44.	3929-61-1	*L*-Glutamic acid, *N*-*L*-α-glutamyl-		2027, 2337, 3491	
45.	6899-04-3	Glutamine $H_2N\text{-}CO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	562, 1910, 1914, 2939	1971, 2939, 3705	
46.	56-85-9	*L*-Glutamine	480, 562, 563, 1351, 1668, 1910, 1914, 1965, 2079, 2724, 2858, 2939, 3059, 3266, 3302, 3491, 3797, 4159, 4249	120, 480, 563, 622, 749, 751–756, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2529, 2532, 2939, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 5079, 5189, 5434, 5437, 5699, 5785, 5811b, 5827, 5831, 5881, 5905, 5907	

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
47.	56-40-6	Glycine $H_2N\text{-}CH_2\text{-}COOH$	1083, 1351, 1914, 2724, 2939, 3302, 3491, 3797, 4249, 5811b	120, 158, 480, 622, 722, 749, 751–756, 826a, 927, 1063–1066, 1068–1074, 1086, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5905, 17B59	
48.	18875-39-3	Glycine, labeled with ^{14}C {glycine-^{14}C}		2099b	
49.	4429-05-4	Glycine, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
50.	88476-94-2	Glycine, *N*-(1-nitroso-*L*-prolyl)-		3951, 4249	
51.	70-18-8	Glycine, *N*-(*N*-*L*-γ-glutamyl-*L*-cysteinyl)- {glutathione}		120, 1351, 1668, 2337, 2939, 3491, 3797, 3974a, 4249, 5079, 5220, 5572, 5811b	
52.	1071-83-6	Glycine, *N*-(phosphonomethyl)-		1121a	
53.	1118-68-9	Glycine, *N,N*-dimethyl- $(H_3C)_2{=}N\text{-}CH_2\text{-}COOH$		4249, 4528	
54.	73360-07-3	Glycine, *N*-[2-(2-aminoethoxy)ethenyl]-		4249	
55.	19246-18-5	Glycine, *N*-*L*-cysteinyl-		429b	
56.	20661-60-3	Glycine, *N*-methyl-*N*-nitro-		992	
57.	13256-22-9	Glycine, *N*-methyl-*N*-nitroso- {NSAR} $H_3C\text{-}N(NO)\text{-}CH_2\text{-}COOH$	1058, 2442, 3256	466, 485, 486, 498, 2442, 3947, 3948, 5001, 5811b	
58.	7006-35-1	Histidine		429b, 3797, 4249, 5699, 5785, 5831	
59.	71-00-1	*L*-Histidine  		120, 158, 553, 622, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5478, 5699, 5785, 5811b, 5831	
60.	332-80-9	*L*-Histidine, 1-methyl-	1083	1086, 1351, 2337, 2597a, 3491, 3797, 3974a, 3972, 4249	
61.	368-16-1	*L*-Histidine, 3-methyl-	1083	1086, 2597a	
62.	62504-27-2	*L*-Histidine, *N*-(1-carboxyethyl)-, (R)-		3565, 4249	
63.	454-29-5	*DL*-Homocysteine $HS\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		172	
64.	498-19-1 672-15-1	Homoserine {2-amino-4-hydroxybutanoic acid} $HO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	3557	1351, 2337, 2939, 3491, 3797, 3974a	

(*continued*)

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
65.	7004-09-3	Isoleucine H_3C-CH_2-CH(CH_3)-CH(NH_2)-COOH		3555, 3705, 3797, 3973, 4249, 4398c, 5079, 5413, 5699, 5785, 5827, 5831, 5905	
66.	1509-34-8	Isoleucine, allo-		3974b	
67.	73-32-5	*L*-Isoleucine H_3C-CH_2-CH(CH_3)-CH(NH_2)-COOH		120, 158, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 5811b	
68.	139681-66-6	*L*-Isoleucine, *N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-valyl)-*L*-phenylalanyl]-*L*-leucyl]-		4249	
69.	7005-03-0	*L*eucine $(H_3C)_2$═CH-CH_2-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5699, 5785, 5827, 5831, 5881, 5905	
70.	61-90-5	*L*-Leucine	5811b	424a, 2338, 3973, 5811b	
71.	139681-65-5	*L*-Leucine, *N*-[*N*-[*N*-[*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-phenylalanyl)-*L*-seryl]-*L*-leucyl]-*L*-leucyl]-*L*-methionyl]-*L*-valyl]-*L*-valyl]-		4249	
72.	6899-06-5	Lysine		429b, 2911c, 3973, 4398c, 5079, 5623, 5785, 17B59	
73.	1190-94-9 28902-93-4	Lysine, hydroxy-		726, 749, 752–754, 4249	
74.	56-87-1	*L*-Lysine H_2N-(CH_2)$_4$-CH(NH_2)-COOH		120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 5811b	
75.	7005-18-7	Methionine		116, 120, 3705, 4249, 5907	

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
76.	63-68-3	*L*-Methionine $H_3C\text{-}S\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		116, 120, 158, 172, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1127b, 1305a, 1329, 1330, 1332, 1351, 1493, 2049, 2270, 2337, 2359, 2532, 2597a, 2795, 2939, 3186, 3188, 3266, 3491, 3499, 3705, 3729, 3797, 3973, 3974a, 3978, 4226, 4249, 4398c, 5079, 5376, 5811b, 5907	
77.	20236-97-9	*D*-Methionine, *N*-(carboxyacetyl)-		4249	
78.	327-57-1 5157-09-5	Norleucine {2-aminohexanoic acid} $H_3C\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		1351, 2337, 2597a, 3491, 3797, 3974a, 3978, 4249	
79.	7006-33-9	Ornithine {2,3-diaminopentanoic acid} $H_2N\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 2858, 2939, 3302, 3491, 3797, 4249	555a, 622, 749, 752–754, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 2597a, 2795, 3491, 3705, 3797, 3973, 3974a, 3978, 4249, 5827, 17B34	
80.	70-26-8	*L*-Ornithine	429b, 5811b	429b, 5811b	
81.	20197-09-5	*L*-Ornithine, *N*2-(1-carboxyethyl)-, (R)-		3565, 4249	
82.	372-75-8	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline} $H_2N\text{-}CO\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		120, 622, 1305a, 1329, 1330, 1332, 1351, 2337, 2939, 3491, 3797, 3973, 3974a, 3978, 4249, 4398c, 5079	
83.	6600-40-4	Pentanoic acid, 2-amino-		5777	
84.	63316-29-0	Pentanoic acid, 5-amino-2-hydroxy-, (R)-		5811, 5811b	
85.	63-91-2	*L*-Phenylalanine $C_6H_5\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3797, 4159, 4249, 5811b	120, 158, 622, 722, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1102, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 02359, 2394a, 2453, 2532, 2597a, 2795, 2903, 2905, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3829, 3973, 3974a, 3975, 3978, 4098a, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5811b, 5831, 5905, 5907	
86.	31105-03-0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
87.	51064-37-0	Phenylalanine, ar,ar-dihydroxy-		4249	

(*continued*)

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

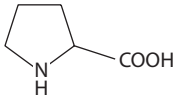
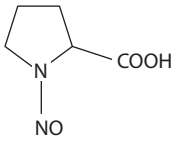
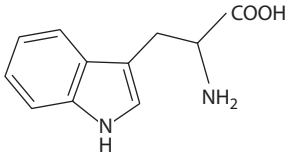
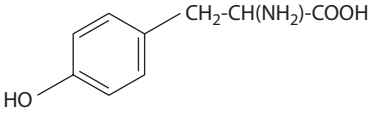
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
88.	147-85-3	*L*-Proline 	1351, 1910, 1914, 1933, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249, 4319	120, 158, 480, 486, 749, 751–756, 826a, 927, 1033, 1053, 1063–1066, 1068–1074, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1933a, 1971, 2133, 2270, 2337, 2394a, 2395, 2453, 2529, 2532, 2592, 2597a, 2795, 2858, 2911c, 2914, 2939, 3059, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4226, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5881, 5896, 5905, 5907	
89.		*L*-Proline, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
90.		Proline, hydroxy-		5907	
91.	18610-59-8	*L*-Proline, 1-hydroxy-		1063–1066, 1068–1074, 1351, 2337, 2394a, 2597a, 3491, 3797, 3973, 3974a, 4224, 4226	
92.	7519-36-0	*L*-Proline, 1-nitroso- {NPRO} 	204–206, 486, 499, 509, 1058, 1673, 1695, 1719, 1870, 1871, 3256, 3260, 3300, 3943a, 3944–3946, 3951	466, 468, 485, 486, 498, 499, 511, 992, 1870, 1871, 3256, 3566, 3943a, 3944–3946, 3947, 3948, 3973, 4130, 4249, 5811b	
93.	147427-29-0	*L*-Proline,1-[1-[1-(1-*L*-seryl-*L*-prolyl)-*L*-prolyl]-*L*-prolyl]-		4249	
94.	62137-28-4	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-,*trans*-		4249, 4429	
95.	62137-29-5	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-ar abinofuranosyl)oxy]-, *trans*-		4249, 4429	
96.	51-35-4	*L*-Proline, 4-hydroxy-, *trans*-		120, 1305a, 5811b	
97.	30310-80-6	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}		486, 3300. 3947, 3948, 5811b	
98.	6898-95-9	Serine $HO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 2858, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1063–1066, 1068–1074, 1223, 1305a, 1351, 1493, 1918, 1919, 2048, 2270, 2337, 2338, 2339b, 2445a, 2453, 2532, 2597a, 2795, 2911a, 2911c, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c 5079, 5699, 5827, 5831, 5881, 5896, 5905, 5907	

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
99.	35688-48-3	*D*-Serine, *N*-(carboxyacetyl)-		2048, 4249, 4728	
100.	56-45-1	*L*-Serine		3973, 5811b	
101.	5147-00-2	*L*-Serine, acetate (ester) CH_3-COO-CH_2-CH(NH_2)-COOH		429b, 4249, 4895	
102.	5692-15-9	*L*-Serine, labeled with ^{14}C {*L*-serine-^{14}C}		4249, 4940	
103.	142785-07-7	*L*-Serine,*L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		4249	
104.	146440-48-4	*L*-Serine,*L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		4249	
105.	72-19-5	*L*-Threonine H_3C-CHOH-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3555, 3797, 4249, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1305a, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5811b, 5827, 5831, 5881	
106.	32190-57-1	*L*-Threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]-		3819a, 4249	
107.		*L*-Threonine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337	
108.	6912-86-3	Tryptophan		3705	
109.	73-22-3	*L*-Tryptophan 		120, 480, 622, 722, 749, 751–756, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 2079, 2270, 2337, 2338, 2359, 2510, 2532, 2597a, 2795, 2902, 2903, 2911c, 2939, 3491, 3705, 3797, 3829, 3973, 3974a, 3978, 4103, 4224, 4244, 4249, 4286b, 4398c, 5079, 5603, 5785, 5811b, 5831, 5881, 5905	
110.	60738-11-6	*L*-Tryptophan, labeled with ^{14}C {*L*-tryptophan-^{14}C}		2562a, 4249, 4876	
111.	55520-40-6	Tyrosine		3705	
112.	587-45-1	Tyrosine, 3-hydroxy-		429b	

(*continued*)

TABLE 4.10 (continued)
Amino Acids and Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
113.	60-18-4	*L*-Tyrosine 		120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1965, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4398c, 5079, 5785, 5811b, 5827, 5905, 5907	
114.	34393-22-1	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
115.	7004-03-7	Valine $(H_3C)_2$═CH-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4249, 4359, 4398c, 5079, 5493, 5785, 5827, 5831, 5881, 5905, 5907	
116.	72-18-4	*L*-Valine	5811b	424a, 429b, 2338, 5811b	
117.		*L*-Valine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	

5 Esters

While no esters were reported in tobacco smoke by Kosak (2170) in his 1954 compilation of reported tobacco smoke components, the number of esters in tobacco and/or its smoke has increased dramatically over the years and now exceeds 1000. In 1955, Latimer (2270) collated and reported component data from chemical abstracts and listed only one set of esters reported in tobacco and its smoke, the "glycerides." In 1959, Johnstone and Plimmer (1971) listed 16 identified esters from these two sources. Between the Johnstone and Plimmer review and that of Stedman (3797) in 1968, the number of identified esters in tobacco and/or smoke escalated to over 300.

The research leading to the major part of the increase involved identification of the following classes of esters: (1) esters from long-chained aliphatic alcohols and saturated and unsaturated acids, (2) esters from solanesol and acetic acid and numerous saturated and unsaturated acids, (3) esters from several phytosterols and numerous saturated and unsaturated acids, and (4) β-amyrin and numerous saturated and unsaturated acids.

One other significant finding that stimulated much subsequent research on sugar esters was the isolation, identification, and synthesis of a specific ester in Oriental tobacco by Schumacher (3535) in 1960 and its identification a year later in Oriental tobacco smoke by Rodgman and Cook (3278). The ester was 6-acetyl-2,3,4-*tris*-*d*-3-methylvaleryl-β-*D*-glucopyranoside, i.e., glucose esterified with the two aliphatic acids, acetic and 4-methylpentanoic (β-methylvaleric). The Schumacher research leading to the identification of this ester was described in detail by Green and Rodgman (1373) during the Symposium of the *50th Tobacco Research Chemists' Conference*.

In his 1968 review of tobacco and smoke components, Stedman [see p. 165 and Table VI in (3797)] discussed at some length the procedures used to identify 272 esters of long-chained aliphatic alcohols in tobacco smoke. However, Stedman not only failed to cite the source of his discussion, an article by Rodgman et al. (3294), but also omitted from his text and ester tabulation that an identical series of esters was identified by Rodgman et al. in an aliphatic ester fraction obtained from Rowland and Latimer who had isolated the fraction from flue-cured tobacco (3358) during their 1958 study of the solanesyl esters in tobacco.

The identification of the numerous esters in the aliphatic ester fraction from tobacco and smoke led to the identification of a series of solanesyl and phytosteryl esters of saturated and unsaturated aliphatic acids in tobacco and smoke (3296) and a similar series of β-amyrin esters in tobacco by Fredrickson (1230).

As mentioned previously, the characterization of the glucose ester in tobacco by Schumacher (3535) and the discovery that it generated the flavorful acid, 4-methylpentanoic (β-methylvaleric) during the smoking process, led many years later to a series of studies aimed at determining the structure of the sucrose esters in tobacco. Despite the numerous studies, seldom was the precise structure of a sucrose ester defined. The various studies included those of Rivers (3185) in the early 1980s and of Severson et al. (3606), Schlotzhauer et al. (3473), Wahlberg et al. (4102), and Danehower (896) in the mid- to late 1980s.

Several studies on tobacco and tobacco smoke composition, including studies of the long-chained aliphatic ester fraction, ultimately led to an interesting extrapolation by Green and Rodgman [see endnote 39 in (1373)] on the number of smoke components. Because of the limitations of analytical technology at the time of the Rodgman et al. study (3294) on the long-chained aliphatic ester fraction from tobacco and smoke, the higher-molecular-weight esters could neither be determined nor characterized. However, it was noted that qualitatively the tobacco ester fraction and the smoke ester fraction were similar: Every ester identified by Rodgman et al. in the smoke ester fraction was found in the tobacco ester fraction. Minor quantitative differences between the levels of individual esters in the two fractions were observed. With much improved analytical technology in the late 1980s, Arrendale et al. (103) in their study on the long-chained aliphatic ester fraction in tobacco were able to identify not only many of the esters identified earlier in tobacco and smoke by Rodgman et al. but also many more higher-molecular-weight esters. Logic would dictate that if every ester identified in the Rodgman et al. study was present in both tobacco and smoke, then every tobacco ester identified by Arrendale et al. when included in the smoke list results in a substantial increase in the number of smoke components.

Examination of the esters listed in Table 5.3 indicates that most of the esters identified in tobacco smoke are found in the particulate phase. An ester that exists predominantly in the vapor phase of tobacco smoke and was identified in cigarette MSS vapor phase by Laurene (2310) in 1959 and Grob (1413) in 1962 was the methyl ester of acetic acid. Since then, acetic acid methyl ester has been identified in cigarette MSS vapor phase in over 50 different studies.

Because many esters have an aroma and/or taste acceptable to the consumer, the list of individual compounds used as tobacco ingredients by U.S. tobacco manufacturers contains numerous esters. Such a list was prepared by Doull et al. (1053) from information provided by the U.S. tobacco product manufacturers. A detailed examination of the Doull et al. list by Rodgman (3266) revealed that many of the added ingredients had been identified in additive-free tobacco and/or its smoke.

As Rodgman noted, the compounds added as ingredients to cigarette tobacco may fall into one of the following categories:

- It is a component of one or more of the tobacco types (flue-cured, Oriental, burley, Maryland) commonly used in cigarette blends.
- It is a component of cigarette MSS.
- It is a component of both tobacco and tobacco smoke.
- It is not a component of either the tobaccos or their smoke.

An ingredient compositionally similar to but not identical with a tobacco leaf or smoke component may be categorized in two ways: It is either an isomer or a homolog of a compound identified in natural tobacco leaf and/or its smoke. As noted, there are compounds used as cigarette ingredients that do not fall into any of the first three categories listed.

In the broad spectrum of chemistry, biochemistry, and biology, cases exist where the properties of one homolog vary significantly from those of another or where the properties of one isomer differ significantly from those of another. For example, whether classified as a "Group 2A carcinogen" by the International Agency for Research on Cancer (IARC) (1868a), or a significant carcinogen in cigarette MSS (1727), or overall as a borderline carcinogen by others (983), the specific tumorigenicity of mouse skin painted or subcutaneously injected benz[*a*]anthracene (B[*a*]A) is insignificant compared to that of its homolog, 7,12-dimethylbenz[*a*]anthracene (DMB[*a*]A), one of the four most potent tumorigenic polycyclic aromatic hydrocarbons (PAHs) known (983). The isomeric $C_{20}H_{12}$ PAHs benzo[*e*]pyrene (B[*e*]P) and benzo[*a*]pyrene (B[*a*]P) differ markedly in their specific tumorigenicities in studies involving mouse skin painting or subcutaneous injection (983). B[*e*]P under the usual laboratory test conditions is found to be essentially nontumorigenic on skin painting or subcutaneous injection, whereas the isomeric B[*a*]P under the same conditions is one of the most potent tumorigens known.

Of the 460 individual ingredients listed by Doull et al. [1053, see Table 1 in (3266)], 117 (25%) are esters (Table 5.1) and all have been approved for use by the U.S. Food and Drug Administration or by the Flavor and Extract Manufacturers Association (FEMA). Of the 117 esters listed by Doull et al., 46 (39%) have been identified in untreated cigarette tobacco and/or its smoke (indicated by + in Table 5.1), and 18 are either a homolog (indicated by H in Table 5.1) or an isomer (indicated by I in Table 5.1) of a known tobacco and/or smoke component.

Doull et al. (1053) also listed 146 mixtures reportedly used by U.S. manufacturers as flavoring ingredients in tobacco products [see Table 2 in (3266)]. Many of these mixtures are obviously multicomponent items, and detailed analyses of several of them (cardamom, cocoa, coffee, davana, licorice) indicated the presence of esters [see Table 3 in (3266)] listed by Doull et al. (1053). A similar situation exists with regard to flavorful mixtures used on tobacco products by non-U.S. manufacturers. Some 34 such mixtures are used on tobacco products by non-U.S. manufacturers [172a, 174a, 174b, 174c, see Table 7B in (3266)].

Compounds (48 in number) other than those in the Doull et al. list are used in tobacco products by manufacturers in countries other than the United States [172a, 174a, 174b, 174c, see Table 7A in (3266)]. Among the 48 esters are 19 (21%) that have been identified in untreated cigarette tobacco and/or its smoke (indicated by + in Table 5.2).*

Table 5.3 lists the 1094 esters identified to date in tobacco and/or tobacco smoke; 643 have been identified in tobacco smoke, 987 in tobacco, and 536 in both tobacco and/or tobacco smoke.

* Inadvertently, two esters (methyl anthranilate and methyl 2-octynate) already included in Table 1 in (3266) were included in Table 7A in (3266).

TABLE 5.1
Esters Used as Tobacco Ingredients by U.S. Tobacco Product Manufacturers (1053)

CAS No.	Chemical Abstracts Nomenclature	Identified in Smoke	Identified in Tobacco
123-86-4	Acetic acid, butyl ester	+	+
151-05-3	Acetic acid, 1,1-dimethyl-2-phenylethyl ester	–	–
115-95-7	Acetic acid, 3,7-dimethyl-1,6-octadien-6-yl ester	–	+
105-87-3	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl ester	–	–
141-78-6	Acetic acid, ethyl ester	+	+
112-06-1	Acetic acid, heptyl ester	H	H
3681-71-8	Acetic acid, 3-hexen-1-yl ester	–	–
142-92-7	Acetic acid, hexyl ester	–	+
123-92-2	Acetic acid, 3-methylbutyl ester	–	–
80-26-2	Acetic acid, 2-(4-methyl-3-cyclohex-1-yl)-2-propyl ester	+	+
89-48-5	Acetic acid, 5-methyl-2-(1-methylethyl)-cyclohexanyl ester	–	–
140-39-6	Acetic acid, 4-methylphenyl ester	–	–
110-19-0	Acetic acid, 2-methylpropyl ester	–	–
143-13-5	Acetic acid, nonyl ester	–	H
2442-10-6	Acetic acid, 1-octen-3-yl ester	–	–
24851-98-7	Acetic acid, 2-pentyl-3-oxo-1-cyclopentyl-, methyl ester	–	–
93-92-5	Acetic acid, 1-phenethyl ester	–	+
103-45-7	Acetic acid, 2-phenethyl ester	+	+
103-54-8	Acetic acid, 3-phenyl-2-propenyl ester	–	–
122-72-5	Acetic acid, 3-phenylpropyl ester	–	–
76-49-3	Acetic acid, *endo*-1,7,7-trimethylbicyclo[2,2,1]heptan-2-yl ester	–	–
125-12-2	Acetic acid, *exo*-1,7,7,-trimethylbicyclo[2,2,1]heptan-2-yl ester	–	–
141-97-9	Acetoacetic acid, ethyl ester	–	–
122-43-0	Benzeneacetic acid, butyl ester	H	H
101-97-3	Benzeneacetic acid, ethyl ester	–	+
102-22-7	Benzeneacetic acid, 3,7-dimethyl-2,6-octadieny-1-yl ester	–	–
5421-17-0	Benzeneacetic acid, hexyl ester	–	–
101-41-7	Benzeneacetic acid, methyl ester	+	+
102-19-2	Benzeneacetic acid, 3-methylbutyl ester	–	–
101-94-0	Benzeneacetic acid, 4-methylphenyl ester	–	–
102-13-6	Benzeneacetic acid, 2-methylpropyl ester	–	–
102-20-5	Benzeneacetic acid, phenylethyl ester	–	H
104-21-2	Benzenemethanol, 4-methoxy-, acetate	+	–
122-91-8	Benzenemethanol, 4-methoxy-, formate	–	–
102-17-0	Benzenemethanol, 4-methoxy-, phenylacetate	–	–
93-89-0	Benzoic acid, ethyl ester	+	+
93-58-3	Benzoic acid, methyl ester	+	+
120-51-4	Benzoic acid, phenylmethyl ester	+	+
134-20-3	Benzoic acid, 2-amino-, methyl ester	–	+
118-61-6	Benzoic acid, 2-hydroxy-, ethyl ester	–	+
119-36-8	Benzoic acid, 2-hydroxy-, methyl ester	–	+
87-19-4	Benzoic acid, 2-hydroxy-, 2-methylpropyl ester	–	–
118-55-8	Benzoic acid, 2-hydroxy-, phenyl ester	–	–
118-58-1	Benzoic acid, 2-hydroxy-, phenylmethyl ester	–	+
121-98-2	Benzoic acid, 4-methoxy-, methyl ester	–	–
94-46-2	Benzoic acid, 3-methylbutyl ester	–	+
106-65-0	Butanedioic acid, dimethyl ester	+	–
109-21-7	Butanoic acid, butyl ester	H	H
10094-34-5	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester	–	–
106-29-6	Butanoic acid, 3,7-dimethyl-2,6-octadien-1-yl ester	–	–
141-16-2	Butanoic acid, 3,7-dimethyl-6-octenyl ester	–	–
105-54-4	Butanoic acid, ethyl ester	+	+

(*continued*)

TABLE 5.1 (continued)
Esters Used as Tobacco Ingredients by U.S. Tobacco Product Manufacturers (1053)

CAS No.	Chemical Abstracts Nomenclature	Identified in	
		Smoke	Tobacco
106-27-4	Butanoic acid, 3-methylbutyl ester	–	–
540-18-1	Butanoic acid, pentyl ester	–	–
103-52-6	Butanoic acid, phenylethyl ester	H	H
103-37-7	Butanoic acid, phenylmethyl ester	+	+
7452-79-1	Butanoic acid, 2-methyl-, ethyl ester	I	I
10032-15-2	Butanoic acid, 2-methyl-, hexyl ester	–	–
109-19-3	Butanoic acid, 3-methyl-, butyl ester	H	H
1009-20-6	Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadieny-1-yl ester	–	
108-64-5	Butanoic acid, 3-methyl-, ethyl ester	+	+
556-24-1	Butanoic acid, 3-methyl-, methyl ester	–	+
659-70-1	Butanoic acid, 3-methyl-, 3-methylbutyl ester	–	–
55066-56-3	Butanoic acid, 3-methyl-, 4-methyylphenyl ester	–	–
140-26-1	Butanoic acid, 3-methyl-, phenethyl ester	–	+
140-27-2	Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester	–	–
10544-63-5	2-Butenoic acid, ethyl ester	–	H
110-40-7	Decanedioic acid, diethyl ester	–	–
110-38-3	Decanoic acid, ethyl ester	–	+
106-33-2	Dodecanoic acid, ethyl ester	–	+
77-83-8	Ethyl methylphenylglycidate	–	–
105-86-2	Formic acid, 3,7-dimethyl-2,6-octadien-1-yl ester	–	–
33467-73-1	Formic acid, 3-hexenyl ester	–	+
110-45-2	Formic acid, 3-methylbutyl ester	–	–
638-49-3	Formic acid, pentyl ester	–	–
	2-Furancarboxylic acid, ethyl ester	H	–
611-13-2	2-Furancarboxylic acid, methyl ester	+	+
126-14-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate	–	–
106-30-9	Heptanoic acid, ethyl ester	–	+
628-97-7	Hexadecanoic acid, ethyl ester	+	+
123-66-0	Hexanoic acid, ethyl ester	+	+
2198-61-0	Hexanoic acid, 3-methylbutyl ester	–	–
123-68-2	Hexanoic acid, 2-propenyl ester	–	–
123-29-5	Nonanoic acid, ethyl ester	–	+
112-63-0	9,12-Octadecadienoic acid (*Z,Z*), methyl ester	+	+
111-61-5	Octadecanoic acid, ethyl ester	–	+
301-00-8	9,12,15-Octadecatrienoic acid, methyl ester	+	+
111-62-6	9-Octadecenoic acid, ethyl ester	–	+
106-32-1	Octanoic acid, ethyl ester	–	+
2035-99-6	Octanoic acid, 3-methylbutyl ester	–	–
638-25-5	Octanoic acid, pentyl ester	–	–
111-12-6	2-Octynoic acid, methyl ester	–	–
539-82-2	Pentanoic acid, ethyl ester	+	+
539-88-8	Pentanoic acid, 4-oxo-, ethyl ester	–	H
102-76-1	1,2,3-Propanetriol, triacetate	+	–
105-53-3	Propanedioic acid, diethyl ester	H	H
105-37-3	Propanoic acid, ethyl ester	+	+
122-63-4	Propanoic acid, phenylmethyl ester	–	–
103-56-0	Propanoic acid, 3-phenyl-2-propenyl ester	–	–
7492-70-8	Propanoic acid, 2-butoxy-, butyl ester	–	–
97-64-3	Propanoic acid, 2-hydroxy-, ethyl ester	+	–
97-89-2	Propanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester	–	–
65416-14-0	Propanoic acid, 2-methyl-, 2-methyl-4-oxo-4*H*-pyran-3-yl ester	–	–
103-93-5	Propanoic acid, 2-methyl-, 4-methylphenyl ester	–	–
109-15-9	Propanoic acid, 2-methyl-, octyl ester	–	–

TABLE 5.1 (continued)
Esters Used as Tobacco Ingredients by U.S. Tobacco Product Manufacturers (1053)

CAS No.	Chemical Abstracts Nomenclature	Identified in Smoke	Identified in Tobacco
103-48-0	Propanoic acid, 2-methyl-, phenylethyl ester	H	H
103-36-6	2-Propenoic acid, 3-phenyl-, ethyl ester	+	–
103-26-4	2-Propenoic acid, 3-phenyl-, methyl ester	H	–
7779-65-9	2-Propenoic acid, 3-phenyl-, 3-methylbutyl ester	H	–
122-67-8	2-Propenoic acid, 3-phenyl-, 2-methylpropyl ester	H	–
103-53-7	2-Propenoic acid, 3-phenyl-, phenylethyl ester	H	–
103-41-3	2-Propenoic acid, 3-phenyl-, phenylmethyl ester	+	–
122-69-0	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester	+	–
	2-Propenoic acid, 3-phenyl-, 3-phenylpropyl ester	–	–
93-60-7	3-Pyridinecarboxylic acid, methyl ester	+	+
124-06-1	Tetradecanoic acid, ethyl ester	–	+
	Undecanoic acid, butyl ester	–	H

H, a homolog of an identified tobacco and/or smoke component; I, an isomer of an identified tobacco and/or smoke component.

TABLE 5.2
Esters Used as Tobacco Ingredients by Tobacco Product Manufacturers Outside of the United States

CAS No.	Chemical Abstracts Nomenclature	Identified in Smoke	Identified in Tobacco
141-12-8	Acetic acid, 3,7-dimethyl-2,8-octadien-1-yl ester	–	–
150-84-5	Acetic acid, 3,7-dimethyl-6-octen-1-yl ester	–	–
2497-18-9	Acetic acid, 2-hexen-1-yl ester	–	+
126-64-7	Benzoic acid, 3,7-dimethyl-1,6-octadien-6-yl ester	–	–
87-20-7	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester	–	+
539-90-2	Butanoic acid, 2-methylpropyl ester	–	–
76-50-6	Butanoic acid, 3-methyl-, *endo*-1,7,7-trimethylbicyclo[2,2,1]heptan-2-yl ester	–	+
103-38-8	Butanoic acid, 3-methyl-, phenylmethyl ester	–	+
16409-46-4	Butanoic acid, 3-methyl-, 5-methyl-2-(1-methylethyl)-cyclohexanyl ester	–	–
104-57-4	Formic acid, phenylmethyl ester	–	+
540-07-8	Hexanoic acid, pentyl ester	–	–
591-68-4	Pentanoic acid, butyl ester	–	–
7549-33-9	Propanoic acid, anisyl ester	–	–
105-68-0	Propanoic acid, 3-methylbutyl ester	–	–
103-28-6	Propanoic acid, 2-methyl-, phenylmethyl ester	–	+
78-35-3	Propanoic acid, 2-methyl-, 3,7-dimethyl-1,6-octadien-6-yl ester	–	–
97-62-1	Propanoic acid, 2-methyl-, ethyl ester	–	–
103-59-3	Propanoic acid, 2-methyl-, 3-phenyl-2-propen-1-yl ester	–	–
110-27-0	Tetradecanoic acid, 1-methylethyl ester	–	–

TABLE 5.3
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

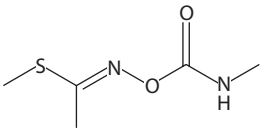
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	5371-49-3	Acetaldehyde, (acetyloxy)-	568b, 3553, 3653, 4249, 5811b	568b, 2336, 2337a, 4249	
2.	16752-77-5	Acetamidic acid, thio-, *N*-[(methylcarbamoyl)oxy]-, methyl ester {Methomyl®} 		1219, 1219b, 1219c, 2650b, 3633, 3977, 4271a	
3.	13831-30-6	Acetic acid, (acetyloxy)- CH_3-COO-CH_2-COOH	568b, 1375a, 1377, 2387, 3553, 4249, 5811b	568b, 2336, 4249	1375a, 1377, 2387
4.	162188-92-3	Acetic acid, bromo-, 7,9,9-trimethyl-8-oxo-1, 4-dioxaspiro[4.5]dec-7-yl ester, (±)-		4249	
5.	123-86-4	Acetic acid, butyl ester {butyl acetate} CH_3-COO-C_4H_9	222–224, 568b, 1140, 1416, 1422, 1445, 3266, 3302, 3797, 4249	172a, 174b, 568b, 1053, 1063, 1422, 2339a, 3186, 3188, 3266, 3905, 4249	
6.	162188-93-4	Acetic acid, (diethoxyphosphinyl)-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro[4.5]dec-7-yl ester, (±)-		4249	
7.	105-87-3	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl, (*E*)- ester {geranyl acetate}		172a, 174b, 1053, 3266, 3370	
8.	141-12-8	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl, (*Z*)- ester {neryl acetate}		174b, 3266	
9.	150-84-5	Acetic acid, 3,7-dimethyl-6-octen-1-yl ester {citronellyl acetate}		174b, 3266	
10.	151-05-3	Acetic acid, 1,1-dimethyl-2-phenylethyl ester		1053, 3266, 3370	
11.	112-66-3	Acetic acid, 1-dodecyl ester CH_3-COO-$(CH_2)_{11}$-CH_3		174b, 568b, 3266, 4249	
12.	108-05-4	Acetic acid, ethenyl ester {vinyl acetate} CH_3-COO-CH═CH_2	239, 1140, 1437, 2782, 2799a, 3219, 3300, 3302, 3308, 3797, 4005–4007, 4249, 5811b, 5869a		642
13.	141-78-6	Acetic acid, ethyl ester {ethyl acetate} CH_3-COO-C_2H_5	565, 1140, 1375, 1375a, 1375b, 1377, 1378, 1413, 1414, 1416, 1418, 1445, 1449, 1590, 1903–1905, 1907, 2088, 2782, 2804, 2858, 2939, 3254, 3266, 3308, 3508, 3530, 3553, 3797, 4249, 4319, 5811b	120, 1053, 1063, 1590, 2339a, 2389, 2544, 2861a, 2939, 3266, 3797, 3973, 3974a, 4249, 5811b	1375a, 1377, 1378
14.	112-06-1	Acetic acid, heptyl ester		1053, 3266	
15.	629-70-9	Acetic acid, 1-hexadecyl ester CH_3-COO-$(CH_2)_{15}$-CH_3		404	
16.	142-92-7	Acetic acid, hexyl ester {hexyl acetate} CH_3-COO-$(CH_2)_5$-CH_3	1157, 4249	172a, 174b, 1053, 1063, 1157, 3266, 3370, 4249	
17.	623-50-7	Acetic acid, hydroxy-, ethyl ester $HOCH_2$-COO-C_2H_5	3255, 3553, 4249		
18.	61892-60-2	Acetic acid, hydroxy-, 2-hydroxypropyl ester $HOCH_2$-COO-CH_2-CHOH-CH_3	568b, 3553, 4249, 5811b	568b, 2389, 2544, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
19.	96-35-5	Acetic acid, hydroxy-, methyl ester $HOCH_2$-COO-CH_3	3553, 3557, 4249, 5811b		
20.	90357-58-7	Acetic acid, hydroxy-, propyl ester $HOCH_2$-COO-C_3H_7	3553	2389, 2544, 3550	
21.		Acetic acid, hydroxymethyl ester CH_3-COO-CH_2OH	2767, 4249		
22.	79-20-9	Acetic acid, methyl ester CH_3-COO-CH_3	37, 38, 112, 314, 568b, 605, 1140, 1284, 1338, 1348–1350, 1365, 1375, 1375a, 1375b, 1377, 1413, 1414, 1416, 1418, 1419, 1449, 1495, 1586, 1589, 1634, 1637, 1875, 2301, 2310, 2543, 2545, 2765, 2767, 2777, 2782, 2804, 2857, 2939, 3132, 3302, 3308, 3530, 3553, 3557, 3797, 4104, 4249, 4257, 4319, 5770, 5811b	568b, 1157, 1550, 2339a, 4249, 5811b	1375a, 1377
23.	624-41-9	Acetic acid, 2-methylbutyl ester CH_3-COO-CH_2-CH(CH_3)-CH_2-CH_3		2339a	
24.	123-92-2	Acetic acid, 3-methylbutyl ester CH_3-COO-$(CH_2)_2$-CH═$(CH_3)_2$		404, 1053, 2339a, 3266	
25.	1191-16-8	Acetic acid, 3-methyl-2-butenyl ester CH_3-COO-CH_2-CH═C═$(CH_3)_2$		404	
26.	108-21-4	Acetic acid, 1-methylethyl ester CH_3-COO-CH═$(CH_3)_2$	568b, 1378, 4249	568b, 2917a, 4249	1378
27.	35897-16-6	Acetic acid, 2-methyl-3-pentyl ester CH_3-COO-CH(C_2H_5)-CH═$(CH_3)_2$		2917a	
28.	140-39-6	Acetic acid, 4-methylphenyl ester {*p*-tolyl acetate}		172a, 174b, 1053, 3266, 3370	
29.	110-19-0	Acetic acid, 2-methylpropyl ester {isobutyl acetate} CH_3-COO-CH_2-CH═$(CH_3)_2$		172a, 174b, 1053, 2339a, 3266, 3370	
30.	143-13-5	Acetic acid, nonyl ester		1053, 3266, 3370, 5811	
31.	2442-10-6	Acetic acid, 1-octen-3-yl ester		1053, 3266, 3370	
32.	112-14-1	Acetic acid, octyl ester		5811	
33.	628-63-7	Acetic acid, pentyl ester CH_3-COO-$(CH_2)_4$-CH_3		1157, 4249	
34.	24851-98-7	Acetic acid, 2-pentyl-3-oxo-1-cyclopentyl-, methyl ester {methyl dihydrojasmonate}		172a, 174b, 1053, 3266	
35.	103-45-7	Acetic acid, 2-phenylethyl ester {2-phenethyl acetate} CH_3-COO-$(CH_2)_2$-C_6H_5	568b, 937, 3224, 3266, 3302, 3794, 4249, 5811b	120, 172a, 174b, 404, 568b, 937, 1053, 1063, 2339a, 2386, 2389, 2544, 2611, 2861a, 2917a, 2939, 3266, 3354, 3370, 3543, 3547, 3560, 3561, 3905, 3973, 3974a, 4249, 5811b	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

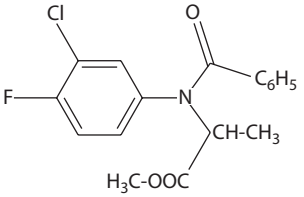
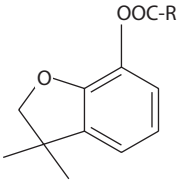
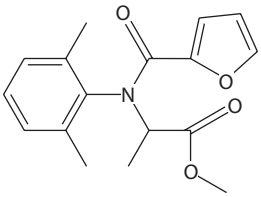
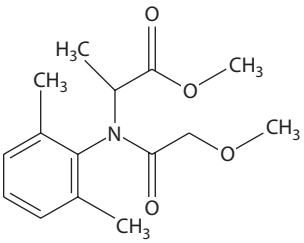
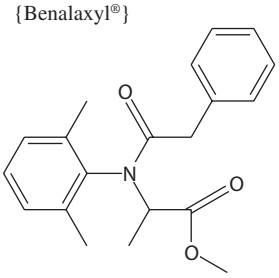
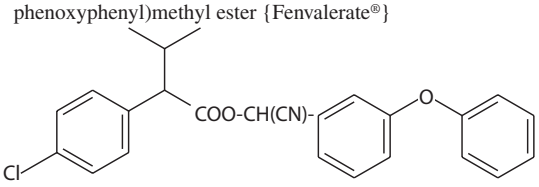
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
36.	140-11-4	Acetic acid, phenylmethyl ester {benzyl acetate} CH_3-COO-CH_2-C_6H_5	568b, 1949, 2088, 3308, 3797, 4249, 5811b	120, 404, 524, 543a, 568b, 1949, 2282, 2339a, 2356, 2386, 2389, 2544, 2722, 2861a, 2917a, 2939, 3219, 3539, 3543, 3547, 3560, 3561, 3797, 3973, 3974a, 3905, 4249, 5811b	
37.	103-54-8	Acetic acid, 3-phenyl-2-propenyl ester {cinnamyl acetate}		172a, 174b, 1053, 3266	
38.	122-72-5	Acetic acid, phenylpropyl ester CH_3-COO-$(CH_2)_3$-C_6H_5		1053, 3266	
39.	109-60-4	Acetic acid, propyl ester {propyl acetate} CH_3-COO-$(CH_2)_2$-CH_3	568b, 2544, 4249	172a, 174b, 568b, 1053, 1590, 2339a, 2389, 2544, 3266, 4249, 5811b	
40.	76-49-3 5655-61-8	Acetic acid, *endo*-1,7,7-trimethylbicyclo[2,2,1]heptan-2-yl ester {bornyl acetate}		568b, 1053, 3266, 3370	
41.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4708	
42.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b	
43.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
44.	22732-83-8	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester		4249	
45.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	
46.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
47.		β-Alanine, *N*-methyl-*N*-nitroso-, methyl ester H_3C-N(NO)-$(CH_2)_2$-$COOCH_3$	4249	4249	
48.	52756-25-9	*DL*-Alanine, *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-, methyl ester {Flamprop-methyl®} 		4271a	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
49.	82560-54-1	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy) carbonyl)methylamino)thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}  R═-NH-S-N[CH(CH_3)$_2$]-(CH_2)$_2$-$COOC_2H_5$		3633	
50.	57646-30-7	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(2-furanylcarbonyl-, methyl ester {Furalaxyl®} 		3633	
51.	57837-19-1	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-, methyl ester {Ridomil®} 		2892a, 3633, 4271	
52.	71626-11-4	*DL*-Alanine, methyl *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)- {Benalaxyl®} 		3633	
53.	51630-58-1	Benzeneacetic acid, 4-chloro- α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®} 	21A19	3585e, 21A19	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

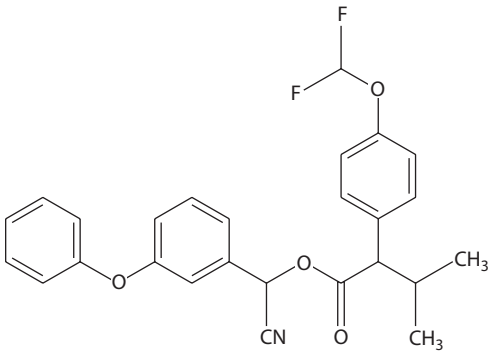
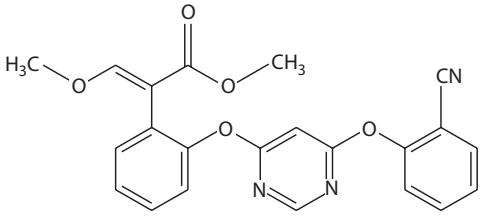
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
54.	70124-77-5	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Flucythrinate®} 		904	
55.	122-43-0	Benzeneacetic acid, butyl ester		1053, 3266, 3370	
56.	102-22-7	Benzeneacetic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl phenylacetate}		1053, 3266	
57.	101-97-3	Benzeneacetic acid, ethyl ester {ethyl phenylacetate}	222–224, 568b, 4249	174b, 568b, 1053, 2389, 2544, 3266, 3555, 4249, 5811b	
58.	131860-33-8	Benzeneacetic acid, methyl (α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)- {Azoxystrobin®} 		5568	
59.	5421-17-0	Benzeneacetic acid, hexyl ester		1053, 3266, 3370	
60.	51-55-8	Benzeneacetic acid, α-(hydroxymethyl)-(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (atropine}		5811, 5811b	
61.	101-41-7	Benzeneacetic acid, methyl ester {methyl phenylacetate}	568b, 2543, 2761, 2762, 2766, 2773, 3266, 4249, 4570a	172a, 174b, 568b, 1053, 1254, 1256, 1662, 2339a, 2389, 2544, 3186, 3188, 3266, 3370, 3547, 3905, 4249, 1254, 1256, 1662, 2339a, 2389, 2544, 3186, 3188, 3266, 3547, 3905, 4249, 5811b	
62.	102-19-2	Benzeneacetic acid, 3-methylbutyl ester	2487	172a, 174b, 1053, 3266, 3370	
63.	101-94-0	Benzeneacetic acid, 4-methylphenyl ester {*p*-tolyl phenylacetate}		1053, 3266, 3370	
64.	102-13-6	Benzeneacetic acid, 2-methylpropyl ester		172a, 174b, 1053, 3266, 3370	
65.	122-45-2	Benzeneacetic acid, octyl ester		5811	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
66.	102-20-5	Benzeneacetic acid, 2-phenylethyl ester	2487	172a, 174b, 404, 1053, 3266, 3370	
67.	102-16-9	Benzeneacetic acid, phenylmethyl ester {benzyl phenylacetate}		3266, 3547, 4249	
68.	7299-89-0	1,2-Benzenedicarboxylic acid, bis(2-ethylbutyl) ester	2777, 4249		
69.	117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	568b, 1375, 1375b, 1586, 1741, 2761, 2762, 2765–2767, 2777, 2807, 3300, 3302, 3553, 3557, 4249, 4570a, 5811b, 5869a	568b, 2339a, 2389, 2544, 2917a, 3547, 3973, 3974a, 4249, 5811b	
70.	131-20-4 27554-26-3	1,2-Benzenedicarboxylic acid, bis(6-methylheptyl) ester {diisooctyl phthalate}	2601a, 4249, 4746, 5777	647, 3973, 4249, 5777	
71.	84-69-5	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester		2917a	
72.	85-69-8	1,2-Benzenedicarboxylic acid, butyl, 2-ethylhexyl ester	2601a	2339a	
73.		1,2-Benzenedicarboxylic acid, butyl, 2-methylbutyl ester		2339a	
74.		1,2-Benzenedicarboxylic acid, butyl, 3-methylbutyl ester		2339a	
75.	85-68-7	1,2-Benzenedicarboxylic acid, butyl, phenylmethyl ester		2339a	
76.		1,2-Benzenedicarboxylic acid, dialkyl ester {four isomers detected}	1360, 1375a, 2508, 4342		1360, 1375a
77.	84-74-2	1,2-Benzenedicarboxylic acid, dibutyl ester {dibutyl phthalate}	568b, 3255, 3553, 3555, 4249, 5777, 5811b	568b, 937, 2339a, 2386, 2917a, 2939, 3547, 3550, 3555, 3797, 3973, 3974a, 3802, 4249, 5777, 5811b	642
78.	84-66-2	1,2-Benzenedicarboxylic acid, diethyl ester {diethyl phthalate}	568b, 1360, 1371, 1375a, 2506, 2507, 2524a, 2601a, 630, 2761, 2762, 2765, 2766, 3410, 3553, 4249, 4570a, 5811b	568b, 937, 984, 1256, 2339a, 3550, 4249	1360, 1375a, 2506, 2507
79.	3648-21-3	1,2-Benzenedicarboxylic acid, diheptyl ester {diheptyl phthalate}		647, 5777	
80.	84-75-3	1,2-Benzenedicarboxylic acid, dihexyl ester		2389, 2544, 4249, 5811b	
81.	131-11-3	1,2-Benzenedicarboxylic acid, dimethyl ester {dimethyl phthalate}	1371, 2761, 2762, 2765, 2766, 3410, 4249	984, 2339a, 4249, 4807, 5811b	
82.	117-84-0	1,2-Benzenedicarboxylic acid, dioctyl ester	1375a, 1377, 3547, 4249, 4342, 5811b	3547, 4249, 5811b	1375a, 1377
83.	131-16-8	1,2-Benzenedicarboxylic acid, dipropyl ester	568b, 3553, 4249, 5811b	568b, 2939, 3797, 3802, 3973, 3974a, 4249, 5811b	
84.	1861-32-1	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester {DCPA®}		2913a, 36333633	
85.	102-29-4	1,2-Benzenediol, monoacetate	2601a		
86.		1,3-Benzenediol, monoacetate	1364		

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

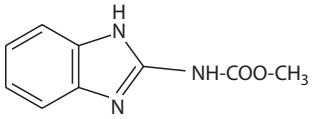
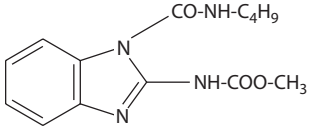
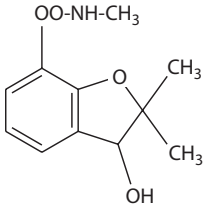
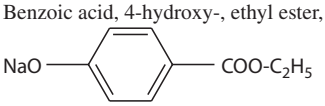
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
87.	3233-32-7	1,4-Benzenediol, monoacetate	568b, 1364, 1365, 1884, 2545, 2767, 3553, 3557, 3712, 4249, 5811b		
88.		1,4-Benzenediol, monopropanoate	1364		
89.	93-92-5	Benzenemethanol, α-methyl-, acetate		172a, 174b, 1053, 2544, 3266, 3547, 4249	
90.	30923-59-2	Benzenemethanol, 2-hydroxy-, α-benzoate		5811, 5811b	
91.	104-21-2	Benzenemethanol, 4-methoxy-, acetate {anisyl acetate}	568b, 3553, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370, 3893, 4249	
92.	122-91-8	Benzenemethanol, 4-methoxy-, formate		172a, 174b, 1053, 3266, 3370	
93.	102-17-0	Benzenemethanol, 4-methoxy-, phenylacetate		172a, 174b, 1053, 3266, 3370	
94.	7549-33-9	Benzenemethanol, 4-methoxy-, propanoate		174b, 3266	
95.	5597-50-2	Benzenepropanoic acid, 4-hydroxy-, methyl ester	568b, 1884, 3553, 3712, 4249, 5811b		
96.	10605-21-7	1*H*-Benzimidazole-2-carbamic acid, methyl ester {Carbendazim®} 		3585b	
97.	17804-35-2	1*H*-Benzimidazole-2-carbamic acid, 1-(butylcarbamomyl)-, methyl ester {Benomyl®} 		928a, 1219b, 1219c, 3585b, 3633, 3661a, 4271a, 21A19	
98.	16655-82-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate) {3-Hydroxycarbofuran®} 	1553, 21A19	1280, 1553, 3481, 5811b, 21A19	
99.	136-60-7	Benzoic acid, butyl ester	1365, 2543, 2773, 4249		
100.	93-89-0	Benzoic acid, ethyl ester {ethyl benzoate}	568b, 1998, 1999, 3266, 4249	174b, 568b, 1053, 2339a, 2389, 2544, 3266, 4249, 5811b	
101.	6789-88-4	Benzoic acid, hexyl ester		1248, 4249	
102.	93-58-3	Benzoic acid, methyl ester {methyl benzoate}	568b, 1371, 2487, 2543, 2722, 2773, 3266, 3410, 4249, 5811b	172a, 174b, 568b, 937, 1053, 2339a, 2389, 2544, 3266, 3905, 4249, 5811b	
103.	2049-96-9	Benzoic acid, pentyl ester {amyl benzoate}	336	336	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
104.	93-99-2	Benzoic acid, phenyl ester		3905	
105.	120-51-4	Benzoic acid, phenylmethyl ester {benzyl benzoate}	568b, 2543, 2553, 2773, 3263, 3266, 3308, 3485, 3504, 3506, 3797, 4249, 5811b	568b, 1053, 3266, 3547, 3797, 3988, 4249, 5811b	
106.	2315-68-6	Benzoic acid, propyl ester	2543, 2773, 4249	2386, 3905, 4249	
107.	50-78-2	Benzoic acid, 2-acetoxy-		5811, 5811b	
108.	7756-96-9	Benzoic acid, 2-amino-, butyl ester		5811	
109.	87-25-2	Benzoic acid, 2-amino-, ethyl ester		5811	
110.	134-20-3	Benzoic acid, 2-amino-, methyl ester {methyl anthranilate}		1053, 1254, 3266, 3370, 4249	
111.	85-91-6	Benzoic acid, 2-(methylamino)-, methyl ester		3905, 4249	
112.	2052-14-4	Benzoic acid, 2-hydroxy-, butyl ester		5811	
113.	118-61-6	Benzoic acid, 2-hydroxy-, ethyl ester {ethyl salicylate}		172a, 174b, 1053, 2386, 2995, 3266, 4249, 5811b	
114.	6259-76-3	Benzoic acid, 2-hydroxy-, hexyl ester		2339a	
115.	119-36-8	Benzoic acid, 2-hydroxy-, methyl ester {methyl salicylate}	568b, 1586, 4249	120, 172a, 174b, 568b, 908, 1053, 2094, 2389, 2544, 2611, 2862, 2939, 3059, 3266, 3370, 3547, 3973, 3974a, 3988, 3974a, 4249, 5811b	
116.	87-20-7	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester {isoamyl salicylate}		174b, 1256, 2339a, 3266, 4249	
117.	87-19-4	Benzoic acid, 2-hydroxy-, 2-methylpropyl ester {isobutyl salicylate}		1053, 3266, 3370	
118.	87-22-9	Benzoic acid, 2-hydroxy-, 2-phenylethyl ester {phenethyl salicylate}		1053, 3266	
119.	118-58-1	Benzoic acid, 2-hydroxy-, phenylmethyl ester {benzyl salicylate}		1053, 2339a, 3266, 3370, 4249	
120.	94-47-3	Benzoic acid, 2-phenylethyl ester {2-phenylethyl benzoate}		3547, 4249	
121.	583-04-0	Benzoic acid, 2-propenyl ester		2389, 2544, 3905, 5811b	
122.	19438-10-9	Benzoic acid, 3-hydroxy-, methyl ester	2767, 3557, 4249		
123.	87513-63-1	Benzoic acid, 3-hydroxy-6-methoxy-, methyl ester		2917a	
124.	54846-63-8	Benzoic acid, 3-methylbutyl ester		1248, 2339a, 4249	
125.	121-79-9	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}	3265	5811b	
126.	126-64-7	Benzoic acid, 3,7-dimethyl-1,6-octadien-6-yl ester {linalyl benzoate}		174b, 3266	
127.	94-26-8 1322-01-6	Benzoic acid, 4-hydroxy-, butyl ester		5811, 5811b	
128.	35285-68-9	Benzoic acid, 4-hydroxy-, ethyl ester, sodium salt 		174b, 3266, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

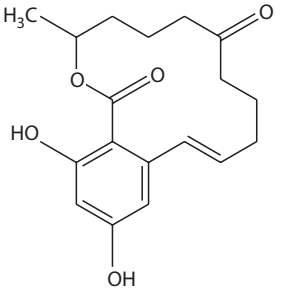
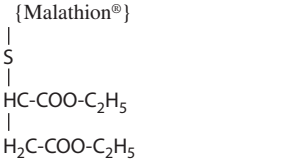
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
129.	99-76-3	Benzoic acid, 4-hydroxy-, methyl ester	1884, 2570, 2769, 3557, 3712, 4249, 5811b		
130.	5026-62-0	Benzoic acid, 4-hydroxy-, methyl ester, sodium salt		174b, 3266, 4249	
131.	94-13-3	Benzoic acid, 4-hydroxy-, propyl ester		1053, 3266, 3370, 5811b	
132.	35285-69-9	Benzoic acid, 4-hydroxy-, propyl ester, sodium salt		174b, 3266, 4249	
133.	617-05-0	Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester		2917a	
134.	3943-74-6	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester	3712	5811b	
135.	121-98-2	Benzoic acid, 4-methoxy-, methyl ester {methyl anisate}		172a, 174b, 1053, 3266	
136.	17924-92-4	1*H*-2-Benzoxacyclotetradecin-1,7(8*H*)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, [S-(*E*)]- 		4249	
137.	125-12-2	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate {isobornyl acetate}		172a, 174b, 1053, 3266	
138.	2756-56-1	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, propanoate, *exo*-		4249, 4787	
139.	32214-91-8	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, acetate {β-caryophyllene acetate}		1590a	
140.	96552-70-4	[2,3′-Bipyridine]-1(2*H*)-carboxylic acid, 3,6-dihydro-, methyl ester, (S)-	4249, 5811b		
141.		1,4-Butanediamine, 3-phenylpropenoyl-		17B02	
142.	121-75-5	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester {Malathion®} 	1618, 1619, 1884, 3634, 4249, 5811b, 21A19	1219b, 1219c, 1618, 1884, 2058a, 2650b, 3633, 3634, 3767a, 3973, 4271a, 21A19	
143.	106-65-0	Butanedioic acid, dimethyl ester {dimethyl succinate}	1235, 3266, 3553, 4249	1053, 3266	
144.	1587-15-1	Butanedioic acid, hydroxy-, dimethyl ester {dimethyl malate; malic acid dimethyl ester} H_3C-OOC-CHOH-CH_2-COO-CH_3	568b, 2570, 3553, 4249, 5811b		
145.	3878-55-5	Butanedioic acid, monomethyl ester HOOC-$(CH_2)_2$-COO-CH_3	568b, 1235, 3302, 3553, 4249, 5811b	5811b	
146.	52642-07-6	Butanediol, monoacetate	2767, 3553, 4249, 5811b		
147.	2432-51-1	Butanethioic acid, *S*-methyl ester	5770		
148.	109-21-7	Butanoic acid, butyl ester		172a, 174b, 1053, 3266, 3370	
149.	10094-34-5	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester		1053, 3266, 3370	
150.	106-29-6	Butanoic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl butyrate}		172a, 174b, 1053, 3266, 3370	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
151.	105-54-4	Butanoic acid, ethyl ester {ethyl butyrate} $H_3C\text{-}(CH_2)_2\text{-}COO\text{-}C_2H_5$	565, 1140, 1971, 2088, 2858, 2939, 3266, 3302, 3308, 3797, 4249, 4319, 5811b	174b, 1053, 2939, 3266, 3797, 3974a, 4249	
152.	26912-31-2	Butanoic acid, hexenyl ester $H_3C\text{-}(CH_2)_2\text{-}COO\text{-}(CH_2)_{4\text{-}n}\text{-}CH{=}CH\text{-}(CH_2)_n\text{-}H$		3547, 4249	
153.	623-42-7	Butanoic acid, methyl ester $H_3C\text{-}(CH_2)_2\text{-}COO\text{-}CH_3$	4570a	2339a, 3556, 4249	
154.	539-90-2	Butanoic acid, 2-methylpropyl ester		174b, 3266	
155.	540-18-1	Butanoic acid, pentyl ester		1053, 3266	
156.		Butanoic acid, phenyl ester $H_3C\text{-}(CH_2)_2\text{-}COO\text{-}C_6H_5$	5770		
157.	103-52-6	Butanoic acid, phenylethyl ester {phenethyl butyrate}		172a, 174b, 1053, 3266, 3370	
158.	103-37-7	Butanoic acid, phenylmethyl ester {benzyl butyrate}	568b, 3263, 3266, 3485, 3504, 3506, 3557, 3797, 4249	172a, 174b, 568b, 1053, 2389, 2544, 3266, 3370, 3561, 3797, 4249, 5811b	
159.	7492-70-8	Butanoic acid, 2-butoxy-1-methyl-2-oxoethyl ester {butyl butyryl lactate}		174b, 3266	
160.	141-16-2	Butanoic acid, 3,7-dimethyl-6-octenyl ester {citronellyl butyrate}		1053, 3266	
161.	7452-79-1	Butanoic acid, 2-methyl-, ethyl ester		172a, 174b, 1053, 2339a, 3266, 3370	
162.	10032-15-2	Butanoic acid, 2-methyl-, hexyl ester		1053, 3266, 3370	
163.	868-57-5	Butanoic acid, 2-methyl-, methyl ester	4570a	2339a	
164.	2445-78-5	Butanoic acid, 2-methyl-, 2-methylbutyl ester		2339a	
165.		Butanoic acid, 2-methyl-, 3-methylbutyl ester		2339a	
166.		Butanoic acid, 2-methyl-, 2-methylpropyl ester		2339a	
167.		Butanoic acid, 2-methyl-, 2-phenylethyl ester		2339a, 2386	
168.	78986-08-0	Butanoic acid, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-2-cyclohexen-1-yl ester		4249	
169.	109-19-3	Butanoic acid, 3-methyl-, butyl ester;		172a, 174b, 1053, 3266, 3370	
170.	1009-20-6	Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadieny-1-yl ester		1053, 3266	
171.	76-50-6	Butanoic acid, 3-methyl-, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, endo- {bornyl isovalerate}		174b, 1590a, 3266, 4249, 4787	
172.	2445-77-4	Butanoic acid, 3-methyl-, 2-methylbutyl ester		2339a	
173.	78-35-3	Butanoic acid, 3-methyl-, 3,7-dimethyl-1,6-octadien-6-yl ester {linalyl isobutyrate}		174a, 3266	
174.	16409-46-4	Butanoic acid, 3-methyl-, 5-methyl-2-(1-methylethyl)-cyclohexanyl ester {menthyl isovalerate}		174b, 3266	
175.	55066-56-3	Butanoic acid, 3-methyl-, 4-methylphenyl ester		1053, 3266	
176.	589-59-3	Butanoic acid, 3-methyl-, 2-methylpropyl ester		2339a	
177.	140-26-1	Butanoic acid, 3-methyl-, 2-phenylethyl ester {phenethyl isovalerate}	318	172a, 174b, 318, 947, 1053, 2339a, 2386, 3266, 3370, 4249	
178.	108-64-5	Butanoic acid, 3-methyl-, ethyl ester {ethyl isovalerate} $(H_3C)_2{=}CH\text{-}CH_2\text{-}COO\text{-}C_2H_5$	565, 1903, 1904, 2858, 2939, 3266, 4249, 4319, 5811b	908, 1053, 2339a, 2389, 2544, 3266, 3974a, 4249, 5811b	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

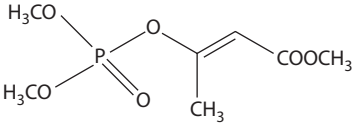
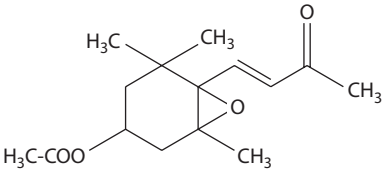
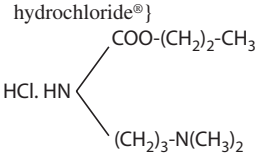
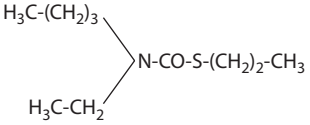
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
179.	556-24-1	Butanoic acid, 3-methyl-, methyl ester {methyl isovalerate} $(H_3C)_2$═CH-CH_2-COO-CH_3		568b, 908, 1053, 2339a, 2389, 2544, 3266, 3370, 4249, 5811b	
180.	659-70-1	Butanoic acid, 3-methyl-, 3-methylbutyl ester {isoamyl isovalerate}	1379, 2487, 5811b	172a, 174b, 1053, 1379, 3266, 3370	
181.		Butanoic acid, 3-methyl-, 4-oxopentyl ester	568b, 4279		
182.	103-38-8	Butanoic acid, 3-methyl-, phenylmethyl ester {benzyl isovalerate}		174b, 2386, 2389, 2544, 3266, 3561, 4249, 5811b	
183.	140-27-2	Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester	2487	1053, 3266, 3370	
184.	106-27-4	Butanoic acid, 3-methylbutyl ester		172a, 174b, 1053, 3266, 3370	
185.	141-97-9	Butanoic acid, 3-oxo-, ethyl ester		172a, 174b, 1053, 3266	
186.	105-45-3	Butanoic acid, 3-oxo-, methyl ester {methyl acetoacetate}		568b, 4249	
187.	67557-56-6	Butanoic acid, 4-(methylnitrosoamino)-, methyl ester CH_3-N(NO)-$(CH_2)_3$-$COOCH_3$	466, 470, 3256, 3300		
188.	94-46-2	1-Butanol, 3-methyl-, benzoate {isoamyl benzoate}	2487	1053, 3266, 4249	
189.	1575-57-1	2-Butanone, 1-(acetyloxy)- H_3C-CH_2-CO-CH_2-OOC-CH_3	1238, 2570, 2731, 2735, 2767, 3553, 3557, 4249, 5811b		3401, 3402, 3404
190.	10150-87-5	2-Butanone, 4-(acetyloxy)- H_3C-CO-CH_2-CH_2-OOC-CH_3	568b, 1586, 2387, 2570, 2767, 3553, 3557, 4249, 5811b		2387
191.	623-91-6	2-Butenedioic acid (*E*)-, diethyl ester {diethyl fumarate}		404	
192.	141-05-9	2-Butenedioic acid (*Z*)-, diethyl ester {diethyl maleate}	3553, 3685, 4249		
193.	624-48-6	2-Butenedioic acid (*Z*)-, dimethyl ester	3553	2356, 4249	
194.	623-70-1 10544-63-5	2-Butenoic acid (*E*)-, ethyl ester {ethyl crotonate}		172a, 174b, 1053, 3266	
195.	623-43-8 18707-60-3	2-Butenoic acid, methyl ester H_3C-CH═CH-COO-CH_3		3186, 3188, 3266, 4249	
196.	37526-88-8	2-Butenoic acid, 2-methyl-, phenylmethyl ester {benzyl tiglate}		404	
197.	39300-45-3	2-Butenoic acid, 2-(1-methylheptyl)-4,6-dinitrophenyl ester {Dinocap®}		3661a, 3633, 4271a	
198.	7786-34-7	2-Butenoic acid, 3[(dimethoxyphosphinyl)oxy]-, methyl ester {Mevinphos®; Phosdrin®} 		1219, 2058a, 3379, 3379a, 3380, 3633, 4271a	
199.	87562-12-7	2-Buten-1-one, 1-[3-(formyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, (*E*)-		4249	
200.	73892-47-4	3-Buten-2-one, 4-[3-(acetyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

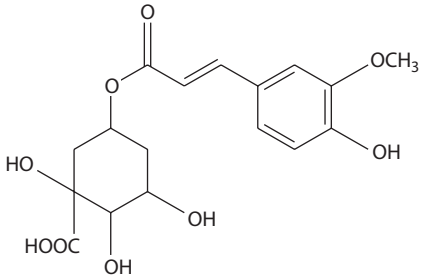
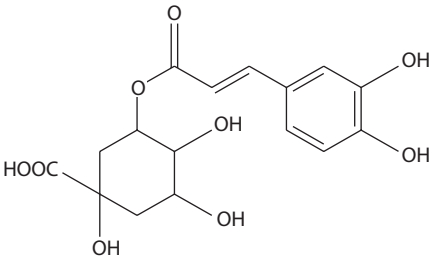
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
201.	50281-40-8	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1R-[1α(*E*), 4β,6α]]- 		1, 4249, 4573	
202.	50281-41-9	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1S-[1α(*E*),4α,6α]]-		1	
203.	101-21-3	Carbamic acid, 3-chlorophenyl-, (1-methylethyl) ester {Chloropropham®}		4271a	
204.	23103-98-2	Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester {Pirimicarb®}		3633, 4249, 4271a	
205.	25606-41-1	Carbamic acid, 3-(dimethylamino)propyl-, propyl ester, hydrochloride {Propamocarb hydrochloride®} 		3633	
206.	51-79-6	Carbamic acid, ethyl ester {urethane} $H_2N\text{-}COO\text{-}C_2H_5$	126a, 239, 757, 1148, 1217, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1870, 1871, 2825, 3255, 3257, 3265, 3300, 3483, 3714, 4005–4007, 4010, 4011, 4249, 5512, 5811b, 5869a	757, 3483, 3973, 3974b, 4249, 5524	
207.	598-55-0	Carbamic acid, methyl ester $H_2N\text{-}COO\text{-}CH_3$		3751, 4249	
208.	1114-71-2	Carbamothioic acid, butylethyl-, *S*-propyl ester {Pebulate®} 		1219b, 1219c, 2913a, 3633, 4271a	
209.	759-94-4	Carbamothioic acid, dipropyl-, *S*-ethyl ester {EPTC®}		3633	
210.	1929-77-7	Carbamothioic acid, dipropyl-, *S*-propyl ester {Vernolate®}		2650a	
211.	2303-17-5	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester {Triallate®}		2650a	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
212.	479-61-8 42617-16-3	Chlorophyll a {Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]-}		120, 537, 543a, 677b, 830a, 832, 835, 838, 840, 1463, 1941, 2038, 2079, 2236, 2270, 2283, 2649, 2914, 2939, 3616, 3630, 3631, 3632, 3797, 3875, 3973, 3974a, 3974b, 4107, 4108, 4222, 4249, 5079, 5189, 5300, 5539, 5811b	
213.		Chlorophyll a, phytol		5539	
214.	519-62-0	{Chlorophyll b} {Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]-}		120, 543a, 677b, 830a, 832, 835, 838, 840, 1941, 2236, 2270, 2914, 2939, 3630, 3631, 3632, 3797, 3875, 3973, 4222, 4249, 5079, 5189, 5300, 5811b	
215.	1406-65-1	Chlorophyll a + b		559, 830a, 832, 876, 877, 1927a, 1941, 2038, 2154, 2236, 2394a, 2914, 3448, 3491, 3630, 3631, 3632, 3797, 3973, 3974b, 4222, 4249, 4424, 5067, 5079, 5108, 5109, 5189, 5300, 5413, 5505, 5517, 5811b	
216.	604-35-3	Cholest-5-en-3-ol (3β)-, acetate {cholesteryl acetate}	5811a, 5811b		
217.	2645-22-4	Cholest-5-en-3-ol (3β)-, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {cholesteryl linolenate}		433	
218.	303-43-5	Cholest-5-en-3-ol (3β)-, 9-octadecenoate, [3β(*Z*),22*E*]- {cholesteryl oleate}		433	
219.	35602-69-8	Cholest-5-en-3-ol (3β)-, octadecanoate, (3β,22*E*)- {cholesteryl stearate}		433	
220.	34214-77-2	Cyclohexanecarboxylic acid, 3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]trihydroxy-, (1α,3α,4α,5β)-	3302, 3792, 4249	1309, 3797, 4249, 5811b	
221.	1899-30-5	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]-, [1S-(1α,3α,4α,5β)]- {*p*-coumaroylquinic acid}		3973, 3974a, 4402	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
222.	1899-29-2 27044-07-1	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)-{3-*O*-feruloylquinic acid}  Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-		3797, 3973, 3974a, 4249, 4402, 4913, 5811b	
223.	2450-53-5	Cyclohexanecarboxylic acid, 3,5-bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4-dihydroxy-, [1R-(1α,3α,4α,5β)]-{isochlorogenic acid}		1309, 4249, 5705	
224.	15016-60-1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*Z*),4α,5α]]-	3302, 3792, 4249	3797, 4249	
225.	15076-00-3	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*E*),4α,5α]]-		4249	
226.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-{chlorogenic acid; 3-*O*-caffeoylquinic acid} 	172, 602, 1884, 3257, 3302, 3792, 3797, 4249, 5811b	69, 72, 120, 254, 385, 486, 598, 602, 657, 665, 677b, 718, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1040, 1063–1066, 1068–1074, 1077b, 1309, 1329, 1333, 1352, 1485, 1625, 1626, 1923, 2014, 2056a, 2079, 2154, 2250a, 2270, 2283, 2313a, 2338, 2361, 2395, 2514, 2531, 2529, 2557a, 2810–2812, 2911c, 2911d, 2914, 2939, 2954, 3029, 3059, 3096, 3161, 3302, 3366a, 3367a, 3400, 3459–3462, 3551, 3616, 3628, 3631, 3641, 3646,	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

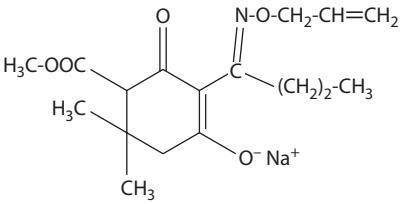
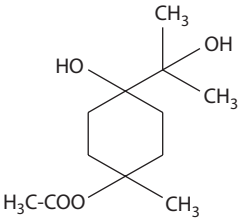
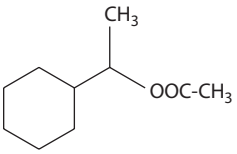
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-{chlorogenic acid; 3-*O*-caffeoylquinic acid} (cont.)		3655b, 3700, 3705, 3738, 3748, 3749, 3751, 3754, 3792, 3794, 3797, 3806, 3973, 3974a, 3974b, 3984, 3999, 4005–4007, 4156, 4221, 4249, 4275, 4279, 4372, 4402, 4403, 4421, 4999, 5079, 5189, 5200, 5246, 5353, 5389, 5576, 5592–5594, 5596, 5604, 5652, 5665, 5672, 5673, 5681, 5697. 5698, 5700, 5705, 5713, 5722, 5737, 5761, 5782, 5784, 5788, 5808–5810, 5811b, 5812, 5827, 5831, 5834, 5839, 5850, 5856, 5889, 3890, 5896, 5900, 5908	
227.	906-33-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-(1α,3α,4α,5β)]-{neochlorogenic acid; 5-*O*-caffeoylquinic acid} Also listed as cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxxy-	3302, 3792, 5811b	120, 602, 830a, 831, 834, 835, 838, 840, 890, 970, 1206a, 1626, 2557a, 2939, 3646, 3738, 3792, 3797, 3973, 3974a, 4249, 4402, 5705, 5811b, 5831	
228.	55635-13-7	Cyclohexanecarboxylic acid, 2,2-dimethyl-2,4-dioxo-3-(1-((2-propenyloxy)amino)butylidene)-, methyl ester, sodium salt {Alloxydim-sodium®} 		3633, 4271a	
229.	24321-18-4	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dioxo-1,5-cyclohexadien-1-yl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-		3533, 3973, 4271a, 5811b	
230.	70898-22-5	Cyclohexanecarboxylic acid, 3-[[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-		4249, 4785, 4984	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
231.	17608-52-5	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy- {4-*O*-caffeoylquinic acid}		831, 834, 835, 838, 840, 890, 1206a, 3646, 3738, 3973, 3974a, 4249, 5705, 5811b, 5889	
232.	534-61-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy- [1S-(1α,3β,4β,5α)]-	5811, 5811b	5811b	
233.	905-99-7	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-, (1α,3α,4α,5β)-		4249, 5811b	
234.		Cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-5-phenyl		5705, 5749	
235.	82612-14-4	1,2-Cyclohexanediol, 4-[1-(acetyloxy)-1-methylethyl]-1-methyl-, (1α,2β,4α)-(±)-		4249, 4664	
236.	88663-71-2	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*E*)- 		4249, 4734	
237.	88663-72-3	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*Z*)-		4249, 4734	
238.	59632-88-1	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*Z*)-		4249, 4734	
239.	59632-87-0	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*E*)-		4249, 4734	
240.	13487-27-9	Cyclohexanemethanol, α-methyl-, acetate 		3547	
241.	10235-63-9	Cyclohexanol, 1-methyl-4-(1-methylethylidene)-, acetate		4249, 4734	
242.	88437-32-5	Cyclohexanol, 4-(2-hydroxy-1-methylethylidene)-1-methyl-, 1-acetate		4249	
243.	89-48-5 16409-45-3	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate {menthyl acetate}		172a, 174b, 1053, 1371, 1375, 3266, 4249	
244.	6082-44-6	1-Cyclohexene-1-carboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]- 4,5-dihydroxy-, (3α,4α,5β)-		4249	
245.	88663-73-4	1-Cyclohexene-1-methanol, 4-(acetyloxy)-α,α,4-trimethyl-		4249, 4734	
246.	80-26-2	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate {α-terpinyl acetate}	3266, 4249	172a, 174b, 1053, 1156, 2389, 2544, 3266, 3370, 4090, 4249, 5811b	
247.	56691-69-1	2-Cyclohexen-1-one, 5-[1-(acetyloxy)-1-methylethyl]-2-methyl-, (R)-		937, 1156, 4090, 4249, 4664	
248.	1211-29-6	Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester {methyl jasmonate}		5811, 5811b	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

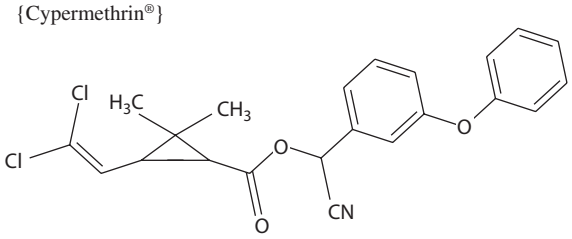
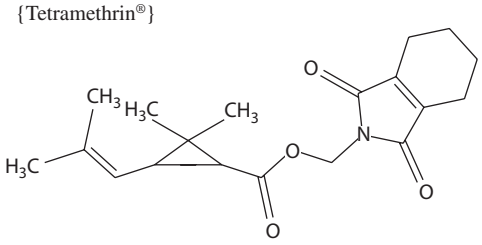
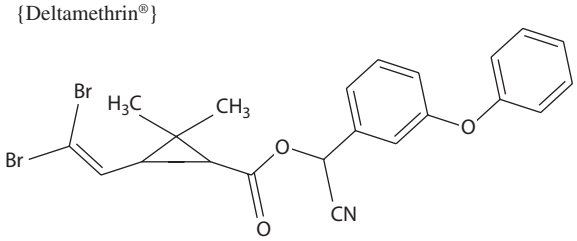
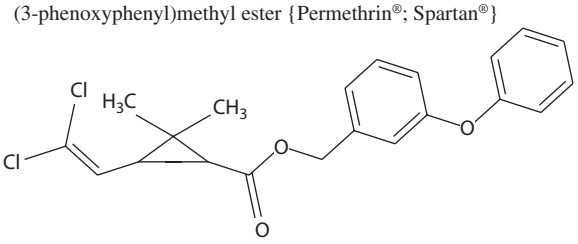
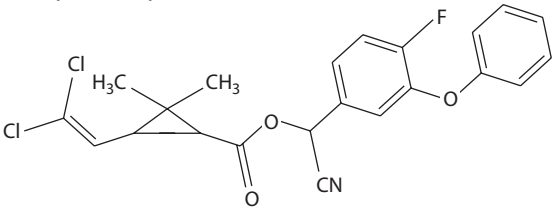
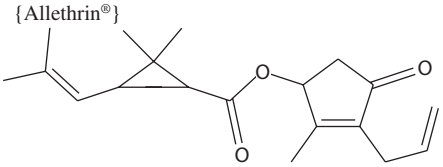
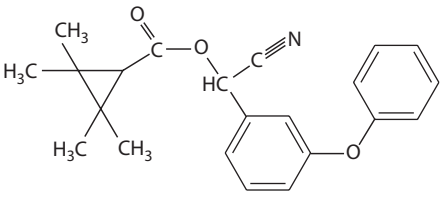
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
249.		2-Cyclopenten-1-one, 4-acetoxy-3-methyl-	568b, 4249		
250.	91465-08-6	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {λ-Cyhalothrin®}	21A19	2650b, 21A19	
251.	52315-07-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {Cypermethrin®} 	21A19	904, 1219b, 1219c, 3188a, 3585e, 3633, 4249, 4271a, 5568, 21A19	
252.	67375-30-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {α-cypermethrin}	21A19	3633, 21A19	
253.	121-29-9	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {pyrethrin II}		3633, 3634	
254.	7696-12-0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, (1-cyclohexene-1,2-dicarboximido)methyl ester {Tetramethrin®} 		904	
255.	121-21-1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {pyrethrin I}		3633, 3634	
256.	10453-86-8	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, (5-phenylmethyl-3-furanyl)methyl ester {Resmethrin®}		21A05	
257.	52918-63-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl)methyl ester {Deltamethrin®} 	21A19	904, 1219b, 1219c, 3585e, 3633, 4271a, 21A19	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
258.	52645-53-1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl)methyl ester {Permethrin®; Spartan®} 		904, 1219a, 1219b, 1219c, 2346, 2892a, 3188a, 3585e, 3633	
259.	68359-37-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl) methyl ester {Cyfluthrin®} 		904, 3633	
260.	97-41-6	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ethyl ester		2917a	
261.	5460-63-9	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, methyl ester		2917a	
262.	25402-06-6	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 3-(2-butenyl)-2-methyl-4-oxo-2-cyclopenten-1-yl ester {cinerin I}		3633	
263.	4466-14-2	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester {jasmolin I}		3633	
264.	584-79-2	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, 2-(1-propenyl)-4-hydroxy-3-methyl-2-cyclopenten-1-one ester {Allethrin®} 		3973, 4271a	
265.	66841-25-6	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-, cyano(3-phenoxyphenyl)methyl ester {Tralomethrin®}		21A05	
266.	39515-41-8	Cyclopropane carboxylic acid, 2,2,3,3-tetramethyl cyano(3-phenoxyphenyl)methyl ester {Fenpropathrin®, Danitol®} 	21A19	21A19	
267.	82657-04-3	Cyclopropanecarboxylic acid, 3-[(1*Z*)-2-chloro-3,3,3-trifluoro-1-propenyl]-2,2-dimethyl-, (2-methyl[1,1′-biphenyl]-3-yl)methyl ester, (1R,3R)-rel- {Bifenthrin®, Biphenthrin®}		21A05	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

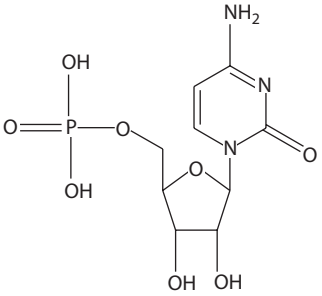
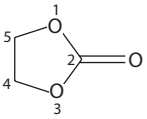
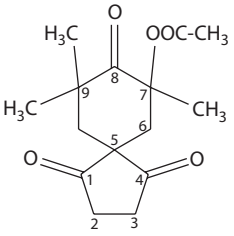
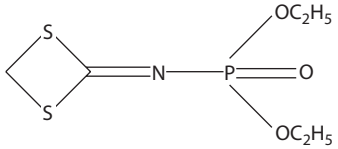
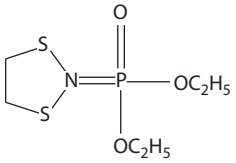
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
268.	2043-08-1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, 3-acetate, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-		4249	
269.	65-47-4	Cytidine 5′-(tetrahydrogen triphosphate)		429b, 4249, 4474, 4505	
270.	63-37-6	5′-Cytidylic acid 		429b, 4249, 4299, 4774	
271.	160115-53-7	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-, methyl ester		4249	
272.	110-40-7	Decanedioic acid, diethyl ester		1053, 3266, 3370	
273.	110-38-3	Decanoic acid, ethyl ester {ethyl caprate} $H_3C\text{-}(CH_2)_8\text{-}COO\text{-}C_2H_5$	3266, 4249	172a, 174b, 908, 1053, 2389, 2544, 3266, 3370, 4249, 5811b	
274.	110-42-9	Decanoic acid, methyl ester $H_3C\text{-}(CH_2)_8\text{-}COO\text{-}CH_3$	568b, 809, 4249	568b, 2093, 3973, 4249	
275.	70898-23-6	Decanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester, (all-*E*)-{solanesyl decanoate}	1231, 3251, 3296, 4336	1893a, 1893b, 2939, 3358, 4249, 4336	
276.	70898-24-7	Decanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		1893, 4249	
277.		$H_3C\text{-}(CH_2)_8\text{-}COO\text{-}CH_2\text{-}CH{=}C(CH_3)\text{-}CH_2[CH_2CH_2CH(CH_3)CH_2]_3\text{-}H$			2387
278.	96-49-1	1,3-Dioxalan-2-one {ethylene glycol carbonate} 	568b, 1375, 1586, 1882, 2570, 2767, 3553, 3557, 4249, 5811b		3405
279.	931-40-8	1,3-Dioxalan-2-one, 4-(hydroxymethyl)- {glycerol carbonate}	568b, 1371, 1375, 3255, 3553, 3557, 4249, 5811b		
280.	108-32-7 9005-37-2	1,3-Dioxalan-2-one, 4-methyl- {1,2-propylene glycol carbonate}	568b, 3553, 4249, 5811b	568b, 2389, 2544, 4249	
281.	162188-91-2	1,4-Dioxaspiro[4.5]decan-8-one, 7-(acetyloxy)-7,9,9-trimethyl-, (±)- 	4249		

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
282.	21548-32-3	1,3-Dithietan-2-ylidenephosphoramidic acid, diethyl ester {Fosthietan®} 		3633	
283.	947-02-4	Dithiolan-2-ylidenephosphoramidic acid, diethyl ester {Cyolane®; Phosfolan®} 		3380	
284.	17671-27-1	Docosanoic acid, docosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
285.	42233-07-8	Docosanoic acid, dodecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
286.	42233-14-7	Docosanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
287.	5908-87-2	Docosanoic acid, ethyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}CH_2\text{-}CH_3$	2601a		
288.	42233-15-8	Docosanoic acid, heneicosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{20}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
289.	121877-99-4	Docosanoic acid, heptacosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{26}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
290.	42233-12-5	Docosanoic acid, heptadecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{16}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
291.	55136-77-1	Docosanoic acid, hexacosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{25}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
292.	42233-11-4	Docosanoic acid, hexadecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{15}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
293.	42233-13-6	Docosanoic acid, nonadecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{18}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
294.	21511-31-9	Docosanoic acid, octacosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{27}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
295.	24271-12-3	Docosanoic acid, octadecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{17}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
296.		Docosanoic acid, pentacosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{24}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
297.	42233-10-3	Docosanoic acid, pentadecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{14}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
298.	42233-17-0	Docosanoic acid, tetracosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{23}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
299.	42233-09-0	Docosanoic acid, tetradecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{13}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
300.	127353-53-1	Docosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl docosanoate} $H_3C\text{-}(CH_2)_{20}\text{-}COOCH_2\text{-}CH{=}C(CH_3)\text{-}CH_2\text{-}[CH_2CH_2CH(CH_3)CH_2]_3\text{-}H$	3287, 3308, 5811		
301.	42233-16-9	Docosanoic acid, tricosyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{32}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
302.	42233-08-9	Docosanoic acid, tridecyl ester $H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{12}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
303.	121877-76-7	Docosanoic acid, 20-methyl-, docosyl ester $H_3C\text{-}CH_2CH(CH_3)\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	103 [see 2809]	103	
304.	121877-62-1	Docosanoic acid, 20-methyl-, eicosyl ester $H_3C\text{-}CH_2CH(CH_3)\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809]	103	
305.	121877-71-2	Docosanoic acid, 20-methyl-, heneicosyl ester $H_3C\text{-}CH_2CH(CH_3)\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{20}\text{-}CH_3$	103 [see 2809]	103	
306.	40596-69-8	2,4-Dodecadienoic acid, 11-methoxy-3,7,11-trimethyl-, 1-methylethyl ester, (*E,E*)- {Methoprene®; Altosid®} $(H_3C)_2{=}C(OCH_3)\text{-}(CH_2)_3\text{-}CH(CH_3)\text{-}CH_2\text{-}CH{=}CH\text{-}C(CH_3){=}CH\text{-}COO\text{-}CH(CH_3)_2$	1242, 1243, 21A19	1053, 1242, 1243, 1588, 2483a, 3266, 3633, 21A19	
307.	71278-23-4 110053-53-7	Dodecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl dodecanoate}	1231, 3251, 3296, 4249, 4336	1893a, 1893b, 3296, 4249, 4336	
308.	71278-24-5 72996-18-0	Dodecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl dodecanoate} $H_3C\text{-}(CH_2)_{10}\text{-}COO\text{-}CH_2\text{-}CH{=}C(CH_3)\text{-}CH_2\ [CH_2CH_2CH(CH_3)CH_2]_3\text{-}H$	3219, 3287, 3308, 4249	1893, 4249	
309.	36617-18-2	Dodecanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{10}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809]	103	
310.	106-33-2	Dodecanoic acid, ethyl ester {ethyl laurate} $H_3C\text{-}(CH_2)_{10}\text{-}COO\text{-}C_2H_5$		172a, 174b, 568b, 908, 1053, 2389, 2544, 3266, 3370, 4249	
311.	111-82-0	Dodecanoic acid, methyl ester $H_3C\text{-}(CH_2)_{10}\text{-}COO\text{-}CH_3$	568b, 3287, 4249	120, 568b, 908, 2339a, 2389, 2544, 2861a, 2939, 3973, 4249, 5811b	
312.	121877-15-4	Dodecanoic acid, 10-methyl-, eicosyl ester $H_3C\text{-}CH_2CH(CH_3)\text{-}(CH_2)_8\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809]	103	
313.	121877-10-9	Dodecanoic acid, 11-methyl-, eicosyl ester $(H_3C)_2{=}CH\text{-}(CH_2)_9\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809]	103	
314.		1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate, (*Z*)- {*cis*-nerolidol acetate}	568b, 4249	568b, 4249	
315.		1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate, (*E*)- {*trans*-nerolidol acetate}	568b, 4249	568b, 4249	
316.	29548-30-9	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, acetate {farnesyl acetate}	1063–1066, 1068–1074	1590a, 3547, 3549, 4249, 5811b	
317.		2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, formate {farnesyl formate}		3547, 4249	
318.	121878-06-6	Dotriacontanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{30}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809]	103	
319.	42232-87-1	Eicosanoic acid, docosyl ester $H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
320.	42232-82-6	Eicosanoic acid, dodecyl ester $H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
321.	22432-80-0	Eicosanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
322.	42218-26-8	Eicosanoic acid, heneicosyl ester $H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{20}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
323.	121877-87-0	Eicosanoic acid, heptacosyl ester $H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{26}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

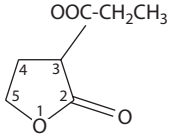
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
324.	36610-58-9	Eicosanoic acid, heptadecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
325.	17318-45-5	Eicosanoic acid, hexacosyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
326.	22413-05-4	Eicosanoic acid, hexadecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
327.	1120-28-1	Eicosanoic acid, methyl ester H_3C-$(CH_2)_{18}$-COO-CH_3		1248, 3667, 4249, 5811b	
328.	36610-60-3	Eicosanoic acid, nonadecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294	
329.	55309-61-0	Eicosanoic acid, octacosyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
330.	22432-79-7	Eicosanoic acid, octadecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
331.	121877-79-0	Eicosanoic acid, pentacosyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{24}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
332.	36665-69-7	Eicosanoic acid, pentadecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
333.	42232-89-3	Eicosanoic acid, tetracosyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
334.	22413-04-3	Eicosanoic acid, tetradecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
335.	71278-14-3	Eicosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl eicosanoate} H_3C-$(CH_2)_{18}$-$COOCH_2$-CH═C(CH_3)-CH_2-[$CH_2CH_2CH(CH_3)CH_2]_3$-H	3219, 3287, 3308, 4249		
336.	42232-88-2	Eicosanoic acid, tricosyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{32}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294	
337.	36610-55-6	Eicosanoic acid, tridecyl ester H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
338.	121877-60-9	Eicosanoic acid, 18-methyl-, docosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{16}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
339.	55682-88-7	11,14,17-Eicosatrienoic acid, methyl ester		2917a	
340.	95-92-1	Ethanedioic acid, diethyl ester		2917a	
341.	542-10-9	1,1-Ethanediol, diacetate	1371, 4249		
342.	111-55-7	1,2-Ethanediol, diacetate	568b, 4249		
343.	542-59-6	1,2-Ethanediol, monoacetate {acetic acid, 2-hydroxyethyl ester} HO-$(CH_2)_2$-OOC-CH_3	568b, 1371, 1375, 1375b, 1586, 2767, 3553, 3557, 4249, 5811b		
344.	23135-22-0	Ethanimidothioic acid, 2-(dimethylamino)-*N*-[[(methylamino) carbonyl]oxy]-2-oxo-, methyl ester {Oxamyl®} $(H_3C)_2$═N-CO-C(S-CH_3)═N-OOC-NH-CH_3		1280, 3633, 3634, 3646a, 3973, 4249, 4271a, 4891	
345.	59669-26-0	Ethanimidothioic acid, *N*′,*N*′-(thiobis((methylimino)carbonyloxy)) bis-, dimethyl ester {Thiodicarb®} S═[NH-COO-N═C(CH_3)-$SCH_3]_2$		3633	
346.	111-21-7	Ethanol, 2,2′-[1,2-ethanediylbis(oxy)]bis-, diacetate	2762, 4249, 5811b	3593	
347.	1071-23-4	Ethanol, 2-amino-, dihydrogen phosphate (ester)		908, 4249, 4670	
348.	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1) [H_3C-$(CH_2)_3$-O-$(CH_2)_2]_3$≡P═O	3553, 5811b		
349.	19859-79-1	Ethanone, 1-(2-furanyl)-2-(acetyloxy)-	568b, 1375, 1375b, 1586, 2767, 3553, 3557, 5811b		
350.	574-06-1	Ethanone, 1,2-diphenyl-2-(acetyloxy)- {benzoin acetate}	2601a		

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
351.	2243-35-8	Ethanone, 1-phenyl-2-(acetyloxy)-		4249	
352.	592-84-7	Formic acid, butyl ester		5811	
353.	105-86-2	Formic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl formate}		172a, 174b, 1053, 3266, 3370	
354.	692-45-5	Formic acid, ethenyl ester	5770		
355.	109-94-4	Formic acid, ethyl ester H-COO-CH_2-CH_3	1412, 1449, 2767, 2782, 2804, 2821, 3302, 3308, 3797, 3882, 4249, 5811b		
356.	629-33-4	Formic acid, hexyl ester H-COO-$(CH_2)_5$-CH_3		3856, 4249	
357.	107-31-3	Formic acid, methyl ester {methyl formate} H-COO-CH_3	239, 722, 1140, 1374, 1375a, 1377, 1412–1414, 1416, 1418, 1437, 1449, 1744, 1842, 2782, 2799a, 2804, 3300, 3302, 3308, 3795, 3797, 3882, 4249, 4257, 4319, 5512, 5811b	2339a	1375a, 1377
358.	110-45-2	Formic acid, 3-methylbutyl ester		1053, 2339a, 3266, 3370	
359.	625-55-8	Formic acid, 1-methylethyl ester H-COO-CH═$(CH_3)_2$	1140, 2782, 2804, 3302, 3308, 3797, 4249, 5811b		
360.	638-49-3	Formic acid, pentyl-ester		1053, 3266, 3370	
361.	104-62-1	Formic acid, 2-phenylethyl ester	5811b	404, 568b, 2339a, 2389, 2544, 3547, 5811b	
362.	104-57-4	Formic acid, phenylmethyl ester {benzyl formate}	5811b	174b, 404, 568b, 937, 2339a, 2389, 2544, 3266, 3547, 4249, 5811b	
363.	110-74-7	Formic acid, propyl ester		5811	
364.	79082-92-1	β-*D*-Fructofuranose, 2,6-bis(dihydrogen phosphate)		429b, 4249	
365.	488-69-7	*D*-Fructose, 1,6-bis(dihydrogen phosphate)		429b, 4249, 4760	
366.	643-13-0	*D*-Fructose, 6-(dihydrogen phosphate)		429b, 4249, 4670	
367.	36119-15-0	*D*-Fructose, mono(dihydrogen phosphate)		429b, 4249, 4960	
368.	4915-21-3	2-Furanacetic acid, ethyl ester	568b, 4249		
369.	10551-58-3	2-Furancarboxaldehyde, 5-[(acetyloxy)methyl]-	5811b	404, 3557, 4249	
370.	1334-76-5	Furancarboxylic acid, methyl ester {methyl furoate}	5811, 5811a, 5811b		
371.	61892-61-3	2-Furancarboxylic acid, 2-(acetyloxy)ethyl ester	568b, 2767, 3553, 4249, 5811b	568b, 1883, 4249	
372.	3736-81-0	2-Furancarboxylic acid, 4-[(2,2-dichloroacetyl)-methylamino] phenyl ester	5811, 5811a, 5811b		
373.	614-99-3	2-Furancarboxylic acid, ethyl ester {ethyl 2-furoate}		1053, 3266	
374.	611-13-2	2-Furancarboxylic acid, methyl ester {methyl 2-furoate}	568b, 1884, 3266, 4249, 5811b	568b, 984, 1053, 3266, 4249, 5811b	
375.	3885-29-8	2-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester	568b, 4249, 5811b		
376.	13129-23-2	3-Furancarboxylic acid, methyl ester		2917a	
377.	5204-91-1	3-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester	568b, 3553, 4249		
378.	623-17-6	2-Furanmethanol, acetate	568b, 2337, 2731, 2735, 3555, 4249, 5811b	404, 568b, 2337, 3547, 4092, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
379.	13493-97-5	2-Furanmethanol, formate		568b, 2389, 2544, 3547, 3555, 4249, 5811b	
380.	19405-99-3	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-	568b, 1375, 1375b, 1586, 3553, 3557, 4249, 5811b		
381.	19405-98-2	2(3*H*)-Furanone, 4-(acetyloxy)dihydro-	568b, 2767, 3353, 4249		
382.		2(3*H*)-Furanone, 4-(acetyloxy)dihydro-5-hydroxy-	568b, 4249		
383.	26817-24-3	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-	1586, 2767, 3553, 5811b		3402
384.	61892-43-1	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-4-hydroxy-	568b, 1351, 1352, 1375, 1375b, 1586, 3553, 3557, 4249, 5811b		
385.	61892-44-2	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-4-hydroxy-	1351, 1352, 3553, 5811b		
386.	160115-54-8	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1E,3S*)]]-		4249	
387.	160224-93-1	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5α(1E,3S*)]]-		4249	
388.	25600-22-0	2(3*H*)-Furanone, dihydro-3-(1-oxopropoxy)- 	568b, 3553, 4249, 5811b		
389.	37209-50-0	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, acetate, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberin}		4249, 4594, 4642, 5811b	
390.		α-*D*-Glucopyranose, 1-acetate 2,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
391.	28977-67-5	β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylvalerate) = β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylpentanoate)	1352, 1373, 3251, 3278, 3286, 3302, 4249, 5811b	1352, 1373, 2338, 3185, 3215, 3473, 3539, 3542, 3560, 3561, 3607, 4249, 4575, 5811b	
392.	60517-74-0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)		5811b	
393.	25545-13-5	*D*-Glucopyranose, 4-(4-hydroxybenzoate)		4249, 4915	
394.	23445-11-6	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)		4249, 4915	
395.	41682-52-4	β-*D*-Glucopyranose, 1-(3-phenyl-2-propenoate)		429b, 4269, 4915	
396.	59-56-3	α-*D*-Glucopyranose, 1-(dihydrogen phosphate)		120	
397.	61891-55-2	β-*D*-Glucopyranose, 1,6-anhydro-, monoacetate	568b, 3553, 4249, 5811b		
398.	10139-18-1	α-*D*-Glucopyranose, 1,6-bis(dihydrogen phosphate)		4249	
399.	21056-52-0	β-*D*-Glucopyranose, 1-benzoate		4249, 4915	
400.		α-*D*-Glucopyranose, 1,2,3,4,5-penta((+)-3-methylbutanoate)		3556	
401.	64461-84-3	β-*D*-Glucopyranose, 6-(3-phenyl-2-propenoate)		3367a, 4249, 4915	
402.		α-*D*-Glucopyranose, 1,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
403.		α-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
404.		β-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
405.	126-14-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate		1053, 3266	
406.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-		4990	
407.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-3′-acetyl-		4990	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

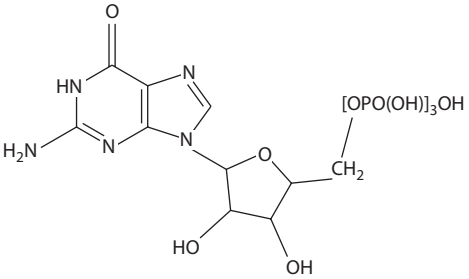
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
408.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-4′-acetyl-		4990	
409.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-,2,3,4-tri-*O*-acyl-		4990	
410.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′-*O*-acetyl-		4990	
411.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-4′-*O*-acetyl-		4990	
412.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′,4′-*O*-diacetyl-		4990	
413.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-1′,3′,4′-*O*-triacetyl-		4990	
414.	98913-58-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 3-methylpentanoate		4249, 5811b	
415.	154063-13-5	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(2-methylbutanoate)		3606	
416.	97614-61-4	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(3-methylpentanoate)		3606, 5811b	
417.	106033-38-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(3-methylpentanoate), [2(S),3(S),4(S)]-		4249, 5811b	
418.	136448-99-2	β-*D*-Glucopyranoside, 2-[5-(acetyloxy)-1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl]-2-hydroxypropyl, 2,3,4,6-tetraacetate, [2R-[2α(S*),5α,8β,8aα]]-		4249, 5811b	
419.	75039-16-6	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl, mono(dihydrogen phosphate) (ester), (*E*)-		4249, 4813	
420.	28905-07-9	α-*D*-Glucuronic acid, methyl ester		4249	
421.		Glycine, *N*-methyl-*N*-nitroso-, methyl ester $H_3C\text{-}N(NO)\text{-}CH_2\text{-}COOCH_3$	3256, 3300	466	
422.	86-01-1	Guanosine 5′-(tetrahydrogen triphosphate) 		4249	
423.	42233-02-3	Heneicosanoic acid, docosyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
424.	42232-93-9	Heneicosanoic acid, dodecyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
425.	42233-00-1	Heneicosanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
426.	42233-01-2	Heneicosanoic acid, heneicosyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{20}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
427.		Heneicosanoic acid, heptacosyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{26}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
428.	42232-98-4	Heneicosanoic acid, heptadecyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{16}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
429.		Heneicosanoic acid, hexacosyl ester $H_3C\text{-}(CH_2)_{19}\text{-}COO\text{-}(CH_2)_{25}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
430.	42232-97-3	Heneicosanoic acid, hexadecyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
431.	42232-99-5	Heneicosanoic acid, nonadecyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
432.	121878-00-0	Heneicosanoic acid, octacosyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809], 3251, 3294, 3302	103, 3251, 3294, 4249	
433.		Heneicosanoic acid, octadecyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
434.		Heneicosanoic acid, pentacosyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
435.	42232-96-2	Heneicosanoic acid, pentadecyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
436.	42233-04-5	Heneicosanoic acid, tetracosyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
437.	42232-95-1	Heneicosanoic acid, tetradecyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
438.	42233-03-4	Heneicosanoic acid, tricosyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
439.	42232-94-0	Heneicosanoic acid, tridecyl ester H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
440.	121877-70-1	Heneicosanoic acid, 19-methyl-, docosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{17}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
441.	121877-61-0	Heneicosanoic acid, 19-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{17}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
442.	71278-17-6	Heneicosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl heneicosanoate} H_3C-$(CH_2)_{19}$-COO-CH_2-CH=$C(CH_3)$-$CH_2[CH_2CH_2CH(CH_3)CH_2]_3$-H	3218, 3287, 3308, 4249		1378, 4249
443.	71278-18-7	Hentriacontanoic acid, hentriacontyl ester H_3C-$(CH_2)_{29}$-COO-$(CH_2)_{30}$-CH_3	1971, 3302, 3308, 3797, 3876, 4249, 4319, 4354		
444.	121877-96-1	Heptacosanoic acid, docosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
445.		Heptacosanoic acid, dodecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
446.	117063-83-9	Heptacosanoic acid, eicosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
447.		Heptacosanoic acid, heneicosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{20}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
448.		Heptacosanoic acid, heptacosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
449.		Heptacosanoic acid, heptadecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
450.		Heptacosanoic acid, hexacosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
451.		Heptacosanoic acid, hexadecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
452.		Heptacosanoic acid, nonadecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
453.		Heptacosanoic acid, octadecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
454.		Heptacosanoic acid, pentacosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
455.		Heptacosanoic acid, pentadecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
456.		Heptacosanoic acid, tetracosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{231}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
457.		Heptacosanoic acid, tetradecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
458.		Heptacosanoic acid, tricosyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
459.		Heptacosanoic acid, tridecyl ester H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
460.	121878-01-1	Heptacosanoic acid, 25-methyl-, docosyl ester H_3C-CH_2–$CH(CH_3)$-$(CH_2)_{23}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
461.	121877-93-8	Heptacosanoic acid, 25-methyl-, heneicosyl ester H_3C-CH_2–$CH(CH_3)$-$(CH_2)_{23}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
462.	37822-80-3	Heptadecadienoic acid, methyl ester		1248, 4249	
463.	42218-25-7	Heptadecanoic acid, docosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
464.	42232-43-9	Heptadecanoic acid, dodecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
465.	36617-53-5	Heptadecanoic acid, eicosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
466.	42232-52-0	Heptadecanoic acid, heneicosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{20}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
467.		Heptadecanoic acid, heptacosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
468.	36617-50-2	Heptadecanoic acid, heptadecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
469.	121877-64-3	Heptadecanoic acid, hexacosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
470.	36617-49-9	Heptadecanoic acid, hexadecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
471.	1731-92-6	Heptadecanoic acid, methyl ester H_3C-$(CH_2)_{15}$-COO-CH_3	2544, 4249	809, 2389, 2544, 4249, 5811b	
472.	36617-52-4	Heptadecanoic acid, nonadecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
473.	36617-51-3	Heptadecanoic acid, octadecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
474.		Heptadecanoic acid, pentacosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
475.	36617-48-8	Heptadecanoic acid, pentadecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
476.	42232-54-2	Heptadecanoic acid, tetracosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
477.	36617-47-7	Heptadecanoic acid, tetradecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
478.	42232-53-1	Heptadecanoic acid, tricosyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
479.	36617-46-6	Heptadecanoic acid, tridecyl ester H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
480.	121877-42-7	Heptadecanoic acid, 15-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
481.	121877-68-7	Heptadecanoic acid, 15-methyl-, hexacosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809]	103	
482.	121877-81-4	Heptadecanoic acid, 15-methyl-, octacosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809]	103	
483.	121877-52-9	Heptadecanoic acid, 15-methyl-, tricosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
484.	150462-99-0	Heptadecanoic acid, 16-methyl-, 2-(acetyloxy)-1-(hydroxymethyl) ethyl ester		4249	
485.	150462-98-9	Heptadecanoic acid, 16-methyl-, 3-(acetyloxy)-2-hydroxypropyl ester		4249	
486.	121877-46-1	Heptadecanoic acid, 16-methyl-, docosyl ester $(H_3C)_2$═CH-$(CH_2)_{14}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
487.	52458-35-2	Heptadecanoic acid, 16-methyl-, ethyl ester $(H_3C)_2$═CH-$(CH_2)_{14}$-COO-C_2H_5		2386, 4249	
488.	121877-36-9	Heptadecanoic acid, 16-methyl-, heneicosyl ester $(H_3C)_2$═CH-$(CH_2)_{14}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
489.	5129-61-3	Heptadecanoic acid, 16-methyl-, methyl ester $(H_3C)_2$═CH-$(CH_2)_{14}$-COO-CH_3		2389, 2544, 2917a, 4249, 5811b	
490.	121877-50-7	Heptadecanoic acid, 16-methyl-, tricosyl ester $(H_3C)_2$═CH-$(CH_2)_{14}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
491.		Heptadecanoic acid, 3,7,11,15,19,23,27,31, 35-nonamethyl- 2,6,10,14,18,22,26,30, 34-hexatriacontanonaenyl ester {solanesyl heptadecanoate}		3298, 3349, 4249	
492.	71278-19-8	Heptadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl heptadecanoate} H_3C-$(CH_2)_{15}$-COO-CH_2-CH═C(CH_3)-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H	3219, 3308, 4249		
493.	37822-82-5	Heptadecatrienoic acid, methyl ester		1248, 4249	
494.	31424-16-5	Heptadecenoic acid, methyl ester H-$(CH_2)_{14-n}$-CH═CH-$(CH_2)_n$-COO-CH_3		1248, 4249, 5811b	
495.	54557-57-2 80114-59-6	4,6-Heptadienoic acid, 6-methyl-3-(1-methylethyl)-, methyl ester, (*E*)-		568b, 3547, 4249	
496.	39815-78-6	Heptanoic acid, 3-oxo-, methyl ester		3858, 4249	
497.	98188-02-4	Heptanoic acid, 7-(2-furanyl)-, methyl ester		2917a	
498.	106-30-9	Heptanoic acid, ethyl ester		172a, 174b, 1053, 3266, 3370, 3474, 4249	
499.	106-73-0	Heptanoic acid, methyl ester		4249, 4573	
500.	30414-57-4	6-Heptenoic acid, 3-oxo-, methyl ester H_2C═CH-$(CH_2)_2$-CO-CH_2-COO-CH_3		3858, 4249	
501.	160115-55-9	6-Hepten-2-one, 7-[4-(acetyloxy)tetrahydro-5-hydroxy-2-methyl-2-furanyl]-5-(1-methylethyl)-		4249	
502.	108657-23-4	Hexacosanoic acid, docosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
503.		Hexacosanoic acid, dodecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
504.	121877-83-6	Hexacosanoic acid, eicosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
505.		Hexacosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl hexacosanoate}	1230	1230	
506.	121877-89-2	Hexacosanoic acid, heneicosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
507.	75696-56-9	Hexacosanoic acid, heptacosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{26}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
508.		Hexacosanoic acid, heptadecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
509.	10210-18-1	Hexacosanoic acid, hexacosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
510.		Hexacosanoic acid, hexadecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
511.		Hexacosanoic acid, nonadecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
512.		Hexacosanoic acid, octadecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
513.		Hexacosanoic acid, pentacosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
514.		Hexacosanoic acid, pentadecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
515.		Hexacosanoic acid, tetracosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
516.		Hexacosanoic acid, tetradecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{193}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
517.	121877-97-2	Hexacosanoic acid, tricosyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
518.		Hexacosanoic acid, tridecyl ester H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
519.	121877-92-7	Hexacosanoic acid, 24-methyl-, docosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{22}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
520.	121877-90-5	Hexacosanoic acid, 24-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{22}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
521.	29961-54-4	Hexadecadienoic acid, methyl ester		4249, 5811b	
522.	111-06-8	Hexadecanoic acid, butyl ester	5811a		
523.	42232-33-7	Hexadecanoic acid, docosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{21}$-CH_3	3251, 3294, 3302, 4249	103, 3251, 3294, 3561, 4249	
524.	42232-29-1	Hexadecanoic acid, dodecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
525.	80252-38-6	Hexadecanoic acid, dotriacontyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{31}$-CH_3	103 [see 2809]	103	
526.	22413-01-0	Hexadecanoic acid, eicosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249, 5811b	
527.	628-97-7	Hexadecanoic acid, ethyl ester {ethyl palmitate} H_3C-$(CH_2)_{14}$-COO-CH_2-CH_3	1371, 2601a, 2775, 3266, 3410, 4249	172a, 174b, 908, 1053, 1157, 2389, 2544, 3266, 3547, 3555, 4249	
528.	42232-32-6	Hexadecanoic acid, heneicosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
529.	94632-82-3	Hexadecanoic acid, heptacosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{26}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
530.	18466-06-3	Hexadecanoic acid, heptadecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
531.	60007-87-6	Hexadecanoic acid, hexacosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
532.	540-10-3	Hexadecanoic acid, hexadecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{15}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

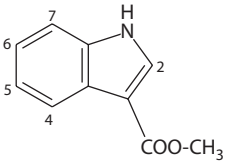
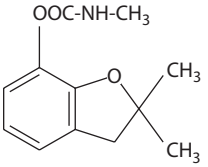
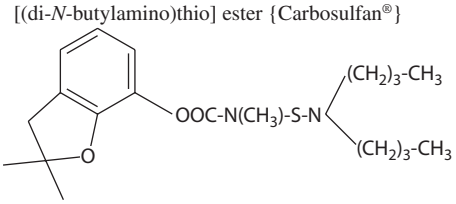
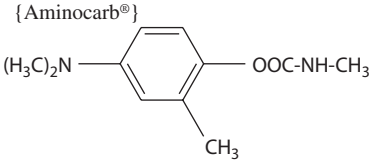
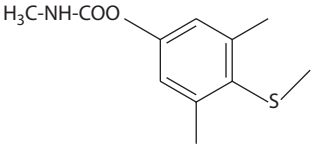
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
533.	23470-00-0	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester H_3C-$(CH_2)_{14}$–COO-CH═$(CH_2OH)_2$ {glyceryl 2-hexadecanoate}	2601a		
534.	112-39-0	Hexadecanoic acid, methyl ester H_3C-$(CH_2)_{14}$-COO-CH_3	568b, 2545, 2601a, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 4249, 4570a	120, 404, 568b, 2339a, 2386, 2389, 2544, 2861a, 2917a, 2940, 3549, 4249, 5811b	
535.	142-91-6	Hexadecanoic acid, (1-methylethyl) ester		2339a	
536.	36617-44-4	Hexadecanoic acid, nonadecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
537.	78509-52-1	Hexadecanoic acid, octacosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
538.	2598-99-4	Hexadecanoic acid, octadecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
539.	94632-81-2	Hexadecanoic acid, pentacosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
540.	18299-77-9	Hexadecanoic acid, pentadecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
541.	42232-35-9	Hexadecanoic acid, tetracosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{33}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
542.	4536-26-9	Hexadecanoic acid, tetradecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
543.	084461-48-3	Hexadecanoic acid, tetratriacontyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{33}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
544.	6027-71-0	Hexadecanoic acid, triacontyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{29}$-CH_3	103 [see 2809]	103	
545.	42232-34-8	Hexadecanoic acid, tricosyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
546.	36617-38-6	Hexadecanoic acid, tridecyl ester H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
547.	121877-41-6	Hexadecanoic acid, 14-methyl-, docosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
548.	121877-33-6	Hexadecanoic acid, 14-methyl-, heneicosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
549.	121877-67-6	Hexadecanoic acid, 14-methyl-, heptacosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{26}$-CH_3	103 [see 2809]	103	
550.	121877-58-5	Hexadecanoic acid, 14-methyl-, hexacosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809]	103	
551.	2490-49-5	Hexadecanoic acid, 14-methyl-, methyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-CH_3	809, 4249	2917a	
552.	121877-74-5	Hexadecanoic acid, 14-methyl-, octacosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809]	103	
553.	121877-39-2	Hexadecanoic acid, 15-methyl-, docosyl ester $(H_3C)_2$═CH-$(CH_2)_{13}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
554.	6929-04-0	Hexadecanoic acid, 15-methyl-, methyl ester $(H_3C)_2$═CH-$(CH_2)_{13}$-COO-CH_3		2389, 2544, 4249, 5811b	
555.	11017-44-0 71607-94-8	Hexadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10, 14,18,22,26,30,34-hexatria contanonaenyl ester {solanesyl palmitate}	1231, 3251, 3296, 4336	1893a, 1893b, 2338, 3348, 3349, 3358, 4249, 4336, 5811b	
556.	1118-77-0	Hexadecanoic acid, 3,7,11,15-tetramethyl-, methyl ester		1248, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
557.	53950-58-6	Hexadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{14}$-COO-CH_2-CH═C(CH_3)-CH_2 [$CH_2CH_2CH(CH_3)CH_2]_3$-H	2939, 3210, 3287, 3308, 4249	1893, 2939, 4249	
558.	37822-81-4	Hexadecatrienoic acid, methyl ester		1248, 4249	
559.	29960-49-4	Hexadecenoic acid, methyl ester		5811, 5811b	
560.	1120-25-8	9-Hexadecenoic acid, methyl ester, (*Z*)- H_3C-$(CH_2)_7$-CH═CH-$(CH_2)_5$-COO-CH_3		1248, 4249	
561.	123-79-5	Hexanedioic acid, dioctyl ester	3559		
562.	103-23-1	Hexanedioic acid, bis(2-ethylhexyl) ester	3559		
563.	626-82-4	Hexanoic acid, butyl ester		5811	
564.	123-66-0	Hexanoic acid, ethyl ester {ethyl caproate} H_3C-$(CH_2)_4$-COO-C_2H_5	565, 568b, 1140, 1416, 1903, 1904, 2858, 2939, 3266, 3302, 4249, 4259, 4319, 5811b	172a, 174b, 568b, 1053, 2389, 2544, 3266, 3370, 3905, 3974a, 4249	
565.	2983-37-1	Hexanoic acid, 2-ethyl-, ethyl ester	568b, 4249		
566.	31501-11-8	Hexanoic acid, *cis*-3-hexenyl ester		568b, 2389, 2544, 4249, 5811b	
567.	6946-90-3	Hexanoic acid, 2-hydroxy-, ethyl ester		5811	
568.	2305-25-1	Hexanoic acid, 3-hydroxy-, ethyl ester		5811	
569.	106-70-7	Hexanoic acid, methyl ester H_3C-$(CH_2)_4$-COO-CH_3		2339a, 2356, 4249	
570.	2198-61-0	Hexanoic acid, 3-methylbutyl ester		172a, 174b, 1053, 3266, 3370	
571.	2177-83-5	Hexanoic acid, 5-methyl-, methyl ester		568b, 4249	
572.	30414-55-2	Hexanoic acid, 5-methyl-3-oxo-, methyl ester		3858, 4249	
573.	1842-56-4	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, methyl ester		3858	
574.	3249-68-1	Hexanoic acid, 3-oxo-, ethyl ester	5811		
575.	13984-57-1	Hexanoic acid, 5-oxo-, ethyl ester	5811		
576.	540-07-8	Hexanoic acid, pentyl ester		174b, 3266	540-07-8
577.	6290-37-5	Hexanoic acid, 2-phenylethyl ester		937, 2336, 4249	
578.	6938-45-0	Hexanoic acid, phenylmethyl ester		568b, 2093, 2386, 2389, 2544, 4249, 5811b	
579.	123-68-2	Hexanoic acid, 2-propenyl ester	5811b	1053, 3266	
580.	626-77-7	Hexanoic acid, propyl ester		5811	
581.	29144-38-5 58000-93-4	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, acetate, stereoisomer {solanesyl acetate}	1373, 2939, 3251, 3270, 3295, 3296, 4249, 5811, 5811a, 5811b	2338, 2939, 3295, 3348, 3349, 3357, 3928, 4249, 5811, 5811a, 5811b	
582.	2396-78-3	3-Hexenoic acid, methyl ester H_3C-CH_2-CH═CH-CH_2-COO-CH_3		1157, 2336, 4249	
583.	2497-18-9	2-Hexen-1-ol, acetate, (*E*)-		172a, 174b, 1053, 3266	
584.	1708-82-3	3-Hexen-1-ol, acetate		1157, 3266, 4249	
585.	3681-71-8	3-Hexen-1-ol, acetate, (*Z*)-		172a, 174b, 1053, 3266, 5811b	
586.	25152-85-6	3-Hexen-1-ol, benzoate, (*Z*)-		4249	
587.	2315-09-5	3-Hexen-1-ol, formate		1157, 4249	
588.	33467-73-1	3-Hexen-1-ol, formate, (*Z*)-		172a, 174b, 1053, 1147, 3266, 4249	
589.	61989-59-1	Hexonic acid, 2,3-dideoxy-, γ-lactone, monoacetate	3553, 4249, 5811b		

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
590.	1912-33-0	1*H*-Indole-3-acetic acid, methyl ester		2675a, 4249, 4467	
591.		1*H*-Indole-3-butanoic acid, methyl ester		4249, 4467	
592.	942-24-5	1*H*-Indole-3-carboxylic acid, methyl ester 		4249, 4467	
593.	5548-09-4	1*H*-Indole-3-propanoic acid, methyl ester		4249, 4467	
594.	27137-10-6	Isotetradecanoic acid, methyl ester	809, 249		
595.	67493-77-0	Lanostane-3,7,11-triol, 3,7-diacetate, (3β,7β,11β)-		4249, 4497	
596.	624-83-9	Methane, isocyanato- {methyl isocyanate} $H_3C\text{-}N{=}C{=}O$	1140, 1284, 1420, 1741, 2722, 2724, 2943, 3300, 3491, 5811b		
597.	17622-35-4	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, acetate, stereoisomer		4249, 4787	
598.	1563-66-2	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester: see 7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate {Furadan®; Carbofuran®} 	1553, 21A19	1280, 1553, 2650b, 3481, 3633, 3973, 4249, 4271a, 5811b, 21A19	
599.	55285-14-8	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl [(di-*N*-butylamino)thio] ester {Carbosulfan®} 		3633	
600.	2032-59-9	Methylcarbamic acid, 4-(dimethylamino)-3-methylphenyl ester {Aminocarb®} 		2650a, 3633, 4271a	
601.	16709-30-1	Methylcarbamic acid, 2,2-dimethyl-3(2*H*)-oxobenzofuran-7-yl ester		5811, 5811b	
602.	2032-65-7	Methylcarbamic acid, 3,5-dimethyl-4-(methylthio)phenyl ester {Methiocarb®} 		3633, 4271a	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

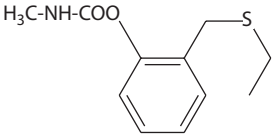
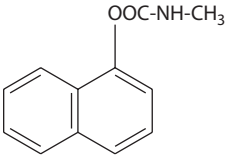
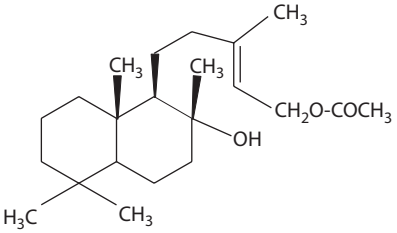
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
603.	29973-13-5	Methylcarbamic acid, 2-((ethylthio)methyl)phenyl ester {Ethiofencarb®} 		3633, 4271a	
604.	114393-99-6	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, 3-acetate, [1R-(1α,3β,4)]		4249, 4454	
605.	61263-48-7	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,8-tetramethyl-, acetate, (R)-		4249, 4928	
606.	63-25-2	1-Naphthalenol, methylcarbamate {Sevin®; Carbaryl®} 	418, 419, 1333, 1457, 3224, 3302, 3634, 21A19	418, 419, 1219a, 1219c, 1280, 1333, 1457, 2650b, 2698, 3481, 3633, 3634, 3637, 3727, 3797, 3973, 3977, 4249, 4271a, 5811b, 21A19	
607.	31149-06-1	2-Naphthalenol, 1-[5-(acetyloxy)-3-methyl-3-pentenyl]decahydro-2,5,5,8a-tetramethyl-, [1R-[1α(*E*),2β,4aβ,8aα]]- 		1156, 2565, 4090, 4101, 4249	
608.	598-58-3	Nitric acid, methyl ester	239, 1437, 3901, 3902		
609.	109-95-5	Nitrous acid, ethyl ester $H_3C\text{-}CH_2\text{-}ON{=}O$	3901, 3902		
610.	624-91-9	Nitrous acid, methyl ester $H_3C\text{-}ON{=}O$	1140, 1420, 1449, 1736, 1955, 2270, 2293, 2310, 2724, 2939, 2941, 3059, 3302, 3308, 3491, 3698, 4058, 4319, 4342, 5811b	984	
611.	121878-05-5	Nonacosanoic acid, docosyl ester $H_3C\text{-}(CH_2)_{27}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	103 [see 2809]	103	
612.	121877-94-9	Nonacosanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{27}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809]	103	
613.	39815-65-1	Nonacosanoic acid, 4-(2-hydroxyethyl)phenyl ester		908, 3219, 4249, 5811b	
614.	42232-76-8	Nonadecanoic acid, docosyl ester $H_3C\text{-}(CH_2)_{17}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
615.	42232-66-6	Nonadecanoic acid, dodecyl ester $H_3C\text{-}(CH_2)_{17}\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	3251, 3294, 3302, 4249	3251, 3294, 4249	
616.	36610-54-5	Nonadecanoic acid, eicosyl ester $H_3C\text{-}(CH_2)_{17}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	103 [see 2809], 3251, 3294, 3302, 4249, 5811b	103, 3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
617.	42232-75-7	Nonadecanoic acid, heneicosyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
618.		Nonadecanoic acid, heptacosyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
619.	36610-51-2	Nonadecanoic acid, heptadecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
620.		Nonadecanoic acid, hexacosyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
621.	36610-50-1	Nonadecanoic acid, hexadecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
622.	1731-94-8	Nonadecanoic acid, methyl ester H_3C-$(CH_2)_{17}$-COO-CH_3		2093, 4249	
623.	36610-53-4	Nonadecanoic acid, nonadecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249, 5811b	3251, 3294, 4249	
624.	36610-52-3	Nonadecanoic acid, octadecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
625.		Nonadecanoic acid, pentacosyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
626.	36610-49-8	Nonadecanoic acid, pentadecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
627.	121877-66-5	Nonadecanoic acid, tetracosyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	93, 3251, 3294, 4249	
628.	36610-48-7	Nonadecanoic acid, tetradecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
629.	42232-77-9	Nonadecanoic acid, tricosyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
630.	36610-47-6	Nonadecanoic acid, tridecyl ester H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
631.	121877-54-1	Nonadecanoic acid, 17-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
632.	121877-69-8	Nonadecanoic acid, 17-methyl-, tetracosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809]	103	
633.	121877-59-6	Nonadecanoic acid, 17-methyl-, tricosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
634.	145090-31-9	Nonadecanoic acid, 18-methyl-, 2-(acetyloxy)-1-(hydroxymethyl) ethyl ester $(H_3C)_2$=CH-$(CH_2)_{16}$-COO-$CH(CH_2OH)$-CH_2-OOC-CH_3		4249	
635.		Nonadecanoic acid, 18-methyl-, eicosyl ester $(H_3C)_2$=CH-$(CH_2)_{16}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
636.	150643-41-7	Nonadecanoic acid, 18-methyl-, ester with 1,2,3-propanetriol monoacetate mono(16-methylheptadecanoate)		4249	
637.	121877-51-8	Nonadecanoic acid, 18-methyl-, heneicosyl ester $(H_3C)_2$=CH-$(CH_2)_{16}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
638.	121877-37-0	Nonadecanoic acid, 18-methyl-, nonadecyl ester $(H_3C)_2$=CH-$(CH_2)_{16}$-COO-$(CH_2)_{18}$-CH_3	103 [see 2809]	103	
639.	71607-90-4	Nonadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]- H_3C-$(CH_2)_{17}$COO-CH_2-CH=C(CH_3)-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H	3210, 3287, 3308, 4249		1375a, 1377, 4249
640.	123-29-5	Nonanoic acid, ethyl ester H_3C-$(CH_2)_7$-COO-C_2H_5		172a, 174b, 908, 1053, 2389, 2544, 3266, 3370, 4249, 5811b	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
641.	1731-84-6	Nonanoic acid, methyl ester H_3C-$(CH_2)_7$-COO-CH_3	568b, 3402, 4249	568b, 908, 2339a, 2389, 2544, 4098a, 4249, 5811b	
642.	37822-76-7	Nonenoic acid, methyl ester		1248, 4249, 5811b	
643.	111-79-5	2-Nonenoic acid, methyl ester		5811, 5811b	
644.	18444-66-1	19-Norlanosta-1,5,23-triene-3,11,22-trione, 25-(acetyloxy)-2,16,20-trihydroxy-9-methyl-, (9β,10α,16α,23*E*)-		4249	
645.	17278-28-3	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3α,9β,10α,16α,23*E*)-		4249	
646.	89647-62-1	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3β,9β,10α,16α,23*E*)-		4249	
647.	121878-02-2	Octacosanoic acid, docosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
648.		Octacosanoic acid, dodecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294	3251, 3294	
649.	121877-91-6	Octacosanoic acid, eicosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
650.		Octacosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl octacosanoate}	1230	1230	
651.	121877-95-0	Octacosanoic acid, heneicosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294	
652.		Octacosanoic acid, heptacosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
653.		Octacosanoic acid, heptadecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
654.		Octacosanoic acid, hexacosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
655.	80756-16-7	Octacosanoic acid, hexadecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
656.		Octacosanoic acid, nonadecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
657.	95415-29-5	Octacosanoic acid, octadecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
658.		Octacosanoic acid, pentacosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
659.		Octacosanoic acid, pentadecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
660.	80252-40-0	Octacosanoic acid, tetracosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
661.	28570-28-7	Octacosanoic acid, tetradecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
662.		Octacosanoic acid, tricosyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
663.		Octacosanoic acid, tridecyl ester H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 4249	3251, 3294, 4249	
664.	121878-04-4	Octacosanoic acid, 26-methyl-, docosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{24}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
665.	97145-16-9	Octadecadienoic acid, 1-[[[(2-aminoethoxy)hydroxyphosphinyl] oxy]methyl]-1,2-ethanediyl ester, (all-*Z*)-		4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
666.	97190-11-9	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) hexadecanoate		4249	
667.	97190-13-1	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecanoate, (*Z,Z*)-		4249	
668.	28061-47-4	Octadecadienoic acid, methyl ester		4249	
669.	97210-24-7	Octadecadienoic acid, monoester with 1,2,3-propanetriol 1,1′-(hydrogen phosphate) mono-3-hexadecenoate, [R-[R*,S*-(*E*)]]-		4249	
670.	26836-36-2	9,12-Octadecadienoic acid (*Z,Z*)-, diester with 1,2,3-propanetriol monohexadecanoate {palmitodilinolein}		5538, 5811, 5811b	
671.	28409-91-8	9,12-Octadecadienoic acid-, diester with 1,2,3-propanetriol mono-9-octadecenoate {oleodilinolein}		5811, 5811b	
672.	29590-02-1	9,12-Octadecadienoic acid-, diester with 1,2,3-propanetriol monooctadecanoate {stearodilinolein}		5811, 5811b	
673.	26836-30-6 99431-70-6	9,12-Octadecadienoic acid-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitolinolein}		5811, 5811b	
674.	26836-32-8	9,12-Octadecadienoic acid, monoester with propanetriol monohexadecanoate and monooctadecanoate {palmitostearolinolein}		5811, 5811b	
675.	26836-35-1	9,12-Octadecadienoic acid (*Z,Z*)-, ester with 1,2,3-propanetriol monohexadecanoate mono[(*Z*)-9-octadecenoate]		4042c, 4249, 5811b	
676.	544-35-4	9,12-Octadecadienoic acid (*Z,Z*)-, ethyl ester {ethyl linoleate} H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COO-C_2H_5		568b, 2386, 404, 2917a, 3555, 4249	
677.	2462-85-3	9,12-Octadecadienoic acid, methyl ester		404, 1590a, 2094, 2386, 4249	
678.	112-63-0	9,12-Octadecadienoic acid (*Z,Z*)-, methyl ester {methyl linoleate} H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COO-CH_3	60, 568b, 2773, 3224, 3266, 4249	60, 568b, 908, 1053, 1590a, 2386, 2389, 2544, 3219, 3266, 3547, 3549, 4249, 5811b	
679.	26836-38-4	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol monooctadecanoate mono-9-octadecenoate, (*Z*)-		4042c, 4249, 5811b	
680.	28880-78-6	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol bis[(*Z*)-9-octadecenoate]		4249, 5811b	
681.	99431-70-6 26836-30-6	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitolinolein}		5538	
682.	34521-51-2	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dioctadecanoate		4249	
683.	70495-60-2 110115-39-4	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecadienoate}	1231, 2939, 3251, 3296, 4249, 4336	1893a, 1893b, 2338, 2939, 3348, 3358, 4249, 4336	
684.	53950-59-7	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]- H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COO-CH_2-CH═C(CH_3)-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H	3219, 3287, 3308, 4249	984, 1590a, 2336, 2389, 2544, 2917a, 3188, 3266, 3547, 3555, 4249	3404, 4249
685.	56847-03-1	Octadecadienoic acid, methyl ester	2601a		
686.	26855-40-3	Octadecanoic acid, diester with 1,2,3-propanetriol dihexadecanoate {dipalmitostearin}		5811, 5811b	
687.	22413-03-2	Octadecanoic acid, docosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
688.	5303-25-3	Octadecanoic acid, dodecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
689.	22413-02-1	Octadecanoic acid, eicosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
690.	111-61-5	Octadecanoic acid, ethyl ester {ethyl stearate} H_3C-$(CH_2)_{16}$-COO-CH_2-CH_3	568b, 2601a, 4249, 5811b	568b, 1053, 2389, 2544, 3266, 3547, 4249, 5811b	
691.	42232-59-7	Octadecanoic acid, heneicosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
692.	121877-78-9	Octadecanoic acid, heptacosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
693.	18299-82-6	Octadecanoic acid, heptadecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
694.	58886-94-5	Octadecanoic acid, hexacosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
695.	1190-63-2	Octadecanoic acid, hexadecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
696.	112-61-8	Octadecanoic acid, methyl ester {methyl stearate} H_3C-$(CH_2)_{16}$-COO-CH_3	568b, 2543, 2545, 2773, 4249	404, 568b, 908, 2092, 2339a, 2389, 2544, 3547, 3549, 4249, 5811b	
697.	121877-86-9	Octadecanoic acid, nonacosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{28}$-CH_3	103 [see 2809]	103	
698.	36610-45-4	Octadecanoic acid, nonadecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{18}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
699.	70495-59-9	Octadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecanoate}	1231, 3251, 3296, 4249, 4332	3349, 3358, 4249	
700.	63317-82-8	Octadecanoic acid, octacosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809]	103	
701.	2778-96-3	Octadecanoic acid, octadecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
702.	121877-65-4	Octadecanoic acid, pentacosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{24}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
703.	18299-80-4	Octadecanoic acid, pentadecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
704.	42232-61-1	Octadecanoic acid, tetracosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
705.	17661-50-6	Octadecanoic acid, tetradecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{13}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
706.	63317-83-9	Octadecanoic acid, triacontyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{29}$-CH_3	103 [see 2809]	103	
707.	42232-60-0	Octadecanoic acid, tricosyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
708.	31556-45-3	Octadecanoic acid, tridecyl ester H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
709.	121877-53-0	Octadecanoic acid, 16-methyl-, docosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{14}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
710.	121877-75-6	Octadecanoic acid, 16-methyl-, hexacosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{14}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809]	103	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
711.		Octadecanoic acid, 17-methyl-, methyl ester $(H_3C)_2$═CH-$(CH_2)_{15}$-COO-CH_3		2389, 2544	
712.	62172-54-7	Octadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{16}$-COO-CH_2-CH═C(CH_3)-$CH_2[CH_2CH_2CH(CH_3)CH_2]_3$-H	3219, 3287, 3308, 4249		
713.	97190-08-4	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecadienoate, (all-*Z*)-		4249	
714.	97229-62-4	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) 2(or 3)-hexadecanoate, (*Z,Z,Z*)-		4249	
715.	97229-63-5	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1,1′-(hydrogen phosphate) 2(or 3)-(3-hexadecenoate), [R-(R*,S*)]-		4249	
716.	29565-44-4	Octadecatrienoic acid, methyl ester		4359a, 5811b	
717.		9,12,15-Octadecatrienoic acid, docosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{21}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
718.		9,12,15-Octadecatrienoic acid, dodecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
719.		9,12,15-Octadecatrienoic acid, eicosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{19}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
720.	1191-41-9	9,12,15-Octadecatrienoic acid, ethyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-$COOC_2H_5$		2386, 3555,4249	
721.		9,12,15-Octadecatrienoic acid, heneicosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{20}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
722.		9,12,15-Octadecatrienoic acid, heptacosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
723.		9,12,15-Octadecatrienoic acid, heptadecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
724.		9,12,15-Octadecatrienoic acid, hexacosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
725.		9,12,15-Octadecatrienoic acid, hexadecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
726.	7361-80-0	9,12,15-Octadecatrienoic acid, methyl ester {methyl linolenate} H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-$COOCH_3$	2543, 2773	404, 908, 1590a, 2386, 3547, 3549	
727.	301-00-8	9,12,15-Octadecatrienoic acid, methyl ester, (*Z,Z,Z*)- {methyl linolenate} H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-CH_3	2543, 2545, 2601a, 2773, 3266, 4249	1053, 1590a, 2917a, 3266, 3547, 4249, 5811b	
728.		9,12,15-Octadecatrienoic acid, nonadecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
729.	28973-74-2	9,12,15-Octadecatrienoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecatrienoate}	1231, 2939, 3251, 3296, 4319, 4336	2939, 3348, 3358, 4336	
730.	17673-60-8	9,12,15-Octadecatrienoic acid, octadecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249, 4319	3251, 3294, 4249	
731.		9,12,15-Octadecatrienoic acid, pentacosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
732.		9,12,15-Octadecatrienoic acid, pentadecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
733.		9,12,15-Octadecatrienoic acid, tetracosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
734.		9,12,15-Octadecatrienoic acid, tetradecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH$═$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
735.		9,12,15-Octadecatrienoic acid, tricosyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
736.		9,12,15-Octadecatrienoic acid, tridecyl ester, (*Z,Z,Z*)- H_3C-$(CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
737.	30452-68-7	9,12,15-Octadecatrienoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E,Z,Z,Z*)]]- H_3C-$(CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-CH_2-$CH{=}C(CH_3)$-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H	3219, 3287, 3308, 4249		
738.	27071-84-7	9-Octadecenoic acid, diester with 1,2,3-propanetriol monohexadecanoate {palmitodiolein}		5811, 5811b	
739.	28409-94-1	9-Octadecenoic acid-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitoolein}		5811, 5811b	
740.	93976-10-4	Octadecenoic acid, docosyl ester, (*Z*)-	3251, 3294, 3302	3251, 3294	
741.		Octadecenoic acid, heneicosyl ester, (*Z*)-	3251, 3294, 3302	3251, 3294	
742.	93976-08-0	Octadecenoic acid, hexacosyl ester, (*Z*)-	3251, 3294, 3302	3251, 3294	
743.	27234-05-5	Octadecenoic acid, methyl ester		2094, 2386, 3549, 4249, 5811b	
744.	93976-09-1	Octadecenoic acid, tetracosyl ester, (*Z*)-	3251, 3294, 3302, 4249	3251, 3294, 4249	
745.	71607-93-7 73037-55-5	9-Octadecenoic acid (*Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester {solanesyl oleate}	1231, 3251, 3296, 4336, 5811	1893a, 1893b, 2338, 3348, 3358, 4336, 5811	
746.	57840-35-4	9-Octadecenoic acid (*Z*)-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(E)]]- H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-CH_2-$CH{=}C(CH_3)$-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H	3287, 3308		
747.		9-Octadecenoic acid (*Z*)-, docosyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{21}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
748.	36078-10-1	9-Octadecenoic acid (*Z*)-, dodecyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
749.	22393-88-0	9-Octadecenoic acid (*Z*)-, eicosyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{19}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
750.	111-62-6	9-Octadecenoic acid (*Z*)-, ethyl ester {ethyl oleate} H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-C_2H_5	2601a	908, 1053, 2389, 2544, 3266, 3547, 4249, 5811b	
751.		9-Octadecenoic acid (*Z*)-, heptacosyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
752.	22393-86-8	9-Octadecenoic acid (*Z*)-, hexadecyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
753.	112-62-9	9-Octadecenoic acid (*Z*)-, methyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-CH_3	568b, 2773, 4249	404, 568b, 908, 2386, 2389, 2544, 3547, 5811b	
754.		9-Octadecenoic acid (*Z*)-, nonadecyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
755.	17673-49-3	9-Octadecenoic acid (*Z*)-, octadecyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
756.		9-Octadecenoic acid (*Z*)-, pentacosyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
757.	69454-18-8	9-Octadecenoic acid (*Z*)-, pentadecyl ester H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
758.		9-Octadecenoic acid (*Z*)-, tetracosyl ester H_3C-$(CH_2)_7$-CH═CH-$(CH_2)_7$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
759.	22393-85-7	9-Octadecenoic acid (*Z*)-, tetradecyl ester H_3C-$(CH_2)_7$-CH═CH-$(CH_2)_7$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
760.		9-Octadecenoic acid (*Z*)-, tricosyl ester H_3C-$(CH_2)_7$-CH═CH-$(CH_2)_7$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
761.	75164-73-7	9-Octadecenoic acid (*Z*)-, tridecyl ester H_3C-$(CH_2)_7$-CH═CH-$(CH_2)_7$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
762.	104077-09-0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-2- [(1-oxo-9-octadecenyl)oxy]ethyl ester, (*Z,Z,Z*)-		4249	
763.	104077-10-3	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-		4249	
764.	104100-34-7	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-1,3-propanediyl ester, (all-*Z*)-		4249	
765.	104077-06-7	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-3-[(1-oxo-9- octadecenyl)oxy]propyl ester, (*Z,Z,Z*)-		4249	
766.	104077-07-8	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl) oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-		4249	
767.	104077-11-4	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl) oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-		4249	
768.	104077-12-5	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl) oxy]-9-octadecenyl]oxy]-,1-(hydroxymethyl)-1,2-ethanediylester,(all-*Z*)-		4249	
769.	104100-35-8	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl) oxy]-9-octadecenyl]oxy]-,2-hydroxy-1,3-propanediylester,(all-*Z*)-		4249	
770.	104077-08-9	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[[1-oxo-18- [(1-oxo-9-octadecenyl) oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-		4249	
771.	104077-13-6	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl) oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-		4249	
772.	2462-84-2	9-Octadecenoic acid, methyl ester		4249	
773.	70687-51-3	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-, methyl ester		4249, 5811b	
774.	115-95-7	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate {linalyl acetate}		172a, 174b, 1053, 2339a, 3198, 3219, 3266, 3354, 3370, 4249	
775.	115-99-1	1,6-Octadien-3-ol, 3,7-dimethyl-, formate {linalyl formate}		2917a	
776.	16409-44-2	2,6-Octadien-1-ol, 3,7-dimethyl-, acetate,		568b, 4249	
777.	106-32-1	Octanoic acid, ethyl ester {ethyl caprylate}	1949	172a, 174b, 908, 1053, 1949, 2389, 2544, 3266, 3370, 4249, 5811b	
778.	111-11-5	Octanoic acid, methyl ester {methyl caprylate}	568b, 3402, 4249	568b, 908, 404, 2093, 2389, 2544, 4249, 5811b	
779.	2035-99-6	Octanoic acid, 3-methylbutyl ester		172a, 174b, 1053, 3266	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

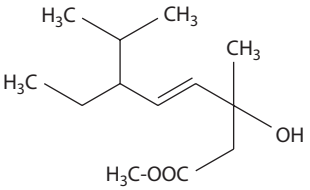
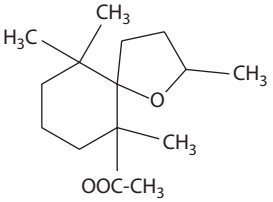
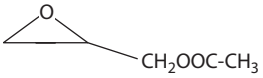
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
780.	70898-30-5	Octanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester, (all-*E*)- {solanesyl octanoate}	1231, 3251, 3296, 4336	1893a, 1893b, 2939, 3358, 4249, 4336	
781.	638-25-5	Octanoic acid, pentyl ester		1053, 3266	
782.	70898-31-6	Octanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]- H_3C-$(CH_2)_6$-COO-CH_2-CH═C(CH_3)-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H		1893, 4249	
783.	20780-49-8	1-Octanol, 3,7-dimethyl-, acetate {tetrahydrogeranyl acetate}		2917a	
784.		4-Octenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-, methyl ester 		404	
785.	111-12-6	2-Octynoic acid, methyl ester H_3C-$(CH_2)_4$-C≡C-COO-CH_3		174b, 1053, 3266	
786.	57893-27-3	1-Oxaspiro[4.5]decane, 6-acetoxy-2,6,10,10-tetramethyl- {6-acetoxydihydrotheaspirane} 		1053, 3266	
787.	77-83-8	Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester {ethyl methylphenylglycidate}		174b, 3266	
788.	61892-62-4	2,3-Oxiranedimethanol, monopropanoate	568b, 3553, 4249, 5811b		
789.	6387-89-9	Oxiranemethanol, acetate {glycidyl acetate} 		568b, 2917a, 4249	
790.	121877-88-1	Pentacosanoic acid, docosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
791.		Pentacosanoic acid, dodecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
792.	121877-80-3	Pentacosanoic acid, eicosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
793.		Pentacosanoic acid, heneicosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{20}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
794.		Pentacosanoic acid, heptacosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
795.		Pentacosanoic acid, heptadecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
796.		Pentacosanoic acid, hexacosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
797.		Pentacosanoic acid, hexadecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

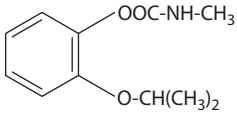
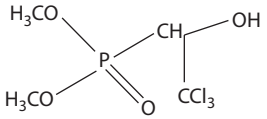
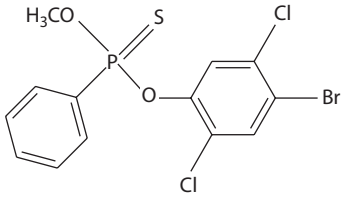
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
798.		Pentacosanoic acid, nonadecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
799.		Pentacosanoic acid, octadecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
800.	10482-74-3	Pentacosanoic acid, pentacosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
801.		Pentacosanoic acid, pentadecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
802.		Pentacosanoic acid, tetracosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
803.		Pentacosanoic acid, tetradecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
804.		Pentacosanoic acid, tricosyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{32}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
805.		Pentacosanoic acid, tridecyl ester H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
806.	121877-85-8	Pentacosanoic acid, 23-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{21}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
807.	102673-27-8	4,9-Pentadecadienal, 6-(acetyloxy)-8-hydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4E,6R*,8R*,9E,11S*)]-		4249	
808.	102734-50-9	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, methyl ester, [6R-(4E,6R*,8S*,9E,11S*)]-		3973, 3974a	
809.	102734-51-0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, methyl ester, [6R-(4E,6R*,8R*,9E,11S*)]-		3973, 3974a	
810.		Pentadecane, 4-acetoxy-		2917a	
811.	42232-23-5	Pentadecanoic acid, docosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
812.	42232-14-4	Pentadecanoic acid, dodecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
813.	36617-37-5	Pentadecanoic acid, eicosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
814.	41114-00-5	Pentadecanoic acid, ethyl ester H_3C-$(CH_2)_{13}$-COO-CH_2-CH_3	2386, 4249	4359a	
815.	42232-22-4	Pentadecanoic acid, heneicosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{20}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
816.		Pentadecanoic acid, heptacosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
817.	36617-34-2	Pentadecanoic acid, heptadecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
818.		Pentadecanoic acid, hexacosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{25}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
819.	36617-33-1	Pentadecanoic acid, hexadecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{15}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
820.	7132-64-1	Pentadecanoic acid, methyl ester H_3C-$(CH_2)_{13}$-COO-CH_3	1878a, 3402, 4249	404, 2389, 2544, 4249, 5811b	
821.	36617-36-4	Pentadecanoic acid, nonadecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
822.	36617-35-3	Pentadecanoic acid, octadecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
823.		Pentadecanoic acid, pentacosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
824.	36617-32-0	Pentadecanoic acid, pentadecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
825.	121877-44-9	Pentadecanoic acid, tetracosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
826.	36617-31-9	Pentadecanoic acid, tetradecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
827.	42232-24-6	Pentadecanoic acid, tricosyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
828.	36617-30-8	Pentadecanoic acid, tridecyl ester H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
829.	121877-18-7	Pentadecanoic acid, 13-methyl-, heptadecyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809]	103	
830.	121877-55-2	Pentadecanoic acid, 13-methyl-, pentacosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COO-$(CH_2)_{24}$-CH_3	103 [see 2809]	103	
831.	121877-43-8	Pentadecanoic acid, 13-methyl-, tricosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COO-$(CH_2)_{32}$-CH_3	103 [see 2809]	103	
832.	121877-31-4	Pentadecanoic acid, 14-methyl-, docosyl ester $(H_3C)_2$=CH-$(CH_2)_{12}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
833.	121877-27-8	Pentadecanoic acid, 14-methyl-, eicosyl ester $(H_3C)_2$=CH-$(CH_2)_{12}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
834.	121877-13-2	Pentadecanoic acid, 14-methyl-, heptadecyl ester $(H_3C)_2$=CH-$(CH_2)_{12}$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809]	103	
835.	121877-20-1	Pentadecanoic acid, 14-methyl-, octadecyl ester $(H_3C)_2$=CH-$(CH_2)_{12}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809]	103	
836.	121877-47-2	Pentadecanoic acid, 14-methyl-, tetracosyl ester $(H_3C)_2$=CH-$(CH_2)_{12}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809]	103	
837.	121877-38-1	Pentadecanoic acid, 14-methyl-, tricosyl ester $(H_3C)_2$=CH-$(CH_2)_{12}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
838.		Pentadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl pentadecanoate}		3295, 3349, 4249	
839.	71607-96-0	Pentadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{13}$-COO-CH_2-CH=C(CH_3)-CH_2 $[CH_2CH_2CH(CH_3)CH_2]_3$-H	3287, 3308, 4249, 4332		
840.	31422-28-3	Pentadecenoic acid, methyl ester		2094, 4249, 5811b	
841.	591-68-4	Pentanoic acid, butyl ester		174b, 3266	
842.	539-82-2	Pentanoic acid, ethyl ester {ethyl valerate} H_3C-$(CH_2)_3$-COO-C_2H_5	565, 1903, 1904, 2858, 2939, 3266, 3302, 4249, 5811b	172a, 174b, 174b, 1053, 3266, 3797, 3973, 3974a, 4249	
843.	624-24-8	Pentanoic acid, methyl ester {methyl valerate} H_3C-$(CH_2)_3$-COO-CH_3	4570a	2993a	
844.	10361-39-4	Pentanoic acid, phenylmethyl ester		1248, 2336, 2389, 2544, 4249, 5811b	
845.	70340-00-0	Pentanoic acid, 2-methylphenyl ester		4249, 5811b	
846.	6376-59-6	Pentanoic acid, 2-oxo-, methyl ester	4249, 4800		
847.	5870-68-8	Pentanoic acid, 3-methyl-, ethyl ester	1903, 1904, 3302, 3797, 4249, 4319, 5811b	3797, 3973, 3974a, 4249	
848.	2177-78-8	Pentanoic acid, 3-methyl-, methyl ester	2939	5811b	
849.	2412-80-8	Pentanoic acid, 4-methyl-, methyl ester	4570a		

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
850.	539-88-8	Pentanoic acid, 4-oxo-, ethyl ester {ethyl levulinate} $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}COO\text{-}CH_2\text{-}CH_3$	1238	1053, 3266	
851.	624-45-3	Pentanoic acid, 4-oxo-, methyl ester {methyl levulinate} $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}COO\text{-}CH_3$	1238	3266, 3543, 3560, 3561, 3858, 4249	
852.	66274-27-9	Pentanoic acid, 5-hydroxy-4-oxo-, methyl ester	3404, 4249, 5811b		3404
853.	5185-97-7	2-Pentanone, 5-(acetyloxy)-	5811b	568b, 3561, 4249	
854.	5164-76-1	2-Pentenedioic acid, dimethyl ester		2356	
855.	24218-00-6	*D*-erythro-2-pentulose, 1,5-bis(dihydrogen phosphate)		4249	
856.	114-26-1	Phenol, 2-(1-methylethoxy)-, methylcarbamate {Undene®; Propoxur®} 		1280, 2698, 3533, 4249, 4271a	
857.	5451-83-2	Phenol, 3-methoxy-, acetate	2601a		
858.					
859.		Pheophytin, 10-hydroxy-		5517	
860.	3147-18-0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2E,7S*,11S*),4β,21β]]- {pheophytin B}		4249, 4445, 5517	
861.	15664-29-6	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, [3S-(3α,4β,21β)]- {pheophorbide A}		4249, 4445, 5517	
862.	603-17-8	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2E,7S*,11S*),4β,21β]]- {pheophytin A		3626a, 4249, 4445, 5517	
863.	52-68-6	Phosphonic acid, 2,2,2-trichloromethyl-1-hydroxyethyl-, dimethyl ester {Trichlorphon®; Dipterex®} 	1333	1333, 2650a, 3380, 3633, 3973, 3977, 4271a	
864.	21609-90-5	Phosphonothioic acid, phenyl-, *O*-(4-bromo-2,5-dichlorophenyl)-, *O*-methyl ester {Phosvel®} 	21A19	3381, 3634, 21A19	
865.	22224-92-6	Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylthio)phenyl ester {Fenamiphos®}		2856a, 3381, 3633, 3646a, 3973, 4249, 4271a, 5811b	
866.	30560-19-1	Phosphoramidothioic acid, *N*-acetyl-, *O,S*-dimethyl ester {Acephate}		1219a, 1219b, 1219c, 2058a, 2650b, 3633, 3634, 3973, 4271a	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

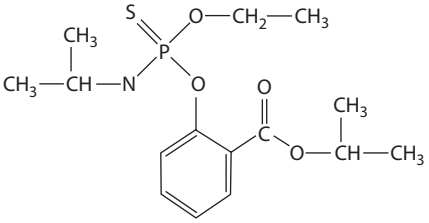
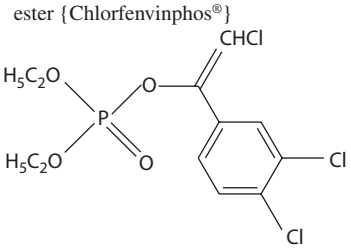
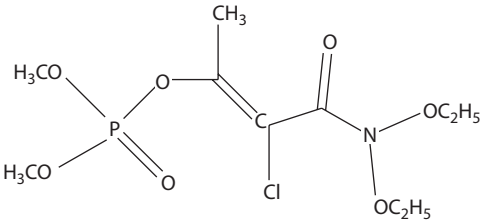
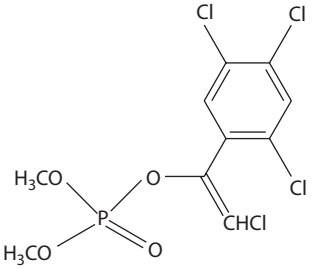
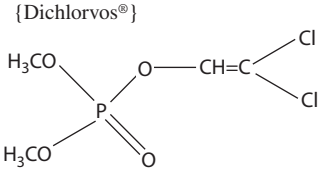
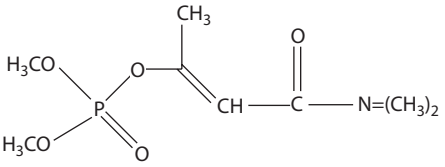
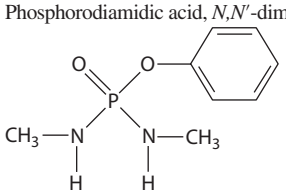
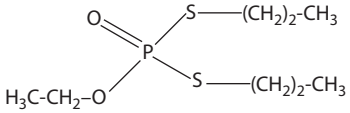
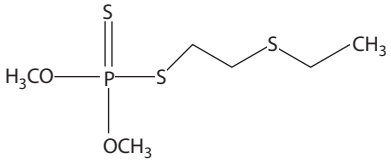
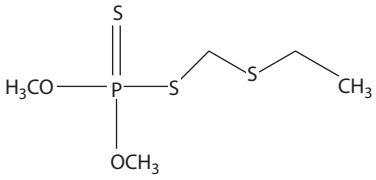
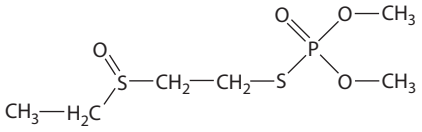
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
867.	10265-92-6	Phosphoramidothioic acid *O,S*-dimethyl ester {Methamidophos®}		2058a, 3633, 4271a, 5811b	
868.	25311-71-1	Phosphoramidothioic acid, *O*-ethyl *O*-2 (1-methylethyl) carbonylphenyl-, (1-methylethyl) ester {Isofenphos®} 		3633, 21A61	
869.	470-90-6	Phosphoric acid, 2-chloro-1-(2-dichlorophenyl)ethenyl-, diethyl ester {Chlorfenvinphos®} 		3381, 3633, 4271a	
870.	13171-21-6	Phosphoric acid, 2-chloro-3-(diethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Phosphamidon®} 		3380, 3633, 4271a	
871.	22248-79-9	Phosphoric acid, 2-chloro-1-(2,4,5-trichlrophenyl)ethenyl-, dimethyl ester {Tetrachlorvinphos®} 		3381, 3633, 4271a	
872.	62-73-7	Phosphoric acid, 2,2,-dichloroethenyl-, dimethyl ester {Dichlorvos®} 		2058a, 3380, 3633, 4271a	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
873.	141-66-2	Phosphoric acid, 3-(dimethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Dicrotophos®} 		3380	
874.	1754-58-1	Phosphorodiamidic acid, *N,N′*-dimethyl-, phenyl ester {Diamidafos®} 	2527	2527	
875.	13194-48-4	Phosphorodithioic acid, *O*-ethyl-*S,S*, dipropyl ester {Ethoprophos®} 		2345, 3381, 3633, 3634, 3646a, 3767a, 3973, 4271a	
876.	13071-79-9	Phosphorodithioic acid, *O,O*-diethyl *S*-[(1,1-dimethylethyl)thio] methyl ester {Terbuphos®}		2650b, 3633	
877.	2497-06-5	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylsulfonyl)ethyl] ester (Thiodemeton sulfone®)		4249	
878.	298-04-4	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester {Disulfoton®} 	1127, 21A19	1127, 2058a, 2345, 3633, 3634, 3973, 4249, 4271a, 5811b, 21A19	
879.	298-02-2	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)methyl] ester {Phorate®} 		2058a, 3381	
880.	301-12-2	Phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(ethylsulfinyl)ethyl] ester {Oxydemeton methyl®} 		3633, 21A22	
881.	640-15-3	Phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Thiometon®}		4271a	
882.	950-37-8	Phosphorodithioic acid, *O,O*-dimethyl-*S*-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl ester {Methidathion®}		2058a, 3633, 3973, 4271a	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

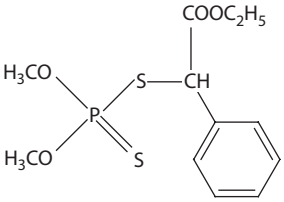
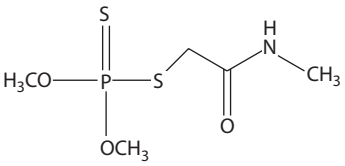
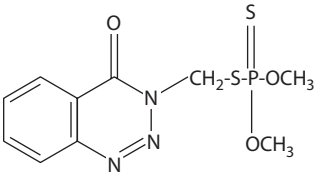
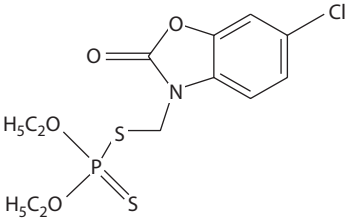
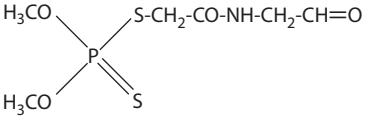
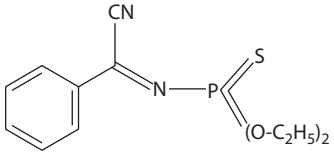
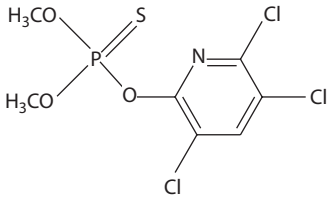
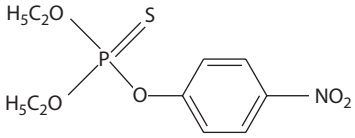
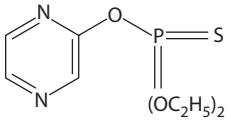
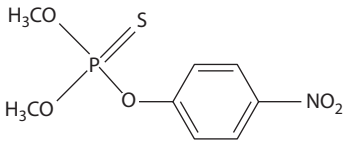
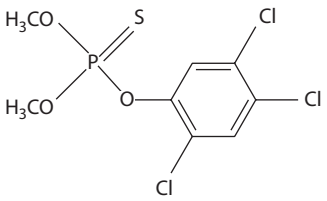
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
883.	2597-03-7	Phosphorodithioic acid, *O,O*-dimethyl-S-(α-ethoxycarbonylbenzyl) ester {Fenthoate®; Phenthoate®} 		3381	
884.	60-51-5	Phosphorodithioic acid, *O,O*-dimethyl-*S*-[2-methylamino)-2-oxoethyl] ester {Dimethoate®} 	5553b, 5811b	3380, 3633, 3797, 3973, 4271a, 5811b	
885.	2642-71-9	Phosphorodithioic acid, *O,O*-diethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Azinphos ethyl}		3633, 4271a	
886.	86-50-0	Phosphorodithioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Guthion®; Azinphos-Methyl®} 	417, 419, 1457, 3302, 21A19	419, 1219a, 1219c, 1457, 2650b, 3381, 3973, 4271a, 21A19	
887.	2310-17-0	Phosphorodithioic acid, *S*-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl) methyl] *O,O*-diethyl ester {Phosalone®} 		3381, 4271a	
888.	2540-82-1	Phosphorodithioic acid, *S*-[2-formylmethylamino)-2-oxoethyl] *O,O*-dimethyl ester {Formothion®} 		2058a, 2650b, 3380, 3633, 4271a	
889.	41198-08-7	Phosphorothioic acid, *O*-(4-bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl ester {Profenophos®}		2058a	
890.	38527-91-2	Phosphorothioic acid, 2-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester {Ethaphos®}	5811, 5811a, 5811b		

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
891.	14816-18-3	Phosphorothioic acid, *O,O*-diethyl *O*-(α-cyanobenzylideneamino)- {Phoxim®} 		1492a, 4271a	
892.	2921-88-2	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyriphos®; Dursban®} 	717, 1333, 5811b, 21A19	717, 1219a, 1219b, 1219c,1333, 2058a, 3381, 3633, 3919, 4249, 3977, 5811b, 21A19	
893.	115-90-2	Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylsulfinyl)phenyl] ester {Fensulfothion®}		2650b, 3381, 3633, 3634, 3973, 4249, 4271a	
894.	56-38-2	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®} 	21A19	2058a, 3381, 3633, 3634, 3973, 4249, 4271a, 5079, 5439, 5811b, 21A19	
895.	297-97-2	Phosphorothioic acid *O,O*-diethyl *O*-pyrazinyl ester {Zinophos®; Thionazine®} 		3633, 4249, 4271a	
896.	298-00-0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-nitrophenyl) {Parathion-methyl®} 	5811b	2058a, 3381, 3633, 3973, 4271a	
897.	299-84-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester {Fenchlorphos®; Phenchlorphos®} 		3381, 3633	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

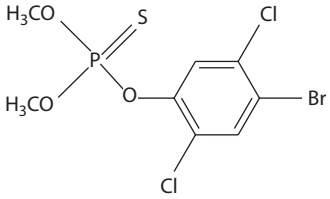
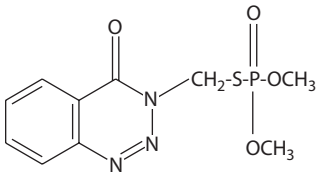
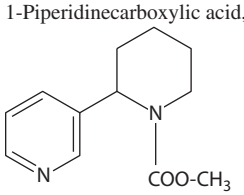
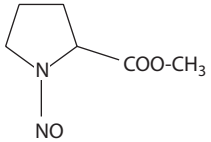
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
898.	2104-96-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-bromo-2,5-dichlorophenyl) ester {Bromophos®} 		3381, 3633, 4271a	
899.	333-41-5	Phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester {Diazinon®}	5811b	1219b, 1219c, 2058a, 2650b, 3633, 3973, 4271a	
900.	24017-47-8	Phosphorothioic acid, *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) ester {Triazophos®}		2650a	
901.	919-86-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Demeton-S-methyl®}		2058a, 3633, 4271a, 5811b	
902.	961-22-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl) methyl] ester 	419, 3302, 4249	419	
903.	20300-00-9	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfinyl]ethyl] ester {Vamidothion sulfoxide®}		3992a, 4249	
904.	2275-23-2	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester {Vamidothion®}		822a, 2650a, 3633, 4249	
905.	70898-34-9	Phosphorothioic acid, *O,O* dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfonyl]ethyl] ester {Vamidothion sulfone®}		4249, 4917	
906.	122-14-5	Phosphorothioic acid, *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester {Fenitrothion}		3633, 3973, 4249, 4271a, 4917	
907.	55-38-9	Phosphorothioic acid *O,O*-dimethyl *O*-(4-methylthio)-3-methylphenyl ester {Fenthion®}		3633, 4271a	
908.	29232-93-7	Phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-dimethyl ester {Pirimiphos-methyl}		4249	
909.	40626-35-5	Phosphorothioic acid, *O*-ethyl *O*-phenyl S-propyl ester {Heterophos®}	5811, 5811a, 5811b		
910.	56078-09-2	1-Piperidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)- 	1578, 2220, 3491, 4249, 5811b	1578, 4249, 5811b	
911.	35909-01-4	*L*-Proline, 1-nitroso-, methyl ester 	3256, 3300	466, 485, 3256	
912.	142-10-9	Propanal, 2,3-dihydroxy-, 3-phosphate		555b	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
913.	105-53-3	Propanedioic acid, diethyl ester	5811b	1053, 3266, 3370	
914.	108-59-8	Propanedioic acid, dimethyl ester $H_2C{=}(COO\text{-}CH_3)_2$	3266	2356, 3266, 4249	
915.	607-81-8	Propanedioic acid, (phenylmethyl)-, diethyl ester	2601a		
916.	627-69-0	1,2-Propanediol, 1-acetate $H_3C\text{-}CHOH\text{-}CH_2\text{-}OOC\text{-}CH_3$	568b, 2543, 2773, 3553, 3559, 4249, 4319, 5811b	568b, 2389, 2544, 3905, 4249, 5811b	
917.	6214-01-3	1,2-Propanediol, 2-acetate $H_3C\text{-}CH(OOC\text{-}CH_3)\text{-}CH_2OH$	568b, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 3905, 4249	
918.	10602-14-9	1,2-Propanediol, 1-(dihydrogen phosphate)		429b, 4249, 4570	
919.	54541-18-3	1,2-Propanediol, 2-propanoate	568b, 3553, 4249, 5811b		
920.		1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monomethyl ester	1375a, 1377		1375a, 1377
921.	77-93-0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester {triethyl citrate}	3190, 3992	172a, 174b, 1053, 2386, 3266, 4249	
922.	61892-59-9	1,2,3-Propanetriol, 1-acetate 2-formate	568b, 3553, 4249, 5811b		
923.	25395-31-7	1,2,3-Propanetriol, diacetate {diacetin}	568b, 1063–1066, 1068–1074, 1371, 1375, 1375b, 1586, 2543, 2601a, 2765–2767, 2773, 3553, 4249, 4570a	568b, 3905, 4249, 4751	
924.	29860-16-0	1,2,3-Propanetriol, 1,2-diacetate {1,2-diacetin}	568b, 4249	568b, 4249, 5811b	
925.	105-70-4	1,2,3-Propanetriol, 1,3-diacetate {1,3-diacetin}	568b, 4249	568b, 4249	
926.	57-03-4	1,2,3-Propanetriol, 1-(dihydrogen phosphate)		429b	
927.	927-20-8	1,2,3-Propanetriol, 1-(dihydrogen phosphate), magnesium salt (1:1)		429b, 4249, 4975	
928.	17603-42-8	1,2,3-Propanetriol, 1-(dihydrogen phosphate), sodium salt		4249, 4908a	
929.	1335-34-8	1,2,3-Propanetriol, mono(dihydrogen phosphate), potassium salt		4249, 4908a	
930.	106-61-6 26446-35-5	1,2,3-Propanetriol, monoacetate {monoacetin}	568b, 1350, 1354, 1360, 1371, 1375a, 1375, 1375a, 1375b, 1586, 2543, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 3255, 3553, 3557, 4249, 4570a, 5811, 5811b	568b, 2389, 2544, 4249, 5811, 5811b	1354, 1360, 1375a
931.	72692-68-3	1,2,3-Propanetriol, monoformate	4249, 4810a		
932.	11046-98-3	1,2,3-Propanetriol, propanoate	5811, 5811a, 5811b		
933.	62244-24-0	1,2,3-Propanetriol, 1-propanoate, (R)-	3553, 4249		
934.	102-76-1	1,2,3-Propanetriol, triacetate {triacetin}	173a, 332, 568b, 1063–1066, 1068–1074, 1302, 1340, 1364, 1365, 1371, 1586, 2410, 2487, 2506, 2507, 2522, 2543, 2545, 2601a, 2761, 2762, 2765, 2773, 2777, 3228, 3255, 3266, 3308, 3559, 3797, 3835, 4249, 4259, 4268, 4570a, 5811b	172a, 174b, 568b, 1053, 2410, 3266, 3354, 3370, 3593, 3905, 4249, 4259, 4751, 5018, 5089, 5543, 5555, 5811b	2506, 2507
935.	555-44-2	1,2,3-Propanetriol, trihexdecanoate {tripalmitin}		5538	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

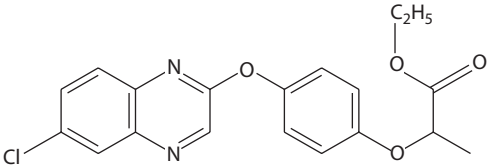
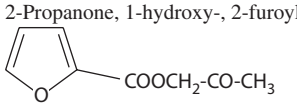
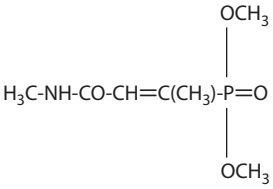
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
936.	122-32-7	1,2,3-Propanetriol, tri-9-octadecenoate {triolein}		5811, 5811b	
937.	537-40-6	1,2,3-Propanetriol, tri-9,12-octadecadienoate {trilinolein}	4249, 4875	5538	
938.	68334-00-9	1,2,3-Propanetriol, trioctadecanoate {tristearin}		5538	
939.	139-45-7	1,2,3-Propanetriol, tripropanoate	1368, 4249		
940.	555-45-3	1,2,3-Propanetriol, tritetradecanoate {trimyristin}		116	
941.	590-01-2	Propanoic acid, butyl ester		2339a	
942.	76578-14-8	Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester {Quizalofop-Et®} 		3633	
943.	138-22-7	Propanoic acid, 2-hydroxy-, butyl ester {butyl lactate}	5811		
944.	97-64-3	Propanoic acid, 2-hydroxy-, ethyl ester {ethyl lactate} H_3C-CHOH-COO-C_2H_5	568b, 1371, 1884, 2761, 2762, 2765, 2766, 2777, 3266, 3553, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370	
945.	547-64-8	Propanoic acid, 2-hydroxy-, methyl ester H_3C-CHOH-COO-CH_3	1371, 2761, 2762, 2765, 2766, 2777, 3410, 4249		3404
946.	97-89-2	Propanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester		1053, 3266, 3370	
947.	97-62-1	Propanoic acid, 2-methyl-, ethyl ester		174b, 3266	
948.	37704-28-2	Propanoic acid, 2-methyl-, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-3-cyclohexen-1-yl ester		4740, 4249	
949.	547-63-7	Propanoic acid, 2-methyl-, methyl ester $(H_3C)_2$=CH-COO-CH_3		2339a, 3585, 4249	
950.	2445-69-4	Propanoic acid, 2-methyl-, 2-methylbutyl ester		2339a	
951.	2050-01-3	Propanoic acid, 2-methyl-, 3-methylbutyl ester		2339a	
952.	65416-14-0	Propanoic acid, 2-methyl-, 2-methyl-4-oxo-4*H*-pyran-3-yl ester		1053, 3266, 3370	
953.	103-93-5	Propanoic acid, 2-methyl-, 4-methylphenyl ester {*p*-tolyl isobutyrate}		172a, 174b, 1053, 3266, 3370	
954.	109-15-9	Propanoic acid, 2-methyl-, octyl ester		1053, 3266, 3370	
955.	103-48-0	Propanoic acid, 2-methyl-, phenylethyl ester		172a, 174b, 1053, 3266, 3370	
956.	103-28-6	Propanoic acid, 2-methyl-, phenylmethyl ester {benzyl isobutyrate}	172a	174b, 1248, 2339a, 3266, 4249, 5811b	
957.	103-59-3	Propanoic acid, 2-methyl-, 3-phenyl-2-propen-1-yl ester		174b, 3266	
958.		Propanoic acid, 2-methylbutyl ester		2339a	
959.	105-68-0	Propanoic acid, 3-methylbutyl ester		174b, 2339a, 3266	
960.	13532-18-8	Propanoic acid, 3-(methylthio)-, methyl ester H_3C-S-$(CH_2)_2$-COO-CH_3		172a, 174b, 1053, 3266, 4249	
961.	103-56-0	Propanoic acid, 3-phenyl-2-propenyl ester {cinnamyl propionate}	2487	1053, 3266	
962.	617-35-6	Propanoic acid, 2-oxo-, ethyl ester H_3C-CO-COO-C_2H_5	3410, 4249		
963.	600-22-6	Propanoic acid, 2-oxo-, methyl ester H_3C-CO-COO-CH_3	568b, 4249, 5811b	5811b	
964.	4272-12-2	Propanoic acid, 3-(acetyloxy)- H_3C-COO-$(CH_2)_2$-COOH	1075, 2775, 3553, 4249		
965.		Propanoic acid, 3-hydroxy-, 2-methylamino-, propyl ester	3553, 4249		

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
966.	80657-57-4	Propanoic acid, 3-hydroxy-2-methyl-, methyl ester	568b, 4249		
967.	105-68-0	Propanoic acid, 3-methylbutyl ester		2339a	
968.	122-63-4	Propanoic acid, phenylmethyl ester {benzyl propionate}		1053, 3266, 3370	
969.	103-56-0	Propanoic acid, 3-phenyl-2-propenyl ester {cinnamyl propionate}	2487	1053, 3266	
970.	105-38-4	Propanoic acid, ethenyl ester $H_3C\text{-}CH_2\text{-}COO\text{-}CH{=}CH_2$		3797, 4249,	
971.	105-37-3	Propanoic acid, ethyl ester {ethyl propionate} $H_3C\text{-}CH_2\text{-}COO\text{-}C_2H_5$	625, 1140, 1903, 1904, 2088, 2858, 2939, 3266, 3302, 3308, 3797, 4249, 5811b	172a, 174b, 1053, 2339a, 2939, 3266, 3370, 3797, 3974a, 4249	
972.	554-12-1	Propanoic acid, methyl ester $H_3C\text{-}CH_2\text{-}COO\text{-}CH_3$	3559, 3797, 4249, 5811b	2339a, 3841, 3855, 4249	
973.	592-20-1	2-Propanone, 1-(acetyloxy)- $H_3C\text{-}CO\text{-}CH_2\text{-}OOC\text{-}CH_3$	568b, 1215, 1238, 1375, 1375b, 1378, 2387, 2570, 2731, 2731, 2735, 3553, 3557, 4249, 5770, 5811b	568b, 2386, 4249, 5811b	1378, 2244, 2387, 3401, 3402, 3404
974.	10258-70-5	2-Propanone, 1-(formyloxy)- $H_3C\text{-}CO\text{-}CH_2\text{-}OOC\text{-}H$	5811b		3402, 4249
975.		2-Propanone, 1-hydroxy-, 2-furoyl ester 	1586		
976.	2157-98-4	1-Propene, 1-methyl-3-(methylamino)-3-oxo-, dimethyl phosphate {Monocrotophos®} 		2058a, 2650b, 3633, 3973	
977.	80-62-6	2-Propenoic acid, 2-methyl-, methyl ester		2917a	
978.	82826-13-9	2-Propenoic acid, 3-(2-furanyl)-2-methyl-, ethyl ester		568b, 4249	
979.		2-Propenoic acid, 3-(2-furanylmethyl)-2-methyl-, ethyl ester		568b, 4249	
980.	2309-07-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester {ferulic acid, methyl ester}	3712, 4249, 4553a	5811b	
981.	47018-25-7	2-Propenoic acid, 3-phenyl-, 2-phenylethenyl ester	3219, 3308, 3485, 4249		
982.	122-69-0	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester {cinnamyl cinnamate}	3219, 3224, 3308, 3485, 4249	172a, 174b, 1053, 3266, 3370	
983.	103-36-6	2-Propenoic acid, 3-phenyl-, ethyl ester {ethyl cinnamate}	2478, 3266, 3308, 4249	172a, 174b, 1053, 3266, 3370	
984.	103-26-4	2-Propenoic acid, 3-phenyl-, methyl ester {methyl cinnamate}	1379, 2487, 5811b	172a, 174b, 1053, 1379, 3266, 3370	
985.	7779-65-9	2-Propenoic acid, 3-phenyl-, 3-methylbutyl ester	2487	172a, 174b, 1053, 3266, 3370	
986.	122-67-8	2-Propenoic acid, 3-phenyl-, 2-methylpropyl ester		172a, 174b, 1053, 3266, 3370	
987.	103-53-7	2-Propenoic acid, 3-phenyl-, phenylethyl ester;		172a, 174b, 1053, 3266	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

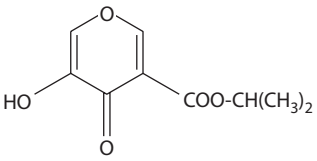
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
988.	103-41-3	2-Propenoic acid, 3-phenyl-, phenylmethyl ester {benzyl cinnamate}	2552, 2553, 3263, 3266, 3308, 3506, 3797, 4249, 5811b	172a, 174b, 1053, 3266, 3370	
989.		2-Propenoic acid, 3-phenyl-, 3-phenylpropyl ester {3-phenylpropyl cinnamate}		1053, 3266	
990.	96-33-3	2-Propenoic acid, methyl ester $H_2C{=}CH\text{-}COO\text{-}CH_3$	1140, 1413, 1414, 1416, 2857, 3302, 3308, 3557, 3797, 4249, 4319, 5811b	984	
991.	21040-45-9	2-Propen-1-ol, 3-phenyl-, acetate, (*E*)-		4249	
992.	85373-77-9	4*H*-Pyran-3-carboxylic acid, 5,6-dihydro-2,6-dimethyl-, methyl ester	568b, 4249		
993.		4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-, (1-methylethyl) ester 	1375a (0), 1377 (0)		1375a, 1377, 4249
994.	614-18-6	3-Pyridinecarboxylic acid, ethyl ester	5811	5811	
995.	93-60-7	3-Pyridinecarboxylic acid, methyl ester {methyl nicotinate}	278, 1568, 3266, 4249, 5811b	1053, 1254, 1256, 1568, 2338, 2339a, 2611, 3266, 3491, 4249	
996.	55557-02-3	3-Pyridinecarboxylic acid, 1,2,5,6-tetrahydro-1-nitroso-, methyl ester		5811, 5811b	
997.	17747-43-2	3-Pyridinol, acetate (ester)	568b, 3553, 4249, 4407, 5811b		
998.	50609-61-5	4*H*-Pyrido[1,2-*a*]pyrimidine-3-acetic acid, 9-hydroxy-4-oxo-, ethyl ester	2601a		
999.	107-49-3	Pyrophosphoric acid, tetraethyl ester {TEPP} $[(H_3C\text{-}CH_2\text{-}O)_2\text{-}P{=}O]_2{=}O$		5079, 5439	
1000.	72692-79-6	1*H*-Pyrrolecarboxylic acid, ethyl ester	2767, 3553, 4249		
1001.	52115-69-2	1*H*-Pyrrole-2-carboxaldehyde, 5-[(acetyloxy)methyl]-		4249, 4788a	
1002.	3284-51-3	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, ethyl ester	568b, 3553, 4249, 5811b		
1003.	1194-97-4	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, methyl ester	568b, 3553, 4249		
1004.	1193-62-0	1*H*-Pyrrole-2-carboxylic acid, methyl ester	1587a, 3650, 4249, 5811b	5811b	
1005.	936-12-9	1*H*-Pyrrole-3-carboxylic acid, 2-methyl-, ethyl ester	568b, 2543, 2773, 4249		
1006.		Pyrrolidine, 2-acetyloxy-methyl-	2767, 4249		
1007.	69730-90-1	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, ethyl ester, (S)-		1156, 2497, 2498, 3742, 4090, 4249	
1008.	56078-08-1	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)-	1578, 3491, 3742, 4249, 5811b	1578, 2497, 2498, 3742, 4249	
1009.	106777-19-9	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-		429b, 4249	
1010.	27442-42-8	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-, 5-(dihydrogen phosphate)		429b, 4249	
1011.	63231-63-0	Ribonucleic acid		4249, 4442, 5863	
1012.	3615-55-2	Ribose, 5-(dihydrogen phosphate)		429b, 4249, 4670	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1013.	5147-00-2	*L*-Serine, acetate (ester) CH_3-COO-CH_2-CH(NH_2)-COOH		429b, 4249, 4895	
1014.	71607-87-9	Stigmasta-5,22-dien-3-ol, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {stigmasteryl linolenate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1015.	71278-15-4	Stigmasta-5,22-dien-3-ol, 9,12-octadecadienoate, [3β(9*Z*,12*Z*),22*E*]- {stigmasteryl linoleate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1016.	31615-93-7	Stigmasta-5,22-dien-3-ol, 9-octadecenoate, [3β(*Z*),22*E*]- {stigmasteryl oleate}	3251, 3296, 4249	2939, 3296, 4249	
1017.	20242-97-1	Stigmasta-5,22-dien-3-ol, dodecanoate, (3β,22*E*)- {stigmasteryl laurate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1018.	2308-84-1	Stigmasta-5,22-dien-3-ol, hexadecanoate, (3β,22*E*)- {stigmasteryl palmitate}	3251, 3296, 4249	2939, 3296, 4249	
1019.	23838-16-6	Stigmasta-5,22-dien-3-ol, octadecanoate, (3β,22*E*)- {stigmasteryl stearate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1020.	20242-98-2	Stigmasta-5,22-dien-3-ol, tetradecanoate, (3β,22*E*)- {stigmasteryl myrsitate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1021.	3177-92-2	Stigmast-5-en-3-ol, 9,12,15-octadecatrienoate, [3β(9*Z*,12*Z*,15*Z*)]- {β-sitosteryl linolenate}	3251, 3296, 4249	2939, 3296, 4249	
1022.	3577-13-7	Stigmast-5-en-3-ol, 9,12-octadecadienoate, [3β(*Z,Z*)]- {β-sitosteryl linoleate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1023.	3712-16-1	Stigmast-5-en-3-ol, 9-octadecenoate, [3β(*Z*)]- {β-sitosteryl oleate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1024.	41005-65-6	Stigmast-5-en-3-ol, dodecanoate, (3β)- {β-sitosteryl laurate}	3251, 3296, 4249	2939, 3296, 4249	
1025.	2308-85-2	Stigmast-5-en-3-ol, hexadecanoate, (3β)- {β-sitosteryl palmitate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1026.	34137-25-2	Stigmast-5-en-3-ol, octadecanoate, (3β)- {β-sitosteryl stearate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1027.	10473-40-2	Stigmast-5-en-3-ol, tetradecanoate, (3β)- {β-sitosteryl myristate}	3251, 3296, 4249	2939, 3296, 4249, 5811b	
1028.	1401-55-4	Tannins {tannic acid}		120, 1053, 2270, 2154, 2939, 2947c, 3266, 3708, 3973, 4249, 5079, 5126, 5381	
1029.	42233-59-0	Tetracosanoic acid, docosyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1030.	42233-49-8	Tetracosanoic acid, dodecyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1031.	42233-57-8	Tetracosanoic acid, eicosyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1032.		Tetracosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl tetracosanoate}	1230	1230	
1033.	42233-58-9	Tetracosanoic acid, heneicosyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1034.		Tetracosanoic acid, heptacosyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1035.	42233-54-5	Tetracosanoic acid, heptadecyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1036.	121878-03-3	Tetracosanoic acid, hexacosyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{25}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1037.	42233-53-4	Tetracosanoic acid, hexadecyl ester H_3C-(CH_2)$_{22}$-COO-(CH_2)$_{15}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1038.	42233-56-7	Tetracosanoic acid, nonadecyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1039.	24897-95-8	Tetracosanoic acid, octacosyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{27}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1040.	42233-55-6	Tetracosanoic acid, octadecyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1041.		Tetracosanoic acid, pentacosyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1042.	42233-52-3	Tetracosanoic acid, pentadecyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1043.	1001-43-0	Tetracosanoic acid, tetracosyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{23}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1044.	42233-51-2	Tetracosanoic acid, tetradecyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{13}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1045.	42233-60-3	Tetracosanoic acid, tricosyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1046.	42233-50-1	Tetracosanoic acid, tridecyl ester H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1047.	121877-84-7	Tetracosanoic acid, 22-methyl-, docosyl ester	103 [see 2809]	103	
1048.	121877-77-8	Tetracosanoic acid, 22-methyl-, eicosyl ester	103 [see 2809]	103	
1049.	71608-05-4	Tetracosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{22}$-COO-CH_2-CH=C(CH_3)-CH_2-[$CH_2CH_2CH(CH_3)CH_2]_3$-H	3287, 3308, 3308, 4249		
1050.	110-36-1	Tetradecanoic acid, butyl ester	5811a		
1051.	42232-05-3	Tetradecanoic acid, docosyl ester H_3C-$(CH_2)_{12}$-COO$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249, 5811b	
1052.	2040-64-4	Tetradecanoic acid, dodecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{11}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1053.	22413-00-9	Tetradecanoic acid, eicosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249, 5811b	
1054.	124-06-1	Tetradecanoic acid, ethyl ester {ethyl myristate} H_3C-$(CH_2)_{12}$-COO-C_2H_5		172a, 174b, 568b, 908, 1053, 2093, 2389, 2544, 3266, 4249, 5811b	
1055.	42218-21-3	Tetradecanoic acid, heneicosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1056.		Tetradecanoic acid, heptacosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1057.	18299-78-0	Tetradecanoic acid, heptadecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1058.	80252-34-2	Tetradecanoic acid, hexacosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1059.	2599-01-1	Tetradecanoic acid, hexadecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{15}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1060.	124-10-7	Tetradecanoic acid, methyl ester H_3C-$(CH_2)_{12}$-COO-CH_3	568b, 809, 3481, 4249	120, 404, 568b, 908, 937, 2339a, 2389, 2544, 2861a, 2917a, 2939, 4249, 5811b	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1061.	110-27-0	Tetradecanoic acid, 1-methylethyl ester H_3C-$(CH_2)_{12}$-COO-CH═$(CH_3)_2$		174b, 2339a, 3266	
1062.	36617-28-4	Tetradecanoic acid, nonadecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{18}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1063.	3234-81-9	Tetradecanoic acid, octadecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1064.	121877-45-0	Tetradecanoic acid, pentacosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{24}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1065.	18299-74-6	Tetradecanoic acid, pentadecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1066.	18653-39-9	Tetradecanoic acid, tetracosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1067.	3234-85-3	Tetradecanoic acid, tetradecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1068.	42232-06-4	Tetradecanoic acid, tricosyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1069.	36617-27-3	Tetradecanoic acid, tridecyl ester H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1070.	121877-30-3	Tetradecanoic acid, 12-methyl-, docosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
1071.	121877-23-4	Tetradecanoic acid, 12-methyl-, eicosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
1072.	121877-28-9	Tetradecanoic acid, 12-methyl-, heneicosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
1073.	121877-56-3	Tetradecanoic acid, 12-methyl-, hexacosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809]	103	
1074.	121877-08-5	Tetradecanoic acid, 12-methyl-, hexadecyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{15}$-CH_3	103 [see 2809]	103	
1075.	121877-17-6	Tetradecanoic acid, 12-methyl-, octadecyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COOH	103 [see 2809]	103	
1076.	121877-48-3	Tetradecanoic acid, 12-methyl-, pentacosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{24}$-CH_3	103 [see 2809]	103	
1077.	121877-40-5	Tetradecanoic acid, 12-methyl-, tetracosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809]	103	
1078.	121877-34-7	Tetradecanoic acid, 12-methyl-, tricosyl ester H_3C-CH_2-CH(CH_3)-$(CH_2)_{10}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
1079.	121877-29-0	Tetradecanoic acid, 13-methyl-, docosyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
1080.	121877-21-2	Tetradecanoic acid, 13-methyl-, eicosyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
1081.	121877-26-7	Tetradecanoic acid, 13-methyl-, heneicosyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
1082.	121877-49-4	Tetradecanoic acid, 13-methyl-, hexacosyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809]	103	
1083.	71801-84-8	Tetradecanoic acid, 13-methyl-, hexadecyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{15}$-CH_3	103 [see 2809]	103	
1084.	121877-12-1	Tetradecanoic acid, 13-methyl-, octadecyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809]	103	
1085.	121877-35-8	Tetradecanoic acid, 13-methyl-, tetracosyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809]	103	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

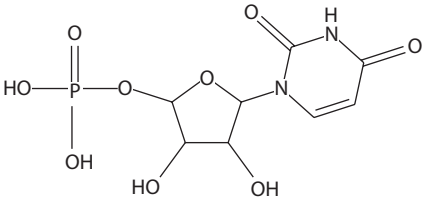
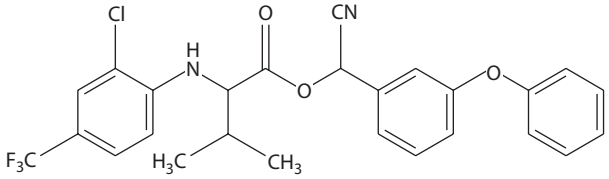
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1086.	121877-32-5	Tetradecanoic acid, 13-methyl-, tricosyl ester $(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{22}$-CH_3	103 [see 2809]	103	
1087.	71607-88-0 110053-62-8	Tetradecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl tetradecanoate}	1231, 2939, 3251, 3296, 4336	1893a, 1893b, 2939, 3348, 3349, 3358, 4336	
1088.	62172-52-5	Tetradecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{12}$-COO-CH_2-CH═$C(CH_3)$-CH_2 [$CH_2CH_2CH(CH_3)CH_2]_3$-H	3219, 3287, 3308, 4249	1893, 4249	
1089.	56219-06-8	9-Tetradecenoic acid, methyl ester, (*Z*)-		4249, 4718	
1090.	656-53-1	Thiazole, 4-methyl-5-(2-acetoxyethyl)-	5811		
1091.	154-87-0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, *P,P′*-dioxide		4051a, 4249, 4798	
1092.	556-64-9	Thiocyanic acid, methyl ester	1587, 4249, 5039, 5770		
1093.	22223-61-6	Thionitrous acid (HNOS), *S*-methyl ester	1140, 1420, 2724, 2939, 2940, 2945, 3491, 4249, 4319, 5811b		
1094.	121878-07-7	Triacontanoic acid, docosyl ester H_3C-$(CH_2)_{28}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
1095.	104932-26-5	Triacontanoic acid, eicosyl ester H_3C-$(CH_2)_{28}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
1096.		Triacontanoic acid, ester with olean-12-en-3-ol, (3β)-{β-amyrenyl triacontanoate}	1230	1230	
1097.	42233-37-4	Tricosanoic acid, docosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1098.	42233-27-2	Tricosanoic acid, dodecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{11}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1099.	42233-35-2	Tricosanoic acid, eicosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{19}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1100.	42233-36-3	Tricosanoic acid, heneicosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{20}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1101.		Tricosanoic acid, heptacosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{26}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1102.	42233-32-9	Tricosanoic acid, heptadecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{16}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1103.	121877-98-3	Tricosanoic acid, hexacosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{25}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1104.	42233-31-8	Tricosanoic acid, hexadecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{15}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	
1105.	2433-97-8	Tricosanoic acid, methyl ester H_3C-$(CH_2)_{21}$-COO-CH_3		404	
1106.	42233-34-1	Tricosanoic acid, nonadecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{18}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1107.	42233-33-0	Tricosanoic acid, octadecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{17}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1108.		Tricosanoic acid, pentacosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{24}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1109.	42233-30-7	Tricosanoic acid, pentadecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{14}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1110.	42233-39-6	Tricosanoic acid, tetracosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{23}$-CH_3	103 [see 2809], 3251, 3294, 3302, 4249	103, 3251, 3294, 4249	

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1111.	42233-29-4	Tricosanoic acid, tetradecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{13}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1112.	42233-38-5	Tricosanoic acid, tricosyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{22}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1113.	42233-28-3	Tricosanoic acid, tridecyl ester H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{12}$-CH_3	3251, 3294, 3302, 4249	3251, 3294, 4249	
1114.	121877-82-5	Tricosanoic acid, 21-methyl-, docosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
1115.	121877-72-3	Tricosanoic acid, 21-methyl-, eicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
1116.	121877-73-4	Tricosanoic acid, 21-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
1117.	121877-63-2	Tricosanoic acid, 21-methyl-, nonadecyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{18}$-CH_3	103 [see 2809]	93	
1118.	71608-06-5	Tricosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{21}$-COO-CH_2-CH=C(CH_3)-CH_2 [$CH_2CH_2CH(CH_3)CH_2]_3$-H	3287, 3308, 4249		1375a, 1377, 4249
1119.	36617-26-2	Tridecanoic acid, eicosyl ester H_3C-$(CH_2)_{11}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
1120.	1731-88-0	Tridecanoic acid, methyl ester H_3C-$(CH_2)_{11}$-COO-CH_3		3198, 3219, 3550, 4249, 5811b	
1121.	121877-24-5	Tridecanoic acid, 11-methyl-, heneicosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_9$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
1122.	121877-57-4	Tridecanoic acid, 11-methyl-, heptacosyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_9$-COO-$(CH_2)_{26}$-CH_3	103 [see 2809]	103	
1123.	121877-07-4	Tridecanoic acid, 11-methyl-, heptadecyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_9$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809]	103	
1124.	121877-16-5	Tridecanoic acid, 11-methyl-, nonadecyl ester H_3C-CH_2-$CH(CH_3)$-$(CH_2)_9$-COO-$(CH_2)_{18}$-CH_3	103 [see 2809]	103	
1125.	121877-25-6	Tridecanoic acid, 12-methyl-, docosyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-$(CH_2)_{21}$-CH_3	103 [see 2809]	103	
1126.	121877-19-8	Tridecanoic acid, 12-methyl-, eicosyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-$(CH_2)_{19}$-CH_3	103 [see 2809]	103	
1127.	121877-22-3	Tridecanoic acid, 12-methyl-, heneicosyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-$(CH_2)_{20}$-CH_3	103 [see 2809]	103	
1128.	121877-14-3	Tridecanoic acid, 12-methyl-, heptadecyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-$(CH_2)_{16}$-CH_3	103 [see 2809]	103	
1129.	5129-58-8	Tridecanoic acid, 12-methyl-, methyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-CH_3		4249	
1130.	121877-11-0	Tridecanoic acid, 12-methyl-, nonadecyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-$(CH_2)_{18}$-CH_3	103 [see 2809]	103	
1131.	121877-09-6	Tridecanoic acid, 12-methyl-, octadecyl ester $(H_3C)_2$=CH-$(CH_2)_{10}$-COO-$(CH_2)_{17}$-CH_3	103 [see 2809]	103	
1132.	71608-07-6	Tridecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]- H_3C-$(CH_2)_{11}$-COO-CH_2-CH=C(CH_3)-CH_2 [$CH_2CH_2CH(CH_3)CH_2]_3$-H	3287, 3308		
1133.	71608-08-7	Undecanoicacid,3,7,11,15-tetramethyl-2-hexadecenylester,[R-[R*,R*-(*E*)]]- H_3C-$(CH_2)_9$-COO-CH_2-CH=C(CH_3)-CH_2 [$CH_2CH_2CH(CH_3)CH_2]_3$-H	3287, 3308, 4249		
1134.	10580-24-2	Undecanoic acid, butyl ester		1053, 3266	

(*continued*)

TABLE 5.3 (continued)
Esters in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1135.	1731-86-8	Undecanoic acid, methyl ester H_3C-$(CH_2)_9$-$COOCH_3$	809, 3481, 4249	1157, 3266, 4249	
1136.	1731-81-3	1-Undecanol, acetate H_3C-$(CH_2)_9$-CH_2-OCO-CH_3		647, 2722, 3797, 3973, 5811b	
1137.	160115-56-0	6-Undecen-2-one, 10-(acetyloxy)-8,11-dihydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-5-hydroxy-2-methyl-2-furanyl)-		4249	
1138.	109-42-2	10-Undecenoic acid, butyl ester		5811	
1139.	692-86-4	10-Undecenoic acid, ethyl ester		1053, 3266	
1140.	133-89-1	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-glucopyranosyl ester		4249, 4489, 4580	
1141.	3616-06-6	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester		429b, 4249	
1142.	19253-25-9	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester		4249, 4459	
1143.	58-97-9	5′-Uridylic acid 		429b, 4249, 4474	
1144.	102851-06-9	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®} 		904, 2346, 3585e	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke.

6 Lactones

At various periods during the past 50 years, lactones in tobacco and tobacco smoke, particularly those in tobacco smoke, were discussed with regard to their toxicity, tumorigenicity, and genotoxicity. However, examination of the numerous lists of tobacco and tobacco smoke components classified as toxic, tumorigenic, and/or genotoxic reveals that seldom is a lactone included. The first significant list, derived from the 1986 International Agency for Research on Cancer (IARC) monograph on tobacco smoke (1870), was published in 1986 by Hoffmann and Wynder (1808). Over the next two decades, the Hoffmann–Wynder list was followed by successive similar but not identical lists by Hoffmann and Hecht (1727) in 1990, Hoffmann et al. (1773) in 1993, the Occupational Safety and Health Administration (OSHA) (2825) in 1994, Hoffmann and Hoffmann (1740, 1741, 1743) in 1997, 1998, and 2001, and Fowles and Bates (1217) in 2001 [see summary of all these lists in Table 2 in Rodgman (3265)].

Based on its February 1985 meeting on tobacco smoking, the IARC working group wrote in 1986 [see p. 107 in (1870)]:

> About 80 lactones have been identified in tobacco smoke. These compounds, especially the γ-butyrolactones, and others, have alkylating potential and some have been reported to be carcinogenic in laboratory animals [Lawley (6A12)]. [See also Appendix 2, pp. 387–394) in (1870)]. Quantitatively, about half the lactones in the smoke consist of γ-butyrolactone [IARC (6A10)] (about 10 µg/cigarette) and its derivatives; δ-valerolactone and some alkylated and unsaturated δ-valerolactones, as well as coumarin [see pp. 427–430 in Wynder and Hoffmann (4332)], 6-methylcoumarin and 3,4-dihydrocoumarin have also been isolated [Schumacher et al. (3553)]. The occurrence of coumarin derivatives in smoke could be due to pyrolysis of polyphenols with a coumarin structure…or of plant extracts added to tobacco to enhance flavour [see pp. 427–430 in Wynder and Hoffmann (4332)]. Coumarin itself is carcinogenic to rats after oral administration [IARC (6A10)].

In its monograph, IARC made no comment on the 10 lactones, including coumarin that Lawley listed as inactive in oncogenesis tests [see Table XXVII in (6A12)], citing the 1965 study on coumarin by Dickens and Jones (6A06). IARC also failed to mention the 1984 listing by Slaga and DiGiovanni (3685) of the report by Wattenberg et al. (4149d) who described the anticarcinogenicity of coumarin toward the potent tumorigenic polycyclic aromatic hydrocarbons (PAHs) benzo[*a*]pyrene (B[*a*]P) and 7,12-dimethylbenz[*a*]anthracene (DMB[*a*]A).

At the time of the writing of the IARC 1986 monograph on tobacco smoking, over 100 lactones had been identified in tobacco smoke.

The information on pp. 387–394 in Appendix 2 in (1870), particularly the information provided by the IARC working group on lactones on p. 391, is as follows:

Compound	Degree of Evidence in Animals (and Humans)
5. *Lactones*	
Coumarin	Limited evidence
γ-Butyrolactone	No evidence

In Figure 5 [see p. 93 in (1870)], only the following five lactones (substituted coumarins) of the nearly two dozen identified in tobacco and/or tobacco smoke were depicted, namely, scopoletin (7-hydroxy-6-methoxy-2*H*-1-benzopyran-2-one), scopolin [7-(β-*D*-glucopyranosyloxy)-6-methoxy-2*H*-1-benzopyran-2-one],esculetin(6,7-dihydroxy-2*H*-1-benzopyran-2-one),cichoriin [7-(β-D-glucopyranosyloxy)-6-hydroxy-2*H*-1-benzopyran-2-one], and scopoletin-β-gentiobioside.

Two lactones that received some attention with regard to tobacco and smoke were aflatoxins, B_1 and B_2, primarily aflatoxin B_1, the more toxic of the two. In 1970, Kaminski et al. (2024) examined the butts, ashes, and mainstream smoke (MSS) vapor phase and particulate phase from machine-smoked commercial nonfilter cigarettes treated with aflatoxin B_1. In six separate smoking experiments, no trace of aflatoxin B_1 was detected in any of the fractions examined. In their 1967 examination of several samples of leaf tobacco, including three types of good-grade tobaccos and heavily molded flue-cured tobacco, and of cigarette smoke condensate (CSC), Tso and Sorokin (3986) failed to detect aflatoxin B_1. They also reported that no aflatoxin B_1 was found in the CSC from cigarettes enriched with authentic aflatoxin B_1 prior to smoking. They concluded that the added aflatoxin B_1 was changed or decomposed during the smoking process. Later, Tso (3970) again reported the results of this aflatoxin B_1 study at the *1967 World Conference on Smoking and Health*. In his 2000 review of scientific publications on aflatoxin B, tobacco, and tobacco smoke, Massey (2484) concluded that aflatoxin B was not a contamination issue on tobaccos and, even if present, would decompose in the burning cigarette and would not transfer to smoke.

As noted in the quotation from the 1986 IARC monograph, orally administered coumarin (2*H*-1-benzopyran-2-one) had been reported as carcinogenic in rats. The results reported from several studies on the tumorigenicity of coumarin eventually resulted in coumarin being removed from the flavor formulations used throughout the tobacco industry on cigarette and pipe tobacco. Coumarin was considered by the consumer as a significantly acceptable contribution to

tobacco smoke. Coumarin was identified by Schumacher and Vestal as a minor component of untreated Oriental tobacco in the early 1960s (3560).

The initial concern in the early 1960s about the addition of coumarin {I} to tobacco products was whether or not it was converted during the smoking process to dicumarol (3,3′-methylenebis[4-hydroxy-2*H*-1-benzopyran-2-one) {II} (Figure 6.1). Dicumarol is a powerful anticoagulant that had been identified in sweet clover hay (6A21).

In previous metabolic studies, it had been reported that coumarin was not a precursor of dicumarol {II} (6A03, 6A15)) or of *o*-coumaric acid [3-(2-hydroxyphenyl)-2-propenoic acid] {III} (6A21). {III} was known to be a precursor of dicumarol via 4-hydroxycoumarin {IV}. Laboratory animals (rats, rabbits) fed coumarin excreted 4-hydroxycoumarin {IV} (6A04). Between 70% and 90% of coumarin administered to humans resulted in excretion of 7-hydroxycoumarin {V} (6A17), a coumarin derivative never indicted as dangerous to any species or proposed as a dicumarol precursor.

Newell reported in 1963 that (1) inclusion in cigarette tobacco of 3-^{14}C-coumarin {I} gave no dicumarol {II} in either the MSS or the sidestream smoke (SSS) and (2) inclusion in cigarette tobacco of unlabeled dicumarol gave no dicumarol {II} in either the MSS or the SSS (2757). Of the 3-^{14}C-coumarin applied to the tobacco blend, Newell reported that 60% appeared unchanged in the MSS and SSS.

To assess the claims of the possible adverse effect of including coumarin in flavor formulations, several reports and memoranda were written in the late 1970s about the coumarin situation in an obvious attempt to put the issue in perspective. In 1978, Buchner (6A05) listed several of the authorities that incorrectly cited negative tumorigenicity results as positive; e.g., in 1976, the National Institute for Occupational Safety and Health (NIOSH) (6A16) incorrectly cited results published in 1955 by Roe and Salaman (6A20). Much weight was given to the reported findings of Griepentrog (6A02, 6A07), the only findings on the induction of bile duct carcinomas in coumarin-fed rats. Buchner (6A05) summarized many of the results of studies that raised questions about the classification of coumarin as a carcinogen, e.g., the negative tumorigenicity results reported by Hagan et al. (6A08) and Hazleton et al. (6A09). He also cited several genotoxicity studies in which coumarin was found to be inactive against human chromosomes (6A22) and

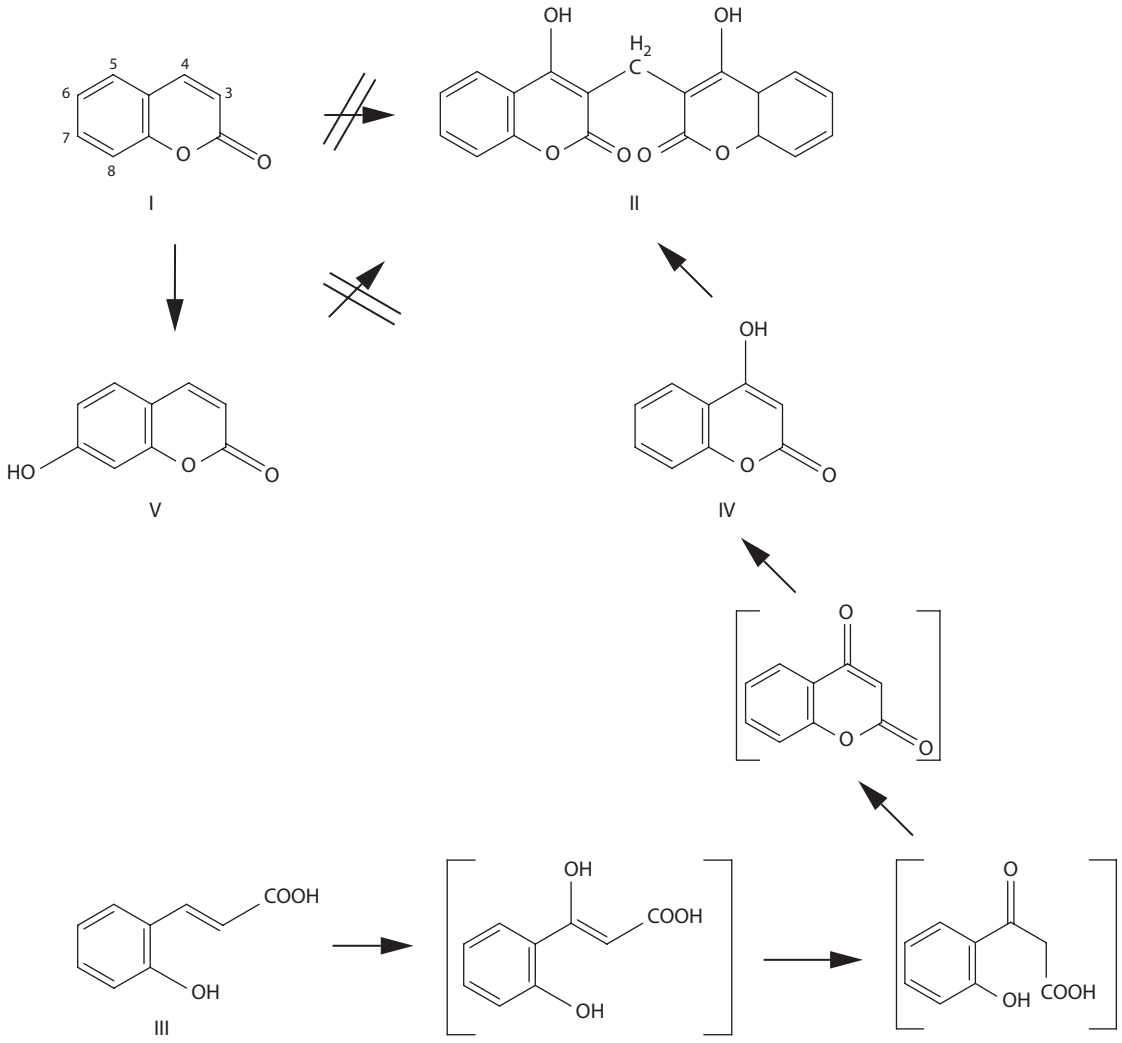


FIGURE 6.1 Relationships between coumarin, its derivatives, and dicumarol.

against *Salmonella typhimurium* strains TA1535, TA1537, TA98, and TA100 in the Ames test [private communication to Buchner, see Reference 26 in (6A22)].

Paralleling the report by Buchner were several memoranda on coumarin by Rodgman in 1978 (6A18) and 1982 (6A19) in which the problems of misinterpretation of data and contrary data pertinent to coumarin were presented. Included in the memoranda were the negative mutagenicity results obtained in Ames tests with five strains (TA1535, TA1537, TA1538, TA898, TA100) of *S. typhimurium* on coumarin conducted in-house by Lee (6A13) at R.J. Reynolds Research and Development. His results were confirmed on a coded coumarin sample among a set of coded samples tested at a contract laboratory (6A14).

Despite the controversies over the tumorigenicity of coumarin, its use in tobacco flavor formulations was subsequently discontinued throughout the tobacco industry worldwide.

In its 2000 evaluation of the tumorigenicity of coumarin (2*H*-1-benzopyran-2-one), IARC (6A11) noted the following as of August 21, 2000:

> Coumarin is a natural product occurring in the essential oils of a large number of plants, such as cinnamon, cassia, lavender and woodruff. It is used for its fragrance in many personal care products (perfumes, deodorants, soaps) and in tobacco, in household and industrial products to mask unpleasant odours and, in some countries, as a flavouring agent in food and beverages. It has also been used to treat several medical conditions. Exposure to coumarin may occur from its production, its natural presence in many plants and essential oils, and its several industrial, medical and consumer uses.

According to IARC, no data were available to its working group on the carcinogenicity of coumarin in humans. After assessment of various studies in which coumarin was administered to laboratory animals, IARC concluded that the evidence was limited in laboratory animals on the carcinogenicity of coumarin. IARC described its overall evaluation of coumarin as a carcinogen as follows: Coumarin is not classifiable as to its carcinogenicity to humans.

In 1998, Abbott (6A01) described the results of the examination of numerous food additives by the World Health Organization. The food additives in this particular study comprised a series of so-called aliphatic lactones. Among the lactones discussed were several that not only are used as foodstuff additives but that also occur in tobacco and/or its smoke and several that are used as tobacco additives. The results of several toxicological studies (acute toxicity, short- and long-term toxicity, carcinogenicity) and genotoxic studies on the lactones were described in detail by Abbott. Table 6.1 presents the results listed by Abbott on those lactones that are used in tobacco products.

Table 6.2 lists the tobacco and/or smoke lactones that, according to the Doull et al. listing (1053), are or have been used recently as components in flavor formulations for tobacco.

The number of lactones identified to date in tobacco and/or tobacco smoke is 336. Of these, 201 have been identified in tobacco smoke, 213 in tobacco, and 78 in both tobacco and tobacco smoke. In Table 6.3 are listed the lactones identified in tobacco and tobacco smoke to date.

TABLE 6.1
Some Biological Properties of Lactones Used as Additives in Foodstuffs as Well as in Tobacco Products (6A01)

	Lactone						
CAS No.	CAS Nomenclature	Common Name	Smoke or Tobacco Component	Flavor Formulation Additive	Genotoxicity[a]	Acute Toxicity, LD_{50}, mg/kg	Short-Term Toxicity, NOEL[b], mg/kg/day
104-50-7	2(3*H*)-Furanone, 5-butyldihydro-	γ-Octalactone	+	+		>5,000 (rat)[c]	
96-48-0	2(3*H*)-Furanone, dihydro-	γ-Butyrolactone	+	+	Negative	1,245 (mouse)	300 (rat) 175 (mouse)
695-06-7	2(3*H*)-Furanone, dihydro-5-ethyl-	γ-Hexalactone	+	+		>5,000 (rat)	
104-67-6	2(3*H*)-Furanone, dihydro-5-heptyl-	γ-Undecalactone	−	+	6 Negative 2 Positive	18,500 (rat)	>14 (rat)
706-14-9	2(3*H*)-Furanone, dihydro-5-hexyl-	γ-Decalactone}	+	+		>5,000 (rat)	
108-29-2	2(3*H*)-Furanone, dihydro-5-methyl-	γ-Valerolactone}	+	+		>5,000 (rat)	>50 (rat)
2305-05-7	2(*3H*)-Furanone, dihydro-5-octyl-	γ-Dodecalactone}	−	+		>5,000 (rat)	
104-61-0	2(3*H*)-Furanone, dihydro-5-pentyl-	γ-Nonalactone}	+	+	3 Negative 3 Positive	9,780 (rat) 3,440 (guinea pig)	>72 (rat)
105-21-5	2(3*H*)-Furanone, dihydro-5-propyl-	γ-Heptalactone	+	+	Negative	>5,000 (rat)	
28664-35-9	2(5*H*)-Furanone, 3-hydroxy-4,5-dimethyl-		−	+			
698-10-2	2(5*H*)-Furanone, 5-ethyl-3-hydroxy-4-methyl-		−	+			>1.3 (rat)
591-12-8	2(3*H*)-Furanone, 5-methyl-	α-Angelica lactone	+	+		2,800 (mouse)	>17 (rat)
7779-50-2	Oxacycloheptadec-7-en-2-one		−	+			
106-02-5	Oxacyclohexadecan-2-one	ω-Pentadecalactone	+	+	2 Negative		
27593-23-3	2*H*-Pyran-2-one, 6-pentyl-	6-Amyl-α-pyrone	−	+			
3301-94-8	2*H*-Pyran-2-one, tetrahydro-6-butyl-	δ-Nonalactone}	−	+			
713-95-1	2*H*-Pyran-2-one, tetrahydro-6-heptyl-	δ-Dodecalactone	−	+			
710-04-3	2*H*-Pyran-2-one, tetrahydro-6-hexyl-	δ-Undecalactone}	−	+			
823-22-3	2*H*-Pyran-2-one, tetrahydro-6-methyl-	δ-Hexalactone	+	−			
705-86-2	2*H*-Pyran-2-one, tetrahydro-6-pentyl-	δ-Decalactone}	−	+		>5,000 (rat)	
698-76-0	2*H*-Pyran-2-one, tetrahydro-6-propyl-	δ-Octalactone}	+	+		>5,000	

[a] References to the various genotoxicity systems used may be found in Abbott [see Table 6 in (6A01)].

[b] NOEL, no observed effect level.

[c] References to procedures used may be found in Abbott [see Table 3 in (6A01)].

TABLE 6.2
Tobacco and/or Smoke Lactones Used in Flavor Formulations

CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Identified in	
			Smoke	Tobacco
50-81-7	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-}	Ascorbic acid	+	+
96-48-0	2(3*H*)-Furanone, dihydro-	4-Hydroxybutanoic acid lactone	+	+
104-50-7	2(3*H*)-Furanone, dihydro-5-butyl-	γ-Octalactone	–	+
695-06-7	2(3*H*)-Furanone, dihydro-5-ethyl-	γ-Hexalactone	–	+
104-67-6	2(3*H*)-Furanone, dihydro-5-heptyl-	γ-Undecalactone	–	H
706-14-9	2(3*H*)-Furanone, dihydro-5-hexyl-	γ-Decalactone	–	+
108-29-2	2(3*H*)-Furanone, dihydro-5-methyl-	γ-Valerolactone	+	+
2305-05-7	2(*3H*)-Furanone, dihydro-5-octyl-	γ-Dodecalactone	–	H
104-61-0	2(3*H*)-Furanone, dihydro-5-pentyl-	γ-Nonalactone	–	+
105-21-5	2(3*H*)-Furanone, dihydro-5-propyl-	γ-Heptalactone	–	+
591-12-8	2(3*H*)-Furanone, 5-methyl-	4-Hydroxy-3-pentenoic acid lactone	+	+
27538-09-6	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl-[a]	3-Ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone[a]	–	–
551-08-6	1(3*H*)-Isobenzofuranone, 3-butylidene-	3-Butylidenephthalide	–	H
564-20-5	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-	Sclareolide	+	+
7779-50-2	Oxacycloheptadec-7-en-2-one	ω-6-Hexadecenlactone	–	H
106-02-5	Oxacyclohexadecan-2-one	ω-Pentadecalactone	–	+
3301-94-8	2*H*-Pyran-2-one, tetrahydro-6-butyl-[a]	δ-Nonalactone[a]	–	H
713-95-1	2*H*-Pyran-2-one, tetrahydro-6-heptyl-	δ-Dodecalactone	–	H
710-04-3	2*H*-Pyran-2-one, tetrahydro-6-hexyl-	δ-Undecalactone	–	H
2721-22-4	2*H*-Pyran-2-one, tetrahydro-6-nonyl-[a]	Tetradecalactone[a]	–	H
705-86-2	2*H*-Pyran-2-one, tetrahydro-6-pentyl-	δ-Decalactone	–	+
698-76-0	2*H*-Pyran-2-one, tetrahydro-6-propyl-	δ-Octalactone	–	+

H, homolog of an identified tobacco and/or smoke component.

[a] This lactone is not included in the Doull et al. list (1053) but is included in flavor formulations used by cigarette manufacturers outside of the United States [see Table 7A in (3266)].

TABLE 6.3
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

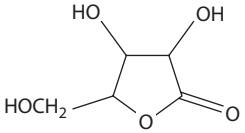
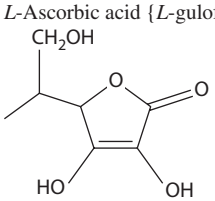
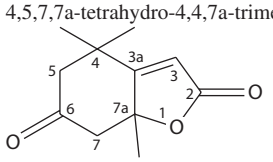
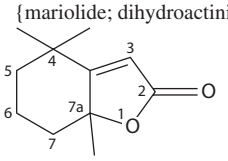
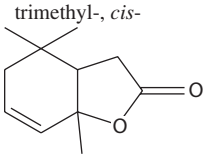
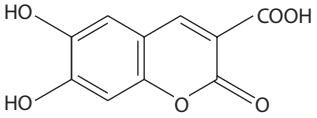
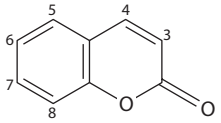
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	20261-96-5	Arabinohexonic acid, 3-deoxy-, γ-lactone	4249	4249	
2.	42400-32-8	*D*-Arabinohexonic acid, 2-deoxy-, γ-lactone		4249	
3.	13280-76-7	Arabinonic acid, γ-lactone 	4249		
4.	50-81-7	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-} 	3257, 3266, 3685, 4249, 4751a	120, 174b, 379, 486, 557, 1053, 1971, 2079, 2270, 2489, 2532, 2939, 3266, 3707, 3922, 4236, 4249, 5079, 5267a, 5811b	
5.	31297-30-0	2,3-Benzofurandione, 2,3-dihydro-4,7-dimethyl-	2601a		
6.	19355-58-9	2,6-Benzofurandione, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl- 		234, 1156, 1254, 1256, 3991, 4090, 4249, 5811b	
7.	13341-72-5	Benzofuranone, dimethyltetrahydro-		1053, 3266, 3370	
8.		Benzofuranone, methyl-	3557, 4249		
9.	553-86-6	2(3*H*)-Benzofuranone	1375a, 1377, 2570, 4249		1375a, 1377
10.	6051-03-2 24871-12-3	2(3*H*)-Benzofuranone, hexahydro-	568b, 4249		
11.	61892-48-6	2(3*H*)-Benzofuranone, hexahydro-3a-hydroxy-	3553, 4249		
12.	54911-63-6	2(3*H*)-Benzofuranone, hexahydro-4-hydroxy-	568b, 4249		
13.	16778-27-1	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl- {mariolide; dihydroactinidiolide} 	1352, 1371, 1375, 1375a, 1375b, 1377, 1586, 2570, 2767, 3557, 4570a	543a, 1063–1066, 1068–1074, 1149, 1149a, 1156, 1352, 1590a, 2034, 2338, 2339a, 2339b, 2386, 2389, 2544, 2917a, 3188, 3198, 3210, 3218, 3219, 3329, 3354, 3539, 3543, 3545, 3547, 3549, 3552, 3558, 3905, 4090, 4159	1375a, 1377
14.	37531-06-9	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-, *cis*-		4249, 4573	
15.	37531-07-0	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-, (*E*)-		4249, 4573	
16.	19432-10-1	2(3*H*)-Benzofuranone, octahydro-4,4,7a-trimethyl- {tetrahydroactinidiolide}		1149, 1149a, 3543, 3546, 5811	
17.	19432-09-8	2(3*H*)-Benzofuranone, 3a,4,5,7a-tetrahydro-4,4,7a-trimethyl-, *cis*- 	2769, 4570a	3218, 3219, 4249	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
18.	75840-26-5	2(4*H*)-Benzofuranone, 5,6-dihydro-3,6-dimethyl-		1053, 3266	
19.	17063-17-1	2(4*H*)-Benzofuranone, 5,7a-dihydro-4,4,7a-trimethyl-, (R)-		3854, 4249, 5811b	
20.	82395-89-9	2(4*H*)-Benzofuranone, 6-(β-*D*-glucopyranosyloxy)-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-		234, 4249, 4714	
21.	10481-90-0	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, *Z*-(±)- {loliolide}	1587, 4249	2389, 2544, 2780, 3218, 4249, 2780	
22.	1133-03-5	2(4*H*)-Benzofuranone,6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-		5811b	
23.	5989-02-6	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-		568b, 4249, 4573, 5811b	
24.	19432-05-4 38725-47-2	2(4*H*)-Benzofuranone, tetrahydro-4,4,7a-trimethyl-		4249	
25.	15356-74-8	2(4*H*)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	568b, 1375, 2545, 2761, 2762, 2765, 2766, 2773, 2775, 3557, 4249	404, 568b, 1256, 2389, 2544, 2917a, 3217, 3219, 3561, 4249, 5811b	
26.	17092-92-1	2(4*H*)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	4249, 4570a	4249, 5811b	
27.		2*H*-1-Benzopyran-3-carboxylic acid, 6,7-dihydroxy-2-oxo- 		4249, 4556	
28.	19484-74-3	2*H*-1-Benzopyran-3-carboxylic acid, 7,8-dihydroxy-2-oxo-		4249, 4752	
29.	91-64-5	2*H*-1-Benzopyran-2-one {coumarin} 	239, 568b, 966, 1364, 1371, 1373, 1427, 1599, 1649, 1842, 2209, 2413, 2543, 2757, 2759, 2767, 2773, 2939, 3193, 3255, 3257, 3263, 3265, 3300, 3302, 3308, 3410, 3474, 3557, 3685, 3753, 3876, 3995, 4025, 4050, 4249, 4354, 5811b	568b, 633, 729, 774, 1156, 1256, 1578, 1649, 1785, 2280, 2543, 2545, 2611, 2699, 2757, 2759, 2761, 2762, 2765, 2766, 3263, 3328, 3329, 3536, 3560, 3643, 3676, 4050, 4090, 4249, 5591, 5711, 5811b	
30.	26093-31-2	2*H*-Benzopyran-2-one, 7-amino-4-methyl-		2917a	
31.	74712-71-3	2*H*-1-Benzopyran-2-one, 7-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-6-methoxy-		4249	
32.	119-84-6	2*H*-1-Benzopyran-2-one, 3,4-dihydro- {dihydrocoumarin}	568b, 1360, 1375a, 2543, 2767, 2773, 2777, 3553, 4050, 4249, 5811b	568b, 2699, 4050, 4249	1360, 1375a
33.	305-01-1	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}	969, 1572, 1626, 1884, 2939, 3059, 3257, 3265, 3302, 3797, 4249, 5811b	969, 970, 1626, 2939, 2954, 3103, 3059, 3194, 3797, 3973, 3974a, 4249, 5711, 5811b, 5888	

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

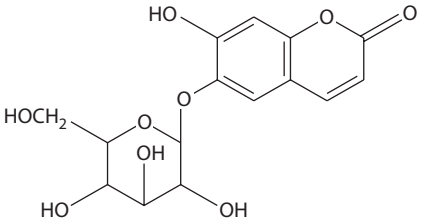
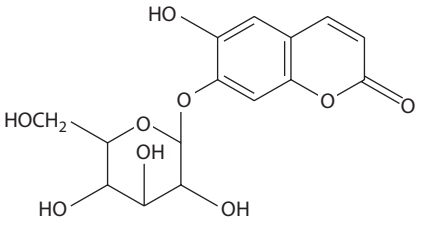
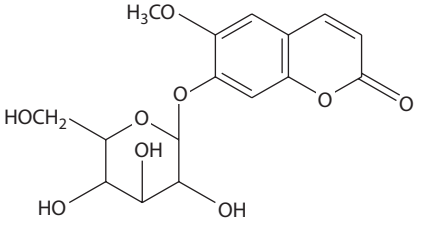
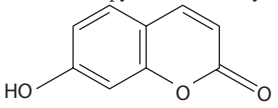
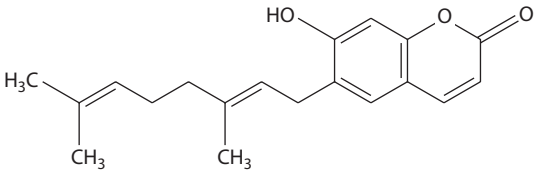
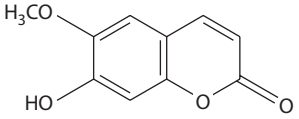
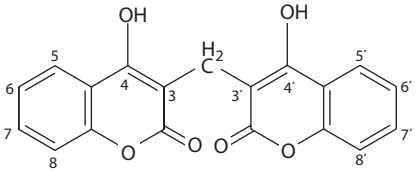
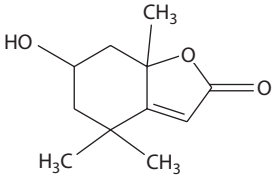
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
34.	60091-00-1	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-		3797, 4249	
35.	531-75-9	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin} 	3257	1309, 2939, 2954, 3103, 3973, 3974a, 4249, 5711, 5811b	
36.	531-58-8	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin} 		1309, 1626, 3797, 4249, 5811b, 5838	
37.	531-44-2	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-methoxy- {scopolin} 		72, 120, 677a, 830a, 831, 834, 835, 840, 890, 966, 1102, 1309, 1626, 1863, 2338, 2395, 2557a, 2911c, 2954, 3194, 3629, 3631, 3646, 3738, 3797, 3973, 3974a, 3974b, 4156, 4249, 4269, 5649, 5650, 5809, 5811b, 5831	
38.	93-35-6	2*H*-1-Benzopyran-2-one, 7-hydroxy- 		3161, 3738, 4249, 4606	
39.	148-83-4	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-(3,7-dimethyl-2,6-octadienyl)- {ostruthin} 		120	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
40.	92-61-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin} 	419, 568b, 1284, 1373, 1626, 1842, 1884, 1898, 2377, 2524a, 2767, 2939, 3059, 3096, 3168, 3302, 3308, 3553, 3602, 3797, 3891, 3995, 4005–4007, 4119, 4121, 4123, 4124, 4164, 4249, 4319, 4373–4375, 5512, 5811b	72, 120, 254, 404, 568b, 677a, 830a, 831, 834, 835, 840, 890, 966, 1063–1066, 1068–1074, 1112, 1626, 1863, 2014, 2270, 2313a, 2338, 2361, 2389, 2531, 2544, 2557a, 2810–2812, 2914, 2939, 2954, 3059, 3103, 3109, 3161, 3194, 3219, 3329, 3631, 3641, 3646, 3705, 3738, 3794, 3797, 3973, 3974a, 3974b, 3984, 4249, 4269, 4373–4375, 5079, 5081, 5127, 5235, 5591, 5616, 5650, 5652, 5704, 5705, 5745, 5766, 5788, 5808, 5811b, 5830, 5831, 5842, 5876, 5888, 5889	
41.	90-33-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-4-methyl-		2917a	
42.	531-59-9	2*H*-1-Benzopyran-2-one, 7-methoxy-		2385a, 4249	
43.		2*H*-1-Benzopyran-2-one, 8-methoxy-		4249, 4897	
44.	71050-53-8	2*H*-1-Benzopyran-2-one, 6-methoxy-7-(β-*D*-xylofuranosyloxy)- {scopoletin glucoside}		2939, 3797, 4249, 5650, 5808, 5809, 5830, 5842, 5888	
45.	18309-73-4	2*H*-1-Benzopyran-2-one, 6-methoxy-7-[(6-*O*-β-*D*-xylopyranosyl-β-*D*-glucopyranosyl)oxy]-		1863a, 2939, 4249, 5811b	
46.	2445-82-1	2*H*-1-Benzopyran-2-one, 3-methyl-	2775, 4249		
47.	92-48-8	2*H*-1-Benzopyran-2-one, 6-methyl- {6-methylcoumarin}	568b, 3553, 3650, 4249, 5811b		
48.	66-76-2	2*H*-1-Benzopyran-2-one, 3,3′-methylenebis[4-hydroxy- {dicumarol} 	2757, 3263, 4249 [**not found in smoke from coumarin-treated tobacco**]		
49.	4430-31-3	2*H*-1-Benzopyran-2-one, octahydro-		4249	
50.	61927-07-9	Bicyclo[4,3,0]non-6-en-8-one, 3-hydroxy-9-oxo-1,5,5-trimethyl- 	5811, 5811a, 5811b		

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

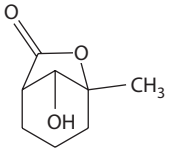
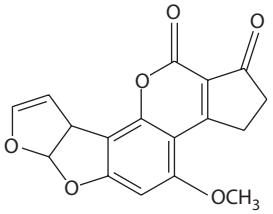
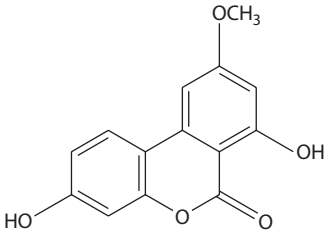
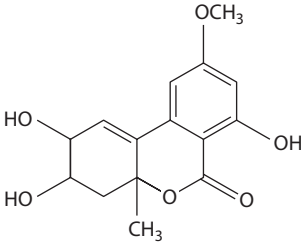
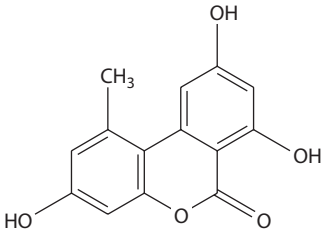
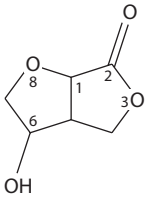
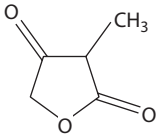
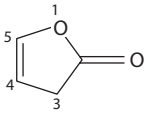
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
51.	110053-64-0	1,3-Cyclohexanecarbolactone, 2-hydroxy-3-methyl- 	5811, 5811a, 5811b		
52.	1162-65-8	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_1} 	158a, 2024, 2484, 3721, 3970, 3986 [**added aflatoxin B_1 not transferred intact to smoke**]	158a, 2024, 2484, 3721, 3970, 3975 [**not found in tobacco**]	
53.	7220-81-7	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,8,9,9a-hexahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_2}		4039b, 4254, 4754	
54.	158815-70-4	4,9-Decadienoicacid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-		736, 4249, 5811b	
55.	160115-53-7	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-, methyl ester		4249	
56.	26894-49-5	6*H*-Dibenzo[*b,d*]pyran-6-one, 3,7(3,9 or 7,9)-dihydroxy-9(7 or 3)-methoxy-1-methyl- 		4249, 4756	
57.	29752-43-0	6*H*-Dibenzo[*b,d*]pyran-6-one, 9-methoxy-4a-methyl-2,3,4,4a-tetrahydro-2,3,7-trihydroxy-(2α,3β,4aβ)- 		4249, 4758	
58.	641-38-3	6*H*-Dibenzo[*b,d*]pyran-6-one, 1-methyl-3,7,9-trihydroxy- 		4249	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
59.	110053-63-9	3,8-Dioxabicyclo[3.3.0]octan-2-one, 6-hydroxy- 	5811, 5811a, 5811b		
60.	3885-29-8	2-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester	568b, 3553, 4249		
61.	5204-91-1	3-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester	568b, 3553, 4249		
62.	1192-51-4	2,4(3*H*,5*H*)-Furandione, 3-methyl- 	5811, 5811a, 5811b		
63.	20825-71-2	2(3*H*)-Furanone {butenolide} 	568b, 1350, 1354, 1371, 1375, 1375a, 1375b, 1377, 1586, 3397, 3410, 3553, 3557	568b, 1063–1066, 1068–1074, 1590a, 2386, 2389, 2544, 3547, 3549, 5811b	1354, 1375a, 1377, 3402, 3404
64.		2(3*H*)-Furanone, acetyl-	2767, 3557		
65.	517-23-7	2(3*H*)-Furanone, 3-acetyldihydro-	568b, 1360, 1375, 1375a, 1375b, 2767, 3553, 3557, 4249, 5811b		1360, 1375a
66.	7400-67-1	2(3*H*)-Furanone, 4-acetyldihydro-	568b, 1375, 1375b, 2767, 3553, 3557, 4249		
67.	29393-32-6	2(3*H*)-Furanone, 5-acetyldihydro-	568b, 1354, 1360, 1375, 1375a, 1375b, 2387, 2761, 2762, 2765–2767, 2777, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 4249	1354, 1375a, 1360, 1375a, 2387, 3404, 3405
68.	19405-99-3	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-	568b, 1375, 1375b, 1586, 3553, 3557, 4249, 5811b		
69.	19405-98-2	2(3*H*)-Furanone, 4-(acetyloxy)dihydro-	568b, 2767, 3353, 4249		
70.		2(3*H*)-Furanone, 4-(acetyloxy)dihydro-5-hydroxy-	568b, 4249		
71.	26817-24-3	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-	1586, 2767, 3553, 5811b		3402
72.	61892-43-1	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-4-hydroxy-	568b, 1351, 1352, 1375, 1375b, 1586, 3553, 3557, 5811b		
73.	61892-44-2	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-4-hydroxy-	1351, 1352, 3553, 5811b		
74.	160115-54-8	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1E,3S*)]]-		4249	

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

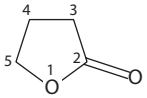
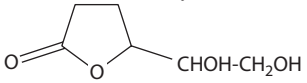
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
75.	160224-93-1	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5α(1E,3S*)]]-		4249	
76.	1192-20-7	2(3*H*)-Furanone, 3-aminodihydro-	2767, 3557, 4249		
77.		2(3*H*)-Furanone, 3-(3-butenyl)-dihydro-		2917a	
78.	104-50-7	2(3*H*)-Furanone, 5-butyldihydro-{γ-octalactone}		172a, 174b, 404, 568b, 1053, 1980, 2339a, 2389, 2544, 3219, 3266, 3370, 3543, 3553, 3555, 3560, 3561, 4098a, 4249	
79.	39212-23-2	2(3*H*)-Furanone, 5-butyldihydro-4-methyl-		2339a	
80.		2(3*H*)-Furanone, 5-butylidene	1378		1378, 4249
81.	96-48-0	2(3*H*)-Furanone, dihydro-{butyrolactone} 	126a, 126b, 237, 568b, 642, 1063–1066, 1068–1074, 1099, 1371, 1375, 1375a, 1375b, 1377, 1445, 1586, 1674, 1881, 1958, 1960, 2387, 2418, 2493, 2506, 2507, 2570, 2731, 2735, 2767, 2775, 2777, 2799a, 3255, 3266, 3300, 3302, 3397, 3553, 3555, 3557, 3559, 4032, 4249, 5811b	404, 568b, 1053, 1590a, 2339a, 2386, 2389, 2544, 2917a, 3188, 3266, 3549, 3550, 3555, 4098a, 4249, 5811b	1375a, 1377, 2387, 2506(0), 2507(0), 3401, 3402, 3404, 3405
82.	13092-55-2	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-	1351, 1352, 1882, 1883, 2777, 3553, 4249		
83.	25596-90-1	2(3*H*)-Furanone, dihydro-3,4-dihydroxy- (3R,4S)	5811, 5811a, 5811b		
84.	17675-99-9	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-, (*Z*)-	2777, 5811b		
85.		2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-	568b, 2321, 4249		
86.	61892-57-7	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-4-methyl-	1351, 1352, 3553, 3557, 4249, 5811b		
87.	63700-30-1	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-	568b, 4249, 5811b		
88.	18465-71-9	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-, (3R-*Z*)-	1351, 1352, 1360, 1375a, 1586, 2767, 3553, 3557		1360, 1375a
89.		2(3*H*)-Furanone, dihydro-3,4-dihydroxy-4-methyl-	1375, 1375b, 1586, 2761, 2762, 2765–2767, 2777, 3553, 3557, 4249		
90.		2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-methyl-	568b, 4249		
91.	61989-58-0	2(3*H*)-Furanone, dihydro-5-(1,2-dihydroxyethyl)- 	5811, 5811a, 5811b		
92.	72902-81-9	2(3*H*)-Furanone, dihydro-3,3-dimethyl-4-hydroxy-	568b, 4249		
93.	38273-97-1	2(3*H*)-Furanone, dihydro-3,3-dimethyl-5-(2-oxopropyl)-		568b, 2389, 2544, 3218, 3543, 3546, 4249, 5811b	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
94.	72693-07-3	2(3*H*)-Furanone, dihydro-3,4-dimethyl-	1586, 2777, 4249	2339a	
95.	5145-01-7	2(3*H*)-Furanone, dihydro-3,5-dimethyl-	1586, 4249	120, 1980, 2270, 2283, 3219, 4249, 5811b	
96.	13861-97-7	2(3*H*)-Furanone, dihydro-4,4-dimethyl-		404, 1157, 4249	
97.		2(3*H*)-Furanone, dihydro-4,4-dimethyl-5-hydroxymethyl-	568b, 4249		
98.	6971-63-7	2(3*H*)-Furanone, dihydro-4,5-dimethyl-	568b, 3553, 4249, 5811b	120, 404, 568b, 1980, 2270, 2283, 2386, 2389, 2544, 3219, 3543, 3560, 3561, 3905, 4249	
99.	90026-55-4	2(3*H*)-Furanone, dihydro-4,5-dimethyl-, (4*R*-Z)-	5811	5811	
100.	110171-22-7	2(3*H*)-Furanone, dihydro-4,5-dimethyl-, (4R-*E*)-	5811		
101.	3123-97-5	2(3*H*)-Furanone, dihydro-5,5-dimethyl-		568b, 1980, 2339a, 3547, 4249	
102.		2(3*H*)-Furanone, dihydro-5-(1,4-dimethyl-1-pentenyl)-		3547, 4249	
103.	1073-11-6	2(3*H*)-Furanone, dihydro-5-ethenyl-5-methyl-	5811b	568b, 2339a, 2389, 2544, 3219, 3543, 3547, 3560, 3561, 4249, 5811b	
104.	16496-51-8	2(3*H*)-Furanone, dihydro-4-ethyl-	5811b	568b, 3547, 3560, 3561, 4249	
105.	695-06-7	2(3*H*)-Furanone, dihydro-5-ethyl- {γ-hexalactone}	4407	172a, 174b, 404, 568b, 1053, 1256, 1980, 2339a, 2389, 2544, 3219, 3266, 3370, 4249, 5811b	
106.	2610-98-2	2(3*H*)-Furanone, dihydro-5-ethyl-3-methyl-	2005, 4249		
107.	2865-82-9	2(3*H*)-Furanone, dihydro-5-ethyl-5-methyl-		2386, 2389, 2544, 3206, 3219, 3547, 4249, 5811b	
108.	158815-74-8	2(3*H*)-Furanone, dihydro-5-(3-ethyl-4-methyl-1-pentenyl)-3-hydroxy-5-methyl-		4249, 5811b	
109.	61892-46-4	2(3*H*)-Furanone, dihydro-4-ethynyl-5-hydroxy-3-methyl-	1351, 1352, 3553, 4249, 5811b		
110.		2(3*H*)-Furanone, dihydro-5-(5-heptenyl)-		2544, 4249	
111.	104-67-6	2(3*H*)-Furanone, dihydro-5-heptyl- {γ-undecalactone}		172a, 174b, 568b, 1053, 2339a, 3266, 3370	
112.	706-14-9	2(3*H*)-Furanone, dihydro-5-hexyl- {γ-decalactone}	5811b	172a, 174b, 1053, 1248, 2611, 3266, 3370, 3545, 3560, 3561, 4249	
113.		2(3*H*)-Furanone, dihydro(hydroxy)-	2570		
114.		2(3*H*)-Furanone, dihydro(hydroxymethyl)-	1360, 1375a, 1586, 2570, 2767, 4249		1360, 1375a
115.	18132-98-4	2(3*H*)-Furanone, dihydro-3-(hydroxymethyl)-	568b, 1350, 1375, 1375b, 2543, 3553, 3557, 4249, 5811b		3402, 3404
116.	1608-63-5	2(3*H*)-Furanone, dihydro-3-(1-methylethyl)-		568b, 2389, 2544, 3219, 3543, 3547, 3561, 3905, 4249, 5811b	
117.	60016-73-1	2(3*H*)-Furanone, dihydro-(2-oxopropyl)-		2544, 4249, 5811b	3402, 3405, 4249

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

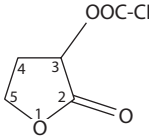
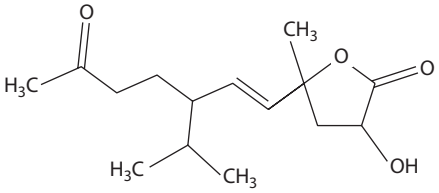
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
118.	25600-22-0	2(3*H*)-Furanone, dihydro-3-(1-oxopropoxy)- 	568b, 3553, 4249, 5811b		
119.	23938-71-8	2(3*H*)-Furanone, dihydro-3-(1-oxopropyl)-	5811, 5811a, 5811b		
120.	71385-84-7	2(3*H*)-Furanone, dihydro-3-(2-oxopropyl)-	568b, 3553, 3557, 4249	568b, 2389, 2544, 4249	3405, 4249
121.	65331-00-2	2(3*H*)-Furanone, dihydro-4-(2-oxopropyl)-	1586, 2767, 3557, 4249		
122.	61892-49-7	2(3*H*)-Furanone, dihydro-5-(1-oxopropyl)-	568b, 1586, 2767, 3553, 3557, 4249, 5811b		
123.	85564-78-9	2(3*H*)-Furanone, dihydro-3,4,5-trimethyl-	568b, 4249		
124.	53155-68-3	2(3*H*)-Furanone, dihydro-3,4,5-trimethyl-, (3α,4α,5α)-		2386, 3457, 4249	
125.	19444-84-9	2(3*H*)-Furanone, dihydro-3-hydroxy-	568b, 1350–1352, 1354, 1360, 1371, 1375, 1375a, 1375b, 2493, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3553, 3557, 4249, 5811b		1354, 1360, 1375a, 3401, 3402, 3404, 3405
126.	19444-86-1	2(3*H*)-Furanone, dihydro-3-hydroxy-3-(hydroxymethyl)-	1351, 1352, 3553, 5811b		
127.	1192-42-3	2(3*H*)-Furanone, dihydro-3-hydroxy-3-methyl-	4249		
128.		2(3*H*)-Furanone, dihydro-3-hydroxy-3,4,4-trimethyl-	568b, 4249		
129.	6969-43-3	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4,5-trimethyl-		2544, 4249	
130.	52126-90-6	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-	568b, 1235, 1351, 1352, 1375, 1375b, 2387, 2570, 2761, 2762, 3302, 3410, 3553, 3557, 4249, 5811b	404, 568b, 1256, 2386, 2389, 2544, 2917a, 3188, 4249	2387
131.	599-04-2	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (R)-	1360, 1375a, 1586, 2543, 2767, 2775, 2777, 3553, 3557	404, 1256, 2389, 2544, 3549, 3550	1360, 1375a
132.		2(3*H*)-Furanone, dihydro-3-hydroxy-5-(1-hydroxyethyl)-	568b, 1351, 1352, 2570, 2765–2767, 2777, 3553, 4249		
133.		2(3*H*)-Furanone, dihydro-3-hydroxy-5-(1-hydroxyethyl)- {isomer}	568b, 4249		
134.	61892-52-2	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-	568b, 1351, 1352, 2570, 2761, 2762, 2767, 3553, 4249, 5811b		
135.	61892-50-0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-5-methyl-	568b, 1351, 1352, 1375, 1375b, 1586, 2767, 3553, 3557, 4249, 5811b		

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
136.	53561-62-9	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-	568b, 1351, 1352, 3553, 4249, 5811b		
137.		2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl- {isomer}	568b, 4249		
138.	158815-71-5	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1E,3S*)]]- 		4249	
139.	5469-16-9	2(3*H*)-Furanone, dihydro-4-hydroxy-	568b, 1351, 1352, 1371, 1586, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3553, 3557, 4249, 5811b	568b, 3550, 4249	3402, 3405
140.	3285-47-0	2(3*H*)-Furanone, dihydro-4-hydroxy-3,3-dimethyl-	2775		
141.	61892-45-3	2(3*H*)-Furanone, dihydro-4-hydroxy-3-(hydroxymethyl)-	568b, 1351, 1352, 3553, 4249, 5811b		
142.	36679-81-9	2(3*H*)-Furanone, dihydro-4-(hydroxymethyl)-	1352, 1360, 1371, 1375, 1375a, 1375b, 1586, 2387, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3553, 3557, 4249, 5811b	2389, 2544	1360, 1375a, 2387
143.	34945-05-6	2(3*H*)-Furanone, dihydro-4-hydroxy-4-methyl-	568b, 1351, 1352, 3553, 4249, 5811b		
144.		2(3*H*)-Furanone, dihydro-4-(2,5,6-trimethyl-5,6-epoxyoctanyl)-		3545	
145.	50768-69-9	2(3*H*)-Furanone, dihydro-5-hydroxy-	1586, 2761, 2762, 2765–2767, 2773, 2775, 4249		
146.	27610-27-1	2(3*H*)-Furanone, dihydro-5-(1-hydroxyethyl)-	1351, 1352, 1586, 3553, 5811b	2389, 2544, 3219	
147.	61892-47-5	2(3*H*)-Furanone, dihydro-5-hydroxy-4-methyl-	1351, 1352, 3553, 4249, 5811b		
148.	10374-51-3	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-	568b, 1351, 1352, 2387, 2543, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3410, 3553, 3557, 4249, 5811b	568b, 3550, 4249	2387, 3405
149.	61892-55-5	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-4-methyl-	1351, 1352, 3553, 4249, 5811b		
150.	1679-47-6	2(3*H*)-Furanone, dihydro-3-methyl-		404, 568b, 2339a, 2386, 2389, 2544, 2917a, 4249, 5811b	

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

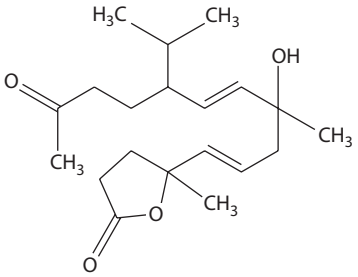
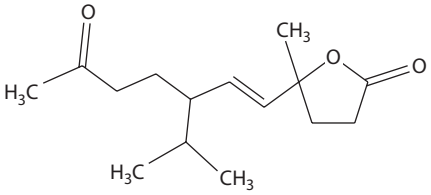
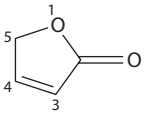
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
151.	1679-49-8	2(3*H*)-Furanone, dihydro-4-methyl-	568b, 1378, 3255, 4249, 5811b	404, 568b, 3543, 3546, 3547, 3560, 3561, 4048, 4249, 5811b	1378, 4249
152.	108-29-2	2(3*H*)-Furanone, dihydro-5-methyl- {γ-valerolactone}	1360, 1371, 1375a, 1883, 2731, 2735, 2775, 3266, 4249	172a, 174b, 404, 1053, 2389, 2544, 2917a, 3219, 3266, 3370, 4249, 5811b	1360, 1375a
153.		2(3*H*)-Furanone, dihydro-5-methyl-5-(3-methyl-1-butenyl)-		568b, 3545, 4249	
154.		2(3*H*)-Furanone, dihydro-5-methyl-5-(3-oxobutyl)-		3543	
155.	80797-69-9	2(3*H*)-Furanone, dihydro-5-(3-methyl-1-butenyl)-		3547, 4249	
156.	2429-94-9	2(3*H*)-Furanone, dihydro-5-(3-methylbutyl)-		1980, 3543, 4249	
157.	10547-88-3	2(3*H*)-Furanone, dihydro-4-(1-methylethyl)-	5811b	404, 568b, 3219, 3543, 3547, 3560, 3561, 4249, 5811b	
158.	38624-29-2	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-		404, 2943a, 3547, 4249	
159.		2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-methyl-1,2-butadienyl)-		3547, 4249	
160.	133561-47-4	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-		5811, 5811b	
161.	129742-48-9	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-, (*E*)-(+)-		4249, 5811b	
162.	2305-05-7	2(*3H*)-Furanone, dihydro-5-octyl- {γ-dodecalactone}		172a, 174b, 1053, 3266, 3370	
163.	76710-90-2	2(3*H*)-Furanone, dihydro-5-(2-pentenyl)-, (*Z*)-		404, 2934b, 3547	
164.	104-61-0	2(3*H*)-Furanone, dihydro-5-pentyl- {γ-nonalactone}	5811b	172a, 174b, 404, 568b, 1053, 2337a, 2339a, 2389, 2544, 3215, 3266, 3370, 3543, 3547, 3555, 3560, 3561, 4098a, 4249, 5811b	
165.	105-21-5	2(3*H*)-Furanone, dihydro-5-propyl- {γ-heptalactone}	568b, 2601a, 4249	120, 172a, 174b, 568b, 1053, 2283, 2270, 3266, 4249	
166.	20971-79-3	2(3*H*)-Furanone, dihydro-5-(3-pyridinyl)-	568b, 3553, 4249, 5811b		
167.	72507-34-7	2(3*H*)-Furanone, dihydro-5-[1-methyl-4-(1-methylethyl)-7-oxo-2-octenyl]-		4249	
168.	102734-52-1	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5S-[5R*(1E,4R*,5E,7R*)]]- 		453, 4089, 4249, 5811b	
169.	102734-53-2	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5S-[5R*(1E,4S*,5E,7R*)]]-		4089, 5811b	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
170.	102734-54-3	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5R-[5R*(1E,4S*,5E,7S*)]]-		4089, 5811b	
171.	102734-55-4	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5R-[5R*(1E,4R*,5E,7S*)]]-		4089, 5811b	
172.	80744-25-8	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-		4249, 4947	
173.		2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl- {stereoisomer}		4249, 4947	
174.		2(3*H*)-Furanone, dihydro-5-methyl-5-(5-methyl-2-furanyl)-		2934b	
175.	60646-31-3	2(3*H*)-Furanone, dihydro-5-methyl-5-(1-methylethyl)-, (S)-	4249, 4749		
176.	57213-51-1	2(3*H*)-Furanone, dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]- 		8, 9, 909, 943, 1151, 1156, 4090, 4249	
177.	3284-93-3	2(3*H*)-Furanone, dihydro-5-methyl-5-propyl-		568b, 3547, 4249	
178.	10008-73-8	2(3*H*)-Furanone, dihydro-5-methylene-	2761, 2762, 2777, 4249		
179.	2981-96-6	2(3*H*)-Furanone, dihydro-4,5,5-trimethyl-	568b, 4249		
180.		2(3*H*)-Furanone, dihydro-5-(1,1,3-trimethyl-2-butenyl)-		3547, 4249	
181.	64291-81-2	2(3*H*)-Furanone, dihydrodimethyl-		1157, 4249, 4359a	
182.		2(3*H*)-Furanone, 3,3-dimethyl-		3543	
183.		2(3*H*)-Furanone, 3,4-dimethyl-	1375, 1375b, 2387	3206	2387
184.	61892-58-8	2(3*H*)-Furanone, 3-(hydroxymethyl)-5-methyl-	568b, 1352, 1371, 2543, 2570, 2773, 2775, 3553, 4249, 5811b		
185.	591-12-8	2(3*H*)-Furanone, 5-methyl- {4-hydroxy-3-pentenoic acid lactone; α-angelica lactone}	568b, 2570, 2769, 2775, 3255, 3257, 3265, 3266, 3553, 3557, 4032, 4407, 5811b	172a, 174b, 568b, 1053, 1980, 2336, 2337a, 2389, 2544, 3266, 4249, 5811b	3401
186.	497-23-4	2(5*H*)-Furanone {crotonolactone} 	568b, 1360, 1375, 1375a, 1375b, 1377, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3553, 3557, 3559, 4249, 4407, 5811b	568b, 2389, 2544, 2917a, 3555, 4249	1360, 1375a, 1377, 3401, 3405
187.		2(5*H*)-Furanone, acetyl-	3557		
188.	80436-91-5	2(5*H*)-Furanone, 3-acetyl-	4249		
189.	38260-27-4	2(5*H*)-Furanone, 4-acetyl-	4249		

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

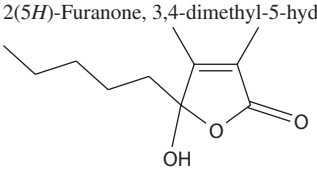
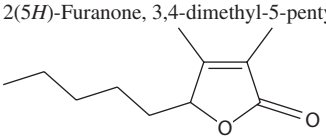
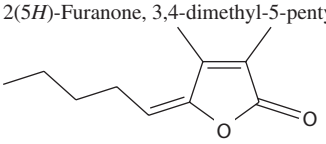
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
190.	61892-53-3	2(5*H*)-Furanone, 5-acetyl-	568b, 2767, 3553, 4249, 5811b		
191.	61892-42-0	2(5*H*)-Furanone, 3-acetyl-4-methyl-	568b, 4249, 5811b		
192.		2(5*H*)-Furanone, 5-butylidene-	1378		1378
193.	14668-67-8	2(5*H*)-Furanone, 3,5-diethyl-	2767, 4249		
194.		2(5*H*)-Furanone, 3,4-dihydroxy-	1883, 4249		
195.	1575-46-8	2(5*H*)-Furanone, 3,4-dimethyl-	568b, 1375, 1378, 3553, 3557, 4249, 5811b	568b, 2544, 4249, 5811b	1378
196.	5584-69-0	2(5*H*)-Furanone, 3,5-dimethyl-	568b, 1371, 2387, 2570, 2767, 2769, 2775, 2777, 3410, 3553, 3557, 4249, 5811b	568b, 3550, 4249	2387
197.	10547-85-0	2(5*H*)-Furanone, 4,5-dimethyl-	568b, 1375, 1375b, 1586, 2387, 2570, 2767, 2775, 3553, 3557, 4249, 5811b	568b, 404, 937, 3543, 4249	1378, 2387
198.	20019-64-1	2(5*H*)-Furanone, 5,5-dimethyl-	937, 4249	404, 937, 2339a, 2389, 2544, 2917a, 4249, 5811b	
199.	150669-55-9	2(5*H*)-Furanone, 5,5-dimethyl-4-ethyl-		2934b	
200.	6067-11-4	2(5*H*)-Furanone, 3,4-dimethyl-5-hydroxy-5-pentyl- 		1248, 1254, 1256, 4249, 5811b	
201.	14300-74-4	2(5*H*)-Furanone, 3,4-dimethyl-5-methylene-	3553, 4249, 5811b		
202.	10547-84-9	2(5*H*)-Furanone, 3,4-dimethyl-5-pentyl- {dihydrobovolide} 	568b, 2767, 4249	404, 568b, 937, 1254, 1256, 2282, 2389, 2544, 2611, 3196, 3198, 3543, 3547, 3550, 4098a, 4249, 5811b	
203.	774-64-1	2(5*H*)-Furanone, 3,4-dimethyl-5-pentylidene- {bovolide} 	1586, 2570, 2767, 2769, 3557, 4249	404, 937, 1254, 1256, 2386, 2389, 2544, 2611, 3188, 3198, 3541, 3543, 3545, 3547, 3550, 3560, 3561, 3905, 4098a, 4249, 5811b	
204.	7935-59-1	2(5*H*)-Furanone, 3,4-dimethyl-5-pentylidene-, dihydro derivative		4249, 5811b	
205.	66309-74-8	2(5*H*)-Furanone, 3,4-dimethyl-5-(1-propenyl)-	1375, 1375b, 1586, 2767, 2769, 3557, 4249		
206.	66309-75-9	2(5*H*)-Furanone, 5-ethenyl-	1586, 2543, 2767, 2769, 3557, 4249		
207.		2(5*H*)-Furanone, 5-ethenyl-3-methyl-	2543, 3557, 4249		
208.		2(5*H*)-Furanone, 4-ethyl-		3543, 3547	
209.	2407-43-4	2(5*H*)-Furanone, 5-ethyl-	568b, 2570, 2769, 4249, 5811b	568b, 2389, 2544, 2917a, 3543, 3546, 4032, 4048, 4249, 5811b	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
210.	698-10-2	2(5*H*)-Furanone, 5-ethyl-3-hydroxy-4-methyl-		172a, 174b, 1053, 3266, 3370	
211.	14668-66-7	2(5*H*)-Furanone, 3-ethyl-5-methyl-	1586, 2769, 3553, 3557, 4249		
212.	54467-53-7	2(5*H*)-Furanone, 4-ethyl-5-methyl-		3547, 4249	
213.	26329-68-0	2(5*H*)-Furanone, 5-ethyl-3-methyl-	568b, 2767, 2775, 3410, 3553, 3557, 4249, 5811b		
214.	52945-87-6	2(5*H*)-Furanone, 5-ethyl-4-methyl-	2543, 2773, 2775, 4249		
215.	6066-62-2	2(5*H*)-Furanone, 5-ethylidene-3,4-dimethyl-	2767, 2769		
216.	71126-48-2	2(5*H*)-Furanone, 5-ethylidene-3-methyl-, (*Z*)-	1371, 2545, 2773, 2775, 3410		
217.	28664-35-9	2(5*H*)-Furanone, 3-hydroxy-4,5-dimethyl-		172a, 174b, 1053, 3255, 4249, 4771, 5811b	
218.		2(5*H*)-Furanone, 3-hydroxy-5-(1-hydroxyethyl)-	3553, 4249		
219.	54621-96-4	2(5*H*)-Furanone, 5-(1-hydroxyethyl)-, [R-(R*,S*)]-	1371, 4249		
220.		2(5*H*)-Furanone, 3-(hydroxymethyl)-	2388, 4249		
221.	80904-75-2	2(5*H*)-Furanone, 4-(hydroxymethyl)-	1351, 3397		
222.	22122-36-7	2(5*H*)-Furanone, 3-methyl-	568b, 1360, 1364, 1371, 1375, 1375a, 1375b, 1378, 1586, 2387, 2570, 2767, 2775, 2777, 3255, 3410, 3553, 3557, 4249, 5034	404, 568b, 937, 1063–1066, 1068–1074, 1590a, 2386, 2389, 2544, 2917a, 3188, 3546, 3550, 3905, 5811b	1360, 1375a, 1378, 2387, 3401, 4249
223.	6124-79-4	2(5*H*)-Furanone, 4-methyl-	568b, 1375, 1375b, 1378, 1586, 2767, 2775, 3255, 3410, 3553, 3557, 5811b	568b, 2389, 2544, 3543, 4249, 5811b	1378, 3401, 3405
224.	591-11-7	2(5*H*)-Furanone, 5-methyl- {β-angelica lactone}	568b, 1371, 1375, 1375a, 1375b, 1377, 1586, 1958, 1960, 2387, 2570, 2767, 2777, 3302, 3553, 3557, 4032, 4249, 4407, 5034, 5811b	404, 568b, 1980, 2336, 2389, 2544, 4249, 5811b	1375a, 1377, 2387, 3401, 3405
225.	108-28-1	2(5*H*)-Furanone, 5-methylene- {protoanemonin}	299, 568b, 1361, 1375, 1375b, 2387, 2545, 2570, 2765, 2766, 2775, 2777, 3255, 3397, 3410, 3553, 3557, 4249, 5034, 5811b	404, 568b, 944, 1063–1066, 1068–1074, 1361, 1590a, 1854, 2386, 2389, 2544, 3547, 4249, 5811b	2387, 3401, 3402
226.	7754-93-0	2(5*H*)-Furanone, 3-(1-methylethyl)-		568b, 2389, 2544, 2611, 3547, 4249, 5811b	
227.	10547-89-4	2(5*H*)-Furanone, 4-(1-methylethyl)-	3553, 3557, 4249, 5811b	937, 3543, 4048, 4249, 5811b	
228.	61892-54-4	2(5*H*)-Furanone, 3-methyl-5-methylene-	568b, 2777, 3553, 4249, 5811b	404, 568b, 3547, 4249	

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

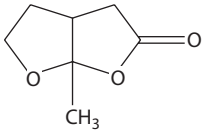
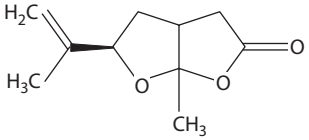
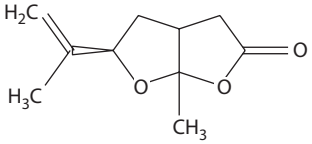
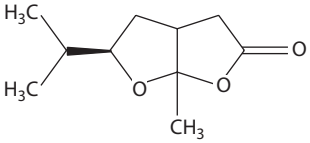
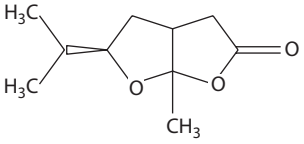
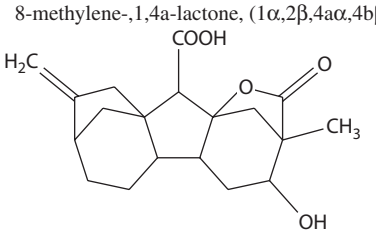
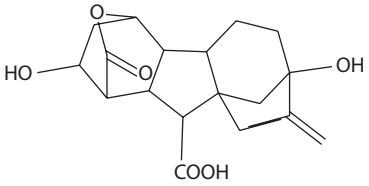
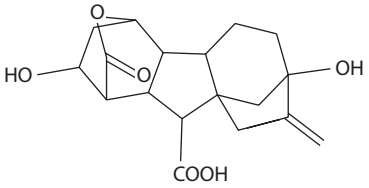
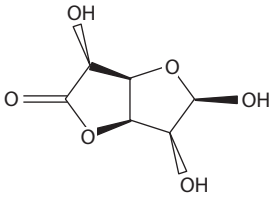
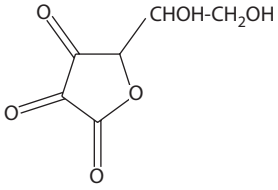
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
229.	150669-54-8	2(5*H*)-Furanone, 5-methyl-5-(1-methylethyl)-		2934b	
230.	150669-57-1	2(5*H*)-Furanone, 4-methyl-5-(3-oxobutyl)		2934b	
231.		2(5*H*)-Furanone, 5-methyl-4-(3-oxo-4-methylpentyl)-		3543	
232.	150669-53-7	2(5*H*)-Furanone, 4-(4-methyl-1-pentyl)-		2934b	
233.	77267-30-2	2(5*H*)-Furanone, 5-(2-pentenyl)-, (*Z*)-		404, 3547	
234.	1963-26-8 21963-26-8	2(5*H*)-Furanone, 5-pentyl-		404, 3547, 4249, 5811b	
235.	33488-51-6	2(5*H*)-Furanone, 3,4,5-trimethyl-	568b, 1375, 1375b, 2387, 2570, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 3547, 4249, 5811b	2387
236.	50598-50-0	2(5*H*)-Furanone, 3,5,5-trimethyl-		3543	
237.	4182-41-6	2(5*H*)-Furanone, 4,5,5-trimethyl-		404, 3543	
238.	484-20-8	7*H*-Furo[3,2-*g*][1]benzopyran-7-one, 4-methoxy-		898a	4249, 4513
239.	60026-27-9	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl- 		2544, 3543, 4249, 5811b	
240.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethenyl)- 		3543	
241.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethenyl)- 		3543	
242.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethyl)- 		3543, 3545	
243.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethyl)- 		3543, 3545	
244.	19147-78-5	Gibbane-1,10-dicarboxylic acid, 2,3-epoxy-4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,3β,4aα,4bβ,10β)-		4249, 4635	
245.	545-97-1	Gibbane-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		429b, 4249, 4831	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
246.	468-44-0	Gibbane-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-,1,4a-lactone, (1α,2β,4aα,4bβ,10β)- 		2260a, 4249, 4635	
247.	561-56-8	Gibb-2-ene-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,4aα,4bβ,10β)-		429b, 4635	
248.	77-06-5	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)- {gibberellic acid} 		527a, 683a, 5804, 5811b	
249.	125-67-7	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, potassium salt {gibberellic acid, potassium salt} 		3633, 4249	
250.	510-75-8	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		429b, 683a	
251.	66537-22-2	Glucometasaccharinic acid, γ-lactone	2493, 5811b	4249	
252.	32449-92-6	*D*-Glucurono-3,6-lactone 	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249		1360, 1375a
253.	33124-69-5	threo-2,3-Hexodiulosonic acid, γ-lactone {2,3-diketogulonic acid, γ-lactone} 		4249	
254.	490-83-5	*L*-threo-2,3-Hexodiulosonic acid, γ-lactone {*L*-2,3-diketogulonic acid, γ-lactone}		429b	

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

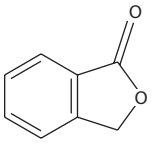
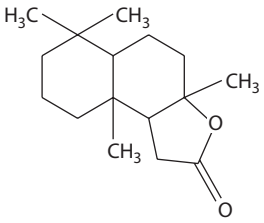
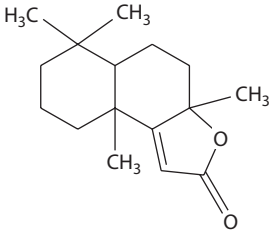
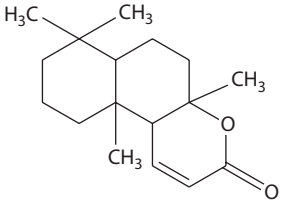
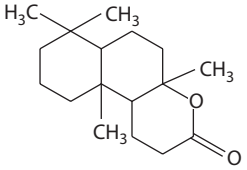
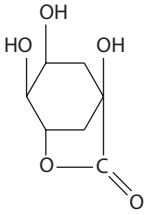
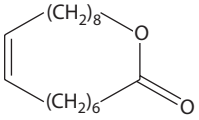
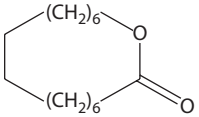
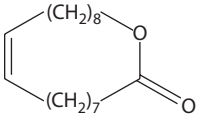
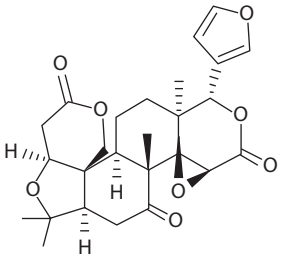
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
255.	61989-59-1	Hexonic acid, 2,3-dideoxy-, γ-lactone, monoacetate	3553, 4249, 5811b		
256.	61892-51-1	Hexonic acid, 3,6-dideoxy-, γ-lactone	3553, 4249, 5811b		
257.	61653-41-6	*D*-lyxo-Hexonic acid, 2-deoxy-, γ-lactone		4249, 4712	
258.	87-41-2	1(3*H*)-Isobenzofuranone {phthalide} 	568b, 1233, 1375, 1375b, 1378, 1586, 2387, 2543, 2767, 2773, 2775, 3302, 3553, 3557, 4249, 5811b	404, 568b, 1254, 2389, 2544, 3198, 3219, 3550, 4249, 5811b	1378, 2387
259.		1(3*H*)-Isobenzofuranone, methyl-			642, 4249
260.	551-08-6	1(3*H*)-Isobenzofuranone, 3-butylidene-		1053, 3266, 3370	
261.	13277-77-5	1(3*H*)-Isobenzofuranone, 3,7-dihydroxy-3,4,5,6-tetramethyl-		4249, 5811b	
262.	17369-59-4	1(3*H*)-Isobenzofuranone, 3-propylidene-		172a, 174b, 1053, 3266, 3370	
263.	66309-76-0	1(3*H*)-Isobenzofuranone, 4,5,6,7-tetrahydro-	2767, 2769, 4249		
264.	564-20-5	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {1,5,5,9-tetramethyl-13-oxatricyclo[8,3,0,0(4,9)]tridecane} {sclareolide} 	568b, 775, 2292, 2756, 2767, 3251, 3267, 3272, 3295, 3557, 4249, 5811b	120, 174e, 568b, 1053, 1296, 1590a, 2292, 2308, 2338, 2386, 2611, 2756, 3198, 3263, 3266, 3267, 3295, 3370, 3533, 3534, 3545, 3547, 3560, 3561, 4249, 5811b	
265.		Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {1,5,5,9-tetramethyl-13-oxatricyclo[8,3,0,0(4,9)] tridecane}, labeled with ^{14}C {sclareolide-^{14}C}	2756, 4249	2756, 4249	
266.	52811-59-3	Naphtho[2,1-*b*]furan-2(3a*H*)-one, 4,5,5a,6,7,8,9,9a-octahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα)]- 	5811b	120, 1297, 2308, 2338, 3561, 4249	
267.	52811-58-2	3*H*-Naphtho[2,1-*b*]pyran-3-one, 4a,5,6,6a,7,8,9,10,10a,10b-decahydro-4a,7,7,10a-tetramethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]- {dehydroambreinolide} 	5811b	1156, 3547, 3560, 3561, 4090, 4249, 4780, 5811b	

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
268.	468-84-8	3*H*-Naphtho[2,1-*b*]pyran-3-one, dodecahydro-4a,7,7,10a-tetramethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]- {ambreinolide} 	5811b	1156, 2031, 3533, 3560, 3561, 4090, 4249, 4780, 5811b	
269.	63626-79-9	3-Oxabicyclo[3.3.1]nonan-2-one, 9-hydroxy-5-methyl-	5811, 5811a, 5811b	5811, 5811a, 5811b	
270.		6-Oxabicyclo[3.2.1]octan-7-one, 6-hydroxy-3-methyl-	568b, 4249		
271.	72693-08-4	6-Oxabicyclo[3.2.1]octan-7-one, 8-hydroxy-1-methyl-	4249		
272.	640-06-2	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy {Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, γ–lactone; quinic acid lactone; quinide} 	1089a, 1364, 1371, 1375, 1375b, 1887a, 2493, 2524a, 2675, 2767, 5811b		
273.	27783-00-2	6-Oxabicyclo[3.2.1]octan-7-one,1,3,4-trihydroxy-,(exo,exo)-	4249, 5811b	4249	
274.	665-27-0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy-,[1S-(exo,exo)]-	4249, 5811b		
275.	7779-50-2	Oxacycloheptadec-7-en-2-one		172a, 174b, 1053, 3266, 3370	
276.	123-69-3	Oxacycloheptadec-8-en-2-one, (*Z*)- {ambrettolide} 	1063–1066, 1068–1074, 2767, 2769, 4249		
277.	106-02-5	Oxacyclohexadecan-2-one {ω-pentadecalactone; exaltolide} 		172a, 174b, 947, 1053, 3266, 3370, 4249	
278.	68985-15-9	Oxacyclononadec-10-en-2-one, (*E*)- 		947, 4249	
279.	1180-71-8	11*H*,13*H*-Oxireno[*d*]pyrano[4′,3′:3,3a]isobenzofuro[5,4-f][2]benzopyran-4,6,13(2H,5aH)-trione,8-(3-furyl) decahydro-2,2,4a,8a-tetramethyl- {limonin} 	5811, 5811a, 5811b		

(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

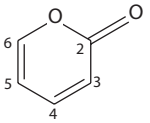
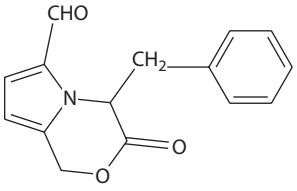
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
280.	61989-60-4	Pentonic acid, 2,3-anhydro-, γ-lactone	4249, 5811b		
281.	9473-19-9	*D*-erythro-Pentonic acid, 3-deoxy-, γ-lactone	4249	4249	
282.	5803-57-6	Pentonic acid, 5-deoxy-, γ-lactone	4249, 5811b		
283.	112468-46-9	2*H*-Pyran-2,5(6*H*)-dione	4249	5811b	
284.	504-31-4	2*H*-Pyran-2-one 	172, 568b, 2388, 4249, 5811b		
285.	20357-65-7	2*H*-Pyran-2-one, 6-chloro-	222–224		
286.		2*H*-Pyran-2-one, 3,4-dihydro-4-(1-methylethyl)-6-methyl-	568b, 4249		
287.	3393-45-1	2*H*-Pyran-2-one, 5,6-dihydro-		404	
288.		2*H*-Pyran-2-one, 5,6-dihydro-4,5-dimethyl-	2767, 4249		
289.		2*H*-Pyran-2-one, 4,5-dihydro-3-hydroxy-	1375, 3553, 3557, 4249		
290.	55100-07-7	2*H*-Pyran-2-one, 5,6-dihydro-4-hydroxy-		3430, 5811b	
291.	54657-94-2	2*H*-Pyran-2-one, 3,4-dihydro-5-methyl-	3404, 4249, 5811b		
292.	2381-87-5	2*H*-Pyran-2-one, 5,6-dihydro-4-methyl-	1586, 3553, 4249, 5811b	404, 937, 2389, 2544, 3550, 3905, 4249, 5811b	
293.	21722-33-8	2*H*-Pyran-2-one, 5,6-dihydro-4-(1-methylethyl)-	568b, 1378, 4249	568b, 937, 1156, 2389, 3219, 3543, 3545, 4090, 4249, 5811b	1378
294.	6400-69-4	2*H*-Pyran-2-one, 5,6-dihydro-6-propyl-	2601a	1256, 4249	
295.	73850-01-8	2*H*-Pyran-2-one, hydroxyethyl-	4097, 4249, 5811, 5811a, 5811b		
296.		2*H*-Pyran-2-one, hydroxymethyl-	3746, 3747		
297.	496-64-0	2*H*-Pyran-2-one, 3-hydroxy-	1375a, 1377, 5811b	3973	1375a, 1377, 4249
298.	73692-69-0	2*H*-Pyran-2-one, 3-hydroxy-6-methyl-		3430	
299.	150669-60-6	2*H*-Pyran-2-one, 4-(1-methylethyl)-	247, 2387, 3553, 3557, 4249	2934b	
300.	27593-23-3	2*H*-Pyran-2-one, 6-pentyl- {6-amyl-α-pyrone}		1053, 3266	
301.	542-28-9	2*H*-Pyran-2-one, tetrahydro- {δ-valerolactone}	568b, 1375, 1375b, 2767, 3553, 3557, 4249, 5811b	568b, 2386, 2389, 2544, 4249, 5811b	3404
302.		2*H*-Pyran-2-one, tetrahydro-3,4-epoxy-5-hydroxy-	1375a (0), 1377 (0)		1375a, 1377
303.	5058-01-5	2*H*-Pyran-2-one, tetrahydro-3-hydroxy-	1586, 2543, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3553, 3557, 5811b		3401, 3402, 3404
304.		2*H*-Pyran-2-one, tetrahydro-methoxy-	1375a (0), 1377 (0)		1375a, 1377
305.		2*H*-Pyran-2-one, tetrahydro-methyl-	1375a (0), 1377 (0)		1375a, 1377
306.	32821-70-8	2*H*-Pyran-2-one, tetrahydro-3-(1-methylethyl)-		297, 2386, 2389, 2544, 4249	
307.	78094-66-3	2*H*-Pyran-2-one, tetrahydro-4,5-dimethyl-, *cis*-(±)-	2767		
308.	3720-20-5	2*H*-Pyran-2-one, tetrahydro-4,6-dimethyl-	568b, 1352, 4249	568b, 3543, 3546, 4249	
309.	710-04-3	2*H*-Pyran-2-one, tetrahydro-6-hexyl- {δ-undecalactone}		172a, 174b, 1053, 3266	
310.	61892-56-6	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-	1351, 3553, 4249		

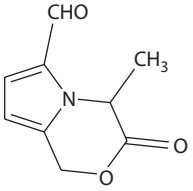
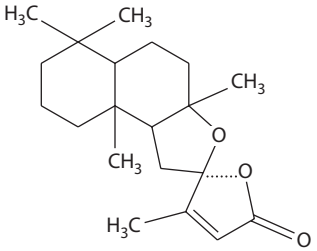
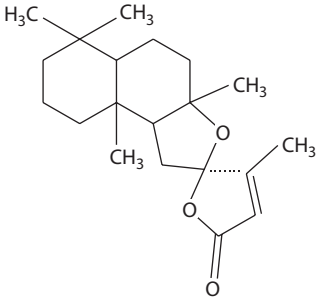
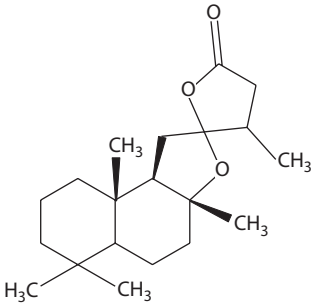
TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
311.	503-48-0 110053-65-1	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-4-methyl-	5811b	323, 4249	
312.	1121-84-2	2*H*-Pyran-2-one, tetrahydro-4-methyl-	568b, 3553, 4249, 5811b	568b, 2386, 2917a, 3543, 3545, 3560, 3561, 3905	
313.	96168-15-9	2*H*-Pyran-2-one, tetrahydro-4-methyl-6-(3,7,11-trimethyldodecyl)-	2601a		
314.	56947-55-8	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-	568b, 3553, 3557, 4249, 5811b	404, 568b, 1063–1066, 1068–1074, 1156, 1256, 1590a, 2282, 2386, 2389, 2544, 3330, 3332, 3543, 3550, 3560, 3561, 3905, 4090, 4249, 5811b	
315.	21754-22-3	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-, (±)-		404, 568b, 4249	
316.	37147-17-4	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-, (*R*)-		5811, 5811b	
317.	10413-18-0 24405-16-1	2*H*-Pyran-2-one, tetrahydro-5,6-dimethyl-	5811b	404, 568b, 2389, 2544, 2917a, 3219, 3546, 3560, 3561, 4249, 5811b	
318.	33691-73-5	2*H*-Pyran-2-one, tetrahydro-5-hydroxy-	568b, 1360, 1375, 1375b, 1586, 2570, 2767, 2777, 3553, 3557, 4249, 5811b		
319.	3301-94-8	2*H*-Pyran-2-one, tetrahydro-6-butyl- {δ-nonalactone}		174b, 3266	
320.	2610-95-9	2*H*-Pyran-2-one, tetrahydro-6,6-dimethyl-		3561, 4249	
321.	59056-32-5	2*H*-Pyran-2-one, tetrahydro-6,6-dimethyl-4-(1-methylethyl)-		568b, 4249	
322.	713-95-1	2*H*-Pyran-2-one, tetrahydro-6-heptyl- {δ-dodecalactone}		172a, 174d, 1053, 3266, 3370	
323.	90-80-2	2*H*-Pyran-2-one, tetrahydro-6-hydroxymethyl, 3,4,5-trihydroxy gluconic acid, δ-lactone}	1360, 4249		
324.	823-22-3 26991-67-3	2*H*-Pyran-2-one, tetrahydro-6-methyl- δ-hexalactone; δ -caprolactone}	1586, 4249	2917a	
325.	21722-34-9	2*H*-Pyran-2-one, tetrahydro-6-methyl-3-(1-methylethyl)- {2 isomers indicated}		568b, 3543, 3547, 3560, 3561, 4249	
326.		2*H*-Pyran-2-one, tetrahydro-6-methyl-4-(1-methylethyl)-		568b, 3543, 4249	
327.	60393-63-7	2*H*-Pyran-2-one, tetrahydro-6-methyl-5-(1-methylethyl)-		568b, 4249	
328.	2721-22-4	2*H*-Pyran-2-one, tetrahydro-6-nonyl- {tetradecalactone}		174b, 3266	
329.	705-86-2	2*H*-Pyran-2-one, tetrahydro-6-pentyl- {δ-decalactone}		1254, 1256, 2611, 3266, 4249	
330.	698-76-0	2*H*-Pyran-2-one, tetrahydro-6-propyl- {δ-octalactone}		172a, 174d, 404, 1053, 1254, 1256, 2389, 2544, 2917a, 3266, 3370, 3561, 4098a, 4249	
331.	60026-28-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-3-oxo-4-(phenylmethyl)-		965, 2337, 2544, 3491, 4249	



(*continued*)

TABLE 6.3 (continued)
Lactones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
332.	35674-33-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-4-methyl-3-oxo- 		965, 2544, 3491, 4249, 5811b	
333.	5989-24-2 30987-48-5	Spiro[furan-2(3*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5(4*H*)-one, decahydro-3,3′a,6′,6′,9′a-pentamethyl- {α-levantenolide} 	323, 799, 801, 1173, 1352, 1373, 2722, 3251, 3302, 3308, 3797, 3971, 4249, 4341, 5811b	1149, 1149a, 1156, 1173, 1290, 1299, 1300, 1352, 2308, 2939, 3797, 3804, 3971, 3973, 3974a, 4090, 4249, 4319, 4341, 5811b	
334.	1235-78-5	Spiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one, 3′a,4′,5′,5′a,6′,7′,8′,9′,9′a,9′b-decahydro-3,3′a,6′,6′,9′a-pentamethyl-, [2′S-(2′α,3′aα,5′aβ,9′aα,9′bβ)]- {β-levantenolide} 	323, 799, 801, 1173, 1373, 3251, 3302, 3308, 3797, 3971, 4249, 4319, 4341, 5811b	1149, 1149a, 1156, 1173, 1290, 1299, 1300, 2308, 2939, 3561, 3797, 3804, 3971, 3973, 3974a, 4090, 4249, 4319, 4341, 5811b	
335.		Spiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one, dodecahydro-3,3′a,6′,6′,9′a-pentamethyl- α_2-levantanolide} 		1149, 1149a, 1156, 1300, 2308, 3973, 3974a, 4090	
336.	82796-87-0	*D*-Xylonic acid, δ-lactone	4249		

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

7 Anhydrides

The number of anhydrides identified in tobacco and tobacco smoke is small. In 1988, Roberts (3215) reported that there were only 10 anhydrides identified in tobacco, 10 identified in tobacco smoke, and 4 in both tobacco and tobacco smoke. The number of anhydrides in tobacco and tobacco smoke has not changed substantially since that time. There are presently 13 anhydrides identified in tobacco, 13 in tobacco smoke, and 6 identified in both tobacco and tobacco smoke.

In his 1984 review of the carcinogenesis induced by alkylating agents, Lawley (Table XXV, p. 434 in 7A04) tabulated the findings of Dickens and Jones on a study of the tumorigenicity (sarcogenicity) of maleic anhydride (7A01) and 2,3-dimethylmaleic anhydride and succinic anhydride (7A02) administered by subcutaneous injection to Wistar rats.

In its 1986 monograph, the International Agency for Research on Cancer (IARC) wrote very little on the few anhydrides in tobacco smoke [see p. 107 in (1870)]. IARC commented as follows:

> At least eight acid anhydrides have been found in cigarette smoke, including maleic anhydride and succinic anhydride and their alkylated derivatives [Schumacher et al. (3553), Newell et al. (2769)]. These smoke constituents are of particular concern because of their alkylating potential. Maleic anhydride, 2,3-dimethylmaleic anhydride and succinic anhydride have produced local tumours in one experiment in rats [Dickens and Jones (7A01, 7A02)], IARC (7A03)].

An inserted comment in the IARC monograph referred the reader to Appendix 2, pp. 389–394 in (1870) which listed the components in tobacco smoke that had been evaluated for carcinogenicity in the IARC monograph series. The tumorigenicity of succinic anhydride was listed as follows:

Compound	Degree of Evidence in Animals (and Humans)
7. *Agricultural chemicals and derivatives*	
Succinic anhydride	Limited evidence

It is obvious from the review by Lawley (7A04) and the data in the Dickens and Jones reports (7A01, 7A02) that the anhydrides are sarcogens, not carcinogens; i.e., they do not fit the definition of a carcinogen, a factor that induces a carcinoma.

At R.J. Reynolds Tobacco Co. (RJRT) R&D, two anhydrides, 3,4-diethyldihydro-2,4-furandione (diethylsuccinic anhydride) and 3,4-dimethyldihydro-2,4-furandione (dimethylsuccinic anhydride), were identified by Jones and Latimer during their research on Oriental tobacco composition. The two anhydrides were listed in their 1943 report on the Oriental tobacco components they identified through the end of 1942 (1980).

In a subsequent RJRT research effort in 1963 and 1964, several anhydrides (see Table 7.1) were isolated from tobacco smoke and identified by Fredrickson (1233, 1235) during his study of the composition of burley tobacco smoke condensate. Two decades later, several additional anhydrides (see Table 7.1) were identified as components of Oriental tobacco by Schumacher (3543).

Table 7.1 lists the 24 anhydrides identified to date in tobacco and/or tobacco smoke: 17 in tobacco smoke, 16 in tobacco, and 9 in both tobacco and tobacco smoke. None of the anhydrides listed in Table 7.1 were included in any of the many publications issued between 1986 and 2001 in which the toxicants in tobacco and/or tobacco smoke were listed (1217, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 2825).

No anhydride was included in the 1994 Doull et al. list (1053) on compounds in flavor formulations used on tobacco products by members of the U.S. tobacco industry.

TABLE 7.1
Anhydrides in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

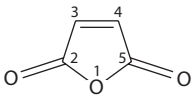
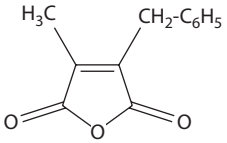
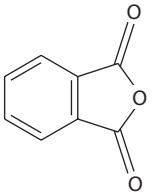
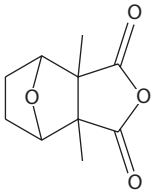
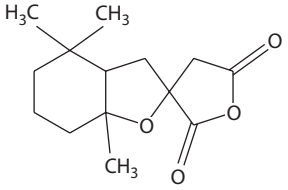
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	108-24-7	Acetic acid, anhydride $(CH_3\text{-}CO)_2O$	568b, 2761, 2762, 2777, 4249		
2.		1,3-Benzofurandione, 5-(1,1-dimethylheptyl)-	2601a		
3.	108-31-6	2,5-Furandione {maleic anhydride} 	239, 568b, 1233, 1375, 1375b, 1375a, 1377, 1586, 2543, 2570, 2767, 3029, 3255, 3257, 3265, 3300, 3553, 3557, 4249, 5811b	568b, 2917a, 4249	1375a, 1377
4.		2,5-^{14}C- 2,5-Furandione {maleic anhydride-2,5-^{14}C}	25A74	25A74	
5.	28843-39-2	2,5-Furandione, 3,4-diethyl-	568b, 4249		
6.	33765-37-6	2,5-Furandione, 3,4-diethyldihydro-, *trans*-		1980, 4249	
7.	108-30-5	2,5-Furandione, dihydro- {succinic anhydride}	568b, 239, 2767, 3300, 3553, 4249, 5811b	568b, 2917a, 3543, 3560, 3561, 4249	
8.	17347-61-4	2,5-Furandione, dihydro-3,3-dimethyl-	3557	2389, 2544, 3561, 5811b	
9.	7475-92-5	2,5-Furandione, dihydro-3,4-dimethyl-	568b, 1233, 1375, 1375b, 2767, 2775, 3553, 3557, 4249, 5811b	568b, 1980, 2389, 2544, 3215, 3541, 3543, 3547, 3560, 3561, 4249	
10.	4100-80-5	2,5-Furandione, dihydro-3-methyl-	568b, 2767, 3553, 3557, 4249, 5811b		
11.	83174-26-9	2,5-Furandione, dihydro-3-propyl-	568b, 4249		
12.	766-39-2	2,5-Furandione, 3,4-dimethyl-	239, 568b, 1233, 1352, 1360, 1371, 1375, 1375a, 1375b, 1586, 2570, 2761, 2762, 2777, 3300, 3410, 3553, 4249, 5811b	568b, 1352, 2386, 2917a, 3188, 3219, 3549	1360, 1375a
13.	3552-33-8	2,5-Furandione, 3-ethyl-4-methyl-	568b, 1233, 1235, 1259, 1352, 1360, 1371, 1375, 1375a, 1375b, 1586, 2543, 2570, 2761, 2762, 2767, 2775, 2777, 3410, 3553, 3557, 4249, 5811b	404, 568b, 937, 1352, 2917a, 3215, 3217, 3219, 3547, 4249, 5811b	1360, 1375a
14.	616-02-4	2,5-Furandione, 3-methyl-	4249	5811b	
15.	72693-16-4	2,5-Furandione, 3-methyl-4-(phenylmethyl)- 	568b, 1235, 3557, 4249		
16.	16493-20-2	2,5-Furandione, 3-methyl-4-propyl-	568b, 3553, 4249, 5811b		
17.	61679-89-8	2,5-Furandione, 3-propyl-	1586, 2767, 2769, 3553, 3557, 4249		
18.	34150-36-2	*D*-Galacturonic acid, anhydro-		4249, 4933	
19.	25249-06-3	*D*-Galacturonic acid, homopolymer		1051a, 1334e, 1971, 4249	
20.	2051-49-2	Hexanoic anhydride		2917a	
21.	85-44-9	1,3-Isobenzofurandione {phthalic anhydride} 	5811b	2389, 2544, 4249, 5811b	

TABLE 7.1 (continued)
Anhydrides in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
22.	56-25-7	1,3-Isobenzofurandione, 3a,7a-dimethyl-4,7-epoxy-hexahydro {cantharidin} 		2917a	
23.	97-73-4	Propanoic acid, 2-hydroxy-, anhydride		4249	
24.	162188-94-5	Spiro[benzofuran-6(2*H*),2′-[1,3]dioxolan]-2-one, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-, (±)- 		4249	

8 Carbohydrates and Their Derivatives

The four macromolecules that have been called the "building blocks of life" are carbohydrates, proteins, lipids, and nucleic acids. Tso (3873) estimated that as much as 75% of all the carbon from CO_2 that is reduced by plants enters into some form of carbohydrate for at least a brief period of time. Via numerous metabolic pathways, these carbohydrates are converted into hundreds of functional molecules necessary to sustain life.

There are 316 components in tobacco and/or tobacco smoke that may be considered as a complete carbohydrate or one in which a carbohydrate is linked to another structure, such as in a glycoside. This number is greater than the 156 listed by Tso in his 1990 book [see Table 1.38 in (3873)] because of our inclusion of the carbohydrate-combined components. The following indicates the difference in numbers:

	Reference	Total	Smoke	Tobacco	Tobacco and Smoke
Tso	Table 1.38 in (3873)	156	30	138	12
Carbohydrates	Table 8.3	316	44	310	38

A great number of carbohydrate-linked components, mostly in tobacco, involve the linkage of a carbohydrate to a 2*H*-1-benzopyran-2-one or 4*H*-1-benzopyran-4-one which may not only be hydroxylated, e.g., 6-(β-*D*-glucopyranosyloxy)-7-hydroxy-2*H*-1-benzopyran-2-one (esculin), but also may have one or more hydroxyphenyl links, e.g., 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one (quercetrin), 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran- 4-one (rutin), and 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one (kaempferol glycoside). Components such as these were classified as polyphenols. Tobacco components such as the latter three may be the precursors of part of the phenols yield in tobacco smoke. Snook et al. (8A08) determined the levels of rutin and kaempferol glycoside in 62 different species of *Nicotiana*. Their levels ranged from <0.005% to 1.6% for rutin and <0.005% to 0.16% for the kaempferol glycoside. There are, of course, in tobacco several carbohydrate-linked benzopyranones that lack a hydroxyphenyl group, e.g., 6-(β-*D*-glucopyranosyloxy)-7-hydroxy-2*H*-1-benzopyran-2-one (esculin) and 7-(β-*D*-glucopyranosyloxy)-6-methoxy-2*H*-1-benzopyran-2-one (scopolin).

As indicated in Table 8.1, only a few tobacco and/or tobacco smoke carbohydrates are used in the flavor formulations used by cigarette manufacturers in the United States (1053) and in other countries (3266). None of those used in that way are linked to a noncarbohydrate entity.

The use on tobacco containing various carbohydrate additives, such as the various sugars listed in Table 8.1, has been the subject of much discussion recently in attempts to link such additives to medical problems induced by cigarette smoke. The major concern was the generation of carbonyl compounds such as formaldehyde and acetaldehyde.

Although Baker (8A02), in his letter to the editor of Food and Chemical Toxicology, agrees with the statements of Talhout et al. (3865b) that addition of sugars to tobacco results in increased yields of formaldehyde in the mainstream smoke (MSS), he also provided numerous references [Baker (8A01), Baker and Bishop (172a, 172b), Baker et al. (172c, 174a, 174b, 174c, 8A03), Baker and Smith (174e), Gori (1332), Massey (2484a), Rodgman (3264), Rustemeier et al. (3370), Seeman et al. (3579, 8A06), Thornton and Massey (3913), Zilkey et al. (4418)] and much discussion to counter the assertions by Talhout et al. (3865b) that sugar addition had an adverse effect on the biological properties of the MSS. Not included in Baker were the facts that (1) Doull et al. (1053), in their detailed 1994 assessment of 599 additives used by members of the U.S. tobacco industry in cigarette manufacture, reported no significant biological problem from the use of sugars in the flavor formulations and (2) Dalhamn et al. (892) had reported in 1968 that a significant percentage of water-soluble MSS vapor-phase components such as formaldehyde, acetaldehyde, and other carbonyls never reached the respiratory tract cilia of the smoker because of their solution in the fluids coating the oral cavity. The findings of Dalhamn et al. (892) were a confirmation of those by Rodgman et al. (3306), Industrial Bio-Research Laboratories, an independent contract laboratory (8A04), and the repeated assertions by Wynder and Hoffmann that such would be the case with water-soluble ciliastats (4330, 4332).

In their mid-1960 publications, Wynder and Hoffmann commented several times on the fact that most of the known ciliastatic components of MSS demonstrated to be ciliastatic in various in vitro systems were water soluble and this property would markedly influence their fate and behavior during and after inhalation. Wynder and Hoffmann (4330) noted:

> As far as human smoking habits are concerned, it remains also to be estimated to which extent volatile smoke components reach the bronchial tree. Preliminary studies indicate that a significant proportion of the gaseous components is being retained within the oral cavity.

TABLE 8.1
Tobacco and/or Smoke Carbohydrates Used in Flavor Formulations

CAS No.	Chemical Abstracts Nomenclature	As Listed by Doull et al. (1053)	Identified in	
			Smoke	Tobacco
57-48-7	*D*-Fructose	Sugars	+	+
59-23-4	*D*-Galactose	Sugars	+	+
50-99-7	α-*D*-Glucose	Sugars	+	+
57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose}	Sugars	+	+
50-99-7	α-*D*-Glucose	Sugars	+	+
31103-86-3	Mannose	Sugars	+	+
50-70-4	Sorbitol[a]	Glucitol	–	+

[a] Sorbitol (glucitol) is not included in the Doull et al. list (1053) but is included in flavor formulations used by cigarette manufacturers outside of the United States [see Table 7A in (3266)].

Later, Wynder and Hoffmann [see p. 542 in (4332)] wrote:

> Water-soluble volatile components, which are primarily responsible for the results of the acute in vitro short-term cilia toxicity tests, are, to a large extent, removed when cigarette smoke contacts the saliva in the mouth and the abundant secretions of the trachea and main bronchi.

They added [see p. 646 in (4332)]:

> In man's manner of smoking, however, volatile components are retained to a significant degree in the oral cavity and may, therefore, be far less important than when tested experimentally.

Baker (8A02), in the letter to the editor of *Food and Chemical Toxicology* in which he responded to the assertions of Talhout et al. (3865b), noted several early studies cited by Talhout et al., those of Thornton and Massey (3913) and Shelar et al. (8A07) in which high levels of a carbohydrate (sugar) were added to the tobacco resulting in a significant increase in the MSS yield of several carbonyl compounds, namely, formaldehyde, acetaldehyde, acrolein. However, the added carbohydrate greatly exceeded the amount usually added in an industrial situation.

As noted by Baker (8A02), Talhout et al. (3865b) commented on the effect on MSS carbonyl component yields produced by additions to tobacco of 12% of three sugars, but they did not describe the effect of the additions of 4% of each sugar, an addition level which more closely resembled that used commercially. Table 8.2 lists the changes reported by Shelar et al. (8A07) in per cigarette MSS yield of formaldehyde, acetaldehyde, acetone, and acrolein by addition of 4% fructose, glucose, or sucrose to two different burley samples.

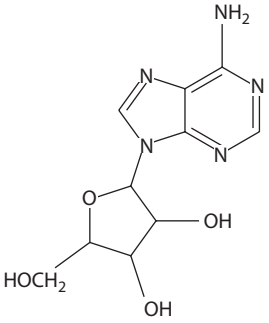
Not discussed by either Baker (8A02) or Talhout et al. (3865b) was a 1970 study by Best (297) in which a flue-cured tobacco sample was treated with sugar to raise its level from 12.6% to 21.0%. Even though the sugar addition to the flue-cured tobacco represented a 66% increase, the MSS yields of carbonyl components increased as follows: formaldehyde from 35.4 to 48.8 µg/cig, a 37.8% increase; acetaldehyde from 998 to 1020 µg/cig, a 2.2% increase; acrolein from 124 to 131 µg/cig, a 5.6% increase.

In his review of the genotoxicity of tobacco smoke and tobacco smoke condensate, DeMarini (933) described in

TABLE 8.2
Effect of Sugars Added to Burley Tobacco on MSS Aldehyde and Ketone Yields (8A07)

	Per Cigarette MSS Yield			
	Formaldehyde	Acetaldehyde	Acetone	Acrolein
Burley 1	16.0	507	269	118
+ 4% Fructose	18.2 (13.8%)	591 (16.6%)	333 (23.8%)	135 (14.4%)
+ 4% Glucose	15.7 (–2%)	553 (9.1%)	335 (24.5%)	123 (4.2%)
+ 4% Sucrose	20.4 (27.5%)	574 (13.2%)	364 (35.3%)	139 (17.8%)
Burley 2	11.2	578	306	118
+ 4% Fructose	12.0 (7.1%)	652 (12.8%)	330 (7.8%)	130 (10.2%)
+ 4% Glucose	18.6 (66.1%)	567 (–2%)	216 (–29.5%)	93 (–21.2%)
+ 4% Sucrose	18.2 (62.5%)	561 (–3%)	270 (–12%)	109 (–7.7%)

TABLE 8.3
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	58-61-7	Adenosine 		429b, 4249, 4828, 5540	
2.	28542-78-1	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-		2371a, 4249, 4523	
3.	6025-53-2	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*E*)-		683a, 2371a, 4066a, 4249	
4.	15896-46-5	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*Z*)-		2371a, 4249, 4582	
5.	26190-61-4	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-		2371a, 4249	
6.	53274-45-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*E*)-		2371a, 4249, 4778	
7.	52049-48-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*Z*)-		2371a, 4249, 4778	
8.	22663-55-4	Adenosine, *N*-(4-hydroxy-3-methylbutyl)-		960a, 2371a, 4249	
9.	7724-76-7	Adenosine, *N*-(3-methyl-2-butenyl)-		2371a, 4249, 4522	
10.	75081-82-2	Adenosine, *N*-[3-methyl-4-[(*O*-phosphono-β-*D*-glucopyranosyl)oxy]-2-butenyl]-, (*E*)-		429b, 4249, 4813	
11.	4294-16-0	Adenosine, *N*-(phenylmethyl)-		2371a	
12.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4708	
13.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1-β-*D*-ribofuranosylpyridinium 3-(aminocarbonyl)-hydroxide, inner salt		429b, 4249	
14.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
15.	22732-83-8	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester		4249, 4617	
16.	40811-89-0	Adenosine 5′′-(trihydrogen diphosphate), *N*-(phenylmethyl)-		2371a	
17.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	
18.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

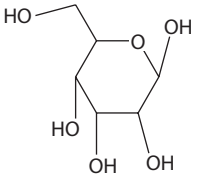
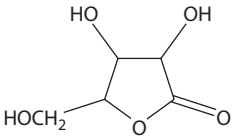
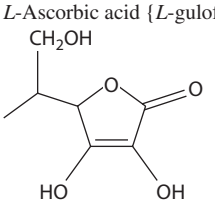
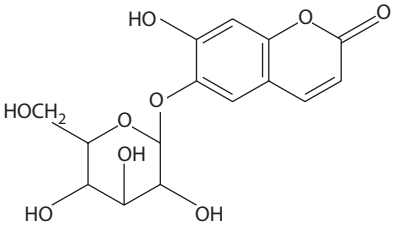
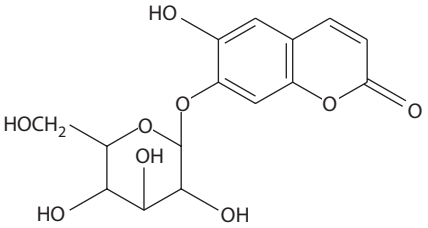
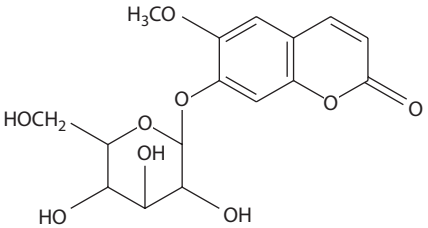
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
19.	2595-97-3	*D*-Allose 		3075	
20.	9005-84-9	Amylodextrin		429b, 4249, 4841a	
21.	9037-22-3	Amylopectin		2338, 2939, 4249, 4614, 5811b	
22.	9005-82-7	Amylose		1971, 2338, 2939, 3430, 4249, 5811b	
23.	11078-27-6	Arabinan		373a, 4249	
24.	20261-96-5	Arabinohexonic acid, 3-deoxy-, γ-lactone	4249	4249	
25.	42400-32-8	*D*-Arabinohexonic acid, 2-deoxy-, γ-lactone		4249	
26.	23675-06-1	α-*D*-Arabinohexopyranoside, 2-deoxy- α-*D*-arabino-hexopyranosyl 2-deoxy-		4249, 4599	
27.	154-17-6	*D*-Arabinohexose, 2-deoxy- {Also known as *D*-Glucose, 2-deoxy-}		429b, 3075, 4249, 4599, 5811b	
28.	16449-30-2	*D*-Arabinohexose, 2-deoxy-4-*O*-β-*D*-glucopyranosyl-		4249, 4599	
29.	13752-83-5	Arabinonic acid $HO\text{-}CH_2\text{-}(CHOH)_3\text{-}COOH$		2362a	
30.	13280-76-7	Arabinonic acid, γ-lactone 	4249		
31.	87-72-9 5328-37-0	*L*-Arabinose $HO\text{-}CH_2\text{-}(CHOH)_3\text{-}CH{=}O$	1351, 2145, 2939, 3302, 4249, 5811	120, 158, 344a, 830a, 1263, 1351, 2070, 2270, 2338, 3059, 3075, 3797, 3973, 3974a, 4249, 5811, 5811b	
32.	147-81-9	*DL*-Arabinose	5580, 5811b	5079, 5785, 5811b	
33.	9040-27-1	Arabinoxylan		429b, 1109, 4249	
34.		Arabitinol, 2,3-di-*O*-methyl- $HO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$		3669	
35.		Arabitinol, 2,5-di-*O*-methyl- $H_3CO\text{-}CH_2\text{-}(CHOH)_2\text{-}(CHOCH_3)\text{-}CH_3$		3669	
36.	98530-09-7	Arabogalactan		1971, 5777	
37.	50-81-7	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-} 	3257, 3266, 3685, 4249, 4751a	120, 174b, 379, 486, 557, 1053, 1971, 2079, 2270, 2489, 2532, 2939, 3266, 3707, 3922, 4236, 4249, 5079, 5267a, 5811b	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
38.	82395-89-9	2(4*H*)-Benzofuranone, 6-(β-*D*-glucopyranosyloxy)-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-		234, 4249, 4714	
39.	10366-91-3	Benzoic acid, 2-(β-*D*-glucopyranosyloxy)-		4249, 5811b	
40.	32142-31-7	Benzoic acid, 4-(β-*D*-glucopyranosyloxy)-3-methoxy-		429b, 4249, 4915	
41.	74712-71-3	2*H*-1-Benzopyran-2-one,7-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-6-methoxy-		4249	
42.	60091-00-1	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-		3797, 4249	
43.	531-75-9	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin} 	3257	1309, 2939, 2954, 3103, 3973, 3974a, 4249, 5711, 5811b	
44.	531-58-8	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin} 		1309, 1626, 3797, 4249, 5811b, 5838	
45.	531-44-2	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-methoxy- {scopolin} 		72, 120, 677a, 830a, 831, 834, 835, 840, 890, 966, 1102, 1309, 1626, 1863, 2338, 2395, 2557a, 2911b, 2954, 3194, 3629, 3631, 3646, 3738, 3797, 3973, 3974a, 3974b, 4156, 4249, 4269, 5649, 5650, 5809, 5811b, 5831	
46.	71050-53-8	2*H*-1-Benzopyran-2-one, 6-methoxy-7-(β-*D*-xylofuranosyloxy)-)- {scopoletin glucoside}		2939, 3797, 4249, 5650, 5808, 5809, 5830, 5842, 5888	
47.	18309-73-4	2*H*-1-Benzopyran-2-one, 6-methoxy-7-[(6-*O*-β-*D*-xylopyranosyl-β-*D*-glucopyranosyl)oxy]-		1863a, 2939, 4249, 5811b	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

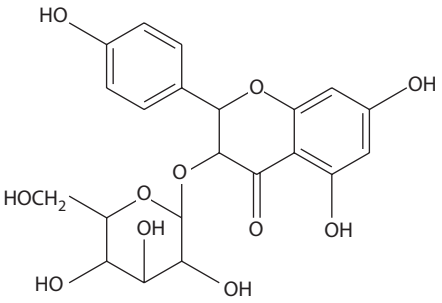
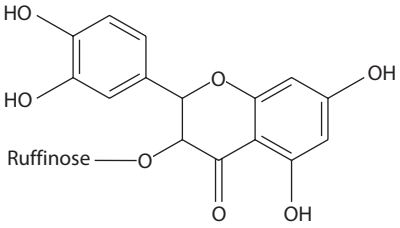
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
48.	21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		120, 1626, 1837a, 1971, 2023, 2270, 2939, 3059, 3194, 3555, 3667, 3794, 3797, 3973, 3974a, 4249, 5079, 5255, 5256, 5724, 5747, 5811b, 5888	
49.	7215-44-3 20188-84-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-b-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy- {quercetin 3,3′-diglucoside}		4249, 5724, 5747, 5811, 5811b, 5888	
50.	491-50-9	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}		3797, 3974a, 4249	
51.	480-10-4	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glucoside; 3,4a,5,7-tetrahydroxyflavone glucoside} 		120, 641, 830a, 835, 838, 840, 966, 970, 1626, 1971, 2023, 2270, 2939, 3059, 3161, 3555, 3646, 3738, 3797, 3974a, 4072a, 4249, 5079, 5724, 5753, 5758	
52.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5,7-tetrahydroxyflavone, 3-glucoside}		1625, 4147, 5353, 5724, 5834, 5888	
53.	55136-76-0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
54.	142235-82-3	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2090b	
55.	19895-95-5	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		42494249, 5724, 5747, 5811, 5811b, 5888	
56.	522-12-3	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl) oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {quercetrin}	970	4036, 4249, 4573	
57.	17912-87-7	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl) oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricitrin}		5811, 5811b	
58.	55696-57-6	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-		4249	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
59.	55804-74-5	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
60.	153-18-4	4*H*-1-Benzopyran-4-one,3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} 		69, 72, 120, 248, 385, 598, 828b, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1063–1066, 1068–1074, 1309, 1329, 1333, 1485, 1626, 1971, 2014, 2079, 2153a, 2270, 2313a, 2338, 2361, 2379, 2395, 2514, 2529, 2531, 2557a, 2704a, 2810–2812, 2939, 3059, 3096, 3161, 3367a, 3400, 3462, 3551, 3555, 3628, 3629, 3631, 3641, 3646, 3700, 3705, 3738, 3767, 3794, 3974a, 3974b, 3984, 3999, 4005–4007, 4036, 4156, 4157, 4249, 4403, 4999, 5079, 5110, 5156, 5157, 5189, 5204, 5217, 5304, 5305, 5310, 5576, 5591, 5596, 5641, 5652, 5661, 5681, 5697, 5698, 5724, 5747, 5750, 5780, 5788, 5808, 5809, 5811b, 5831, 5834, 5888, 5889	
61.	17650-84-9	4*H*-1-Benzopyran-4-one,3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		1309, 4147, 4249, 5811b, 5888	
62.	30311-61-6	4*H*-1-Benzopyran-4-one,3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy- {rutin-7-glucoside}		2023, 4147, 5777, 5811b, 5888	
63.	34336-18-0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	
64.	29859-91-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
65.	27554-19-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxy phenyl)-		1309, 4249	
66.	58934-57-9	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl) glucosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
67.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-glucoside}		4147, 5888	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

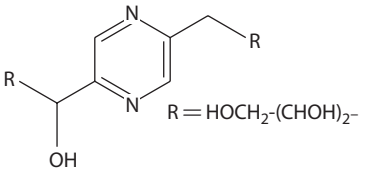
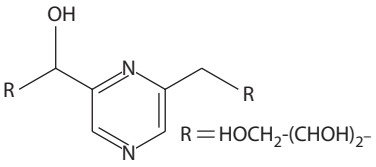
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
23.		4*H*-1-Benzopyran-4-one,7-(β-*D*-rhamnoglucopyranosyloxy)-3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone, 7-rhamnoglucoside}		4147, 5888	
24.		4*H*-1-Benzopyran-4-one,3-(β-*D*-rhamnoglucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-rhamnoglucoside}		3095a, 4372, 5888	
68.	10236-47-2	4*H*-1-Benzopyran-4-one,7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}		970, 1305b, 3797, 3974a, 4249	
69.		4*H*-1-Benzopyran-4-one,2-phenyl-,3′,4′,5,5′,7-pentahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2023, 4249	
70.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,7-tetrahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		4249	
71.	22688-80-8	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride		4249, 4681, 4710	
72.	18719-76-1	1-Benzopyrylium, 3-[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]ox y]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-, chloride		928b, 4249, 4710	
73.	33978-17-5	1-Benzopyrylium, 3-[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride		4249, 4681	
74.	1758-51-6	Butanal, 2,3,4-trihydroxy-, (R*,R*)- {erythrose} $HOCH_2$-$(CHOH)_2$-CH = O		3797, 4249, 5811b	
75.	149-32-6	1,2,3,4-Butanetetrol, (R*,S*)- {erythritol}	2321, 3302, 5580, 5811b	3797, 4249	
76.	68510-02-1	1,2,3,4-Butanetetrol, 1-[5-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,5-deoxyfructosazine} 		480, 1361, 1587a, 2339b, 2420, 2421, 2423, 2424, 4249, 4422, 4747, 5540, 17B57	
77.	68510-03-2	1,2,3,4-Butanetetrol, 1-[6-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,6-deoxyfructosazine} 		480, 1361, 1587a, 2339b, 2420, 2421, 2423, 2424, 4249, 4422, 4747, 5540, 17B57	
78.		2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylaminoribosyl)-		4249, 4514	
79.	62512-25-8	2-Buten-1-one,1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-		4249, 4715	
80.	160550-77-6	2-Buten-1-one,1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		4249, 4715	
81.	9064-51-1 54724-00-4	Callose {1,3-β-*D*-glucan}		1102, 3075, 4249, 4907, 5811b	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
82.	528-50-7	Cellobiose		3075, 3468	
83.	9004-34-6	Cellulose		120, 172, 248, 277, 337, 385, 385a, 420, 451, 535, 539, 601, 602, 629, 665, 722, 1053, 1063–1066, 1068–1074, 1077, 1228, 1289, 1329, 1330, 1333, 1352, 1878a, 1885, 1887, 1933a, 2014, 2042, 2044, 2046, 2070, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2454, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2913, 2919, 2939, 3029, 3059, 3087, 3192, 3264, 3266, 3305, 3371, 3372, 3393, 3395, 3401, 3402, 3404, 3405, 3409, 3430, 3449, 3450, 3462, 3468, 3551, 3665a, 3702, 3797, 3871, 3973, 3974a, 3975, 3976, 4104, 4151, 4249, 4261, 4262, 4418, 4999, 5079, 5189, 5344, 5811b, 5841	
84.		Cellulose, labeled with ^{14}C {cellulose-^{14}C}		2764, 4249	
85.	9000-11-7	Cellulose, carboxymethyl ether		172b, 2086a	
86.	9004-57-3	Cellulose, ethyl ether		429b	
87.	9004-67-5	Cellulose, methyl ether		429b	
88.	70898-22-5	Cyclohexanecarboxylic acid, 3-[[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-		4249, 4785, 4984	
89.	62512-22-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-		4249, 4715, 5811b	
90.	77699-19-5	2-Cyclohexen-1-one,4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-		4249, 4715	
91.	159813-37-3	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [4R-[4R*(1*E*,3S*)]]-		4249, 4715	
92.	54835-70-0	2-Cyclohexen-1-one,4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-4-hydroxy-3,5,5-trimethyl-,[R-[R*,S*-(*E*)]]-		321b, 1361, 4249, 4713	
93.	62512-23-6	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butyl]-3,5,5-trimethyl-		4249, 4715, 5811b	
94.	91048-13-4	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butylidene]-3,5,5-trimethyl-		4249, 4715	
95.	9004-53-9	Dextrin		120, 174b, 2079, 2283, 2939, 2947b, 2947c, 3266, 3449, 4249, 5079, 5189, 5344, 5449, 5811b	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

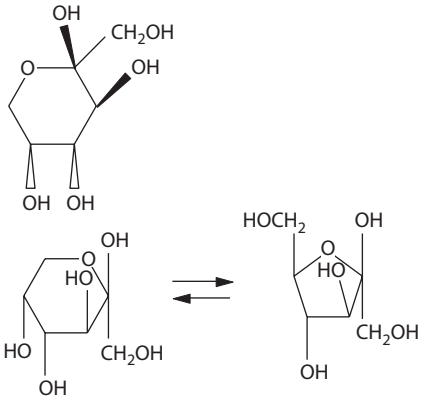
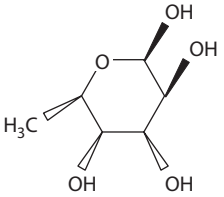
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
96.	29732-48-7	Flavylium, 3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride		4249, 4527, 4710	
97.		Flavylium, 3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-3′,4′,5,7-tetrahydroxy-, chloride		4249, 4527**,** 4644	
98.	9037-90-5	*D*-Fructan		429b, 4249, 4806	
99.	10247-46-8	*D*-Fructofuranose		429b, 3333a	
100.	71385-82-5	β-*D*-Fructofuranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2155, 4249	
101.	79082-92-1	β-*D*-Fructofuranose, 2,6-bis(dihydrogen phosphate)		429b, 4249	
102.	79886-47-8	β-*D*-Fructopyranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		3667, 3668, 4249	
103.	57-48-7	*D*-Fructose {levulose} 	1089a, 1352, 1360, 1361, 1375a, 1587, 1887a, 1944, 2079, 2145, 2321, 2524a, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	71, 120, 321b, 480, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1141, 1142, 1289, 1352, 1361, 1435a, 1916, 1971, 2070, 2270, 2283, 2313a, 2337, 2338, 2381, 2532, 2818, 2911c, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3462, 3551, 3555, 3580, 3667, 3797, 3871, 3913, 3973, 3974a, 3974b, 4159, 4249, 4275, 4411, 5079, 5105, 5108, 5109, 5114, 5189, 5344, 5387, 5449, 5562, 5652, 5748, 5768, 5811b, 5819	1360, 1375a
104.	51767-72-7	*D*-Fructose labeled with ^{13}C {*D*-Fructose-^{13}C}		976a, 4249, 4720, 5644	
105.	29118-61-4	*D*-Fructose, 1-(2-carboxy-1-pyrrolidinyl)-1-deoxy-, (S)-		434, 1063–1066, 1068–1074, 1351, 2337, 2339b, 3555, 3639, 3923, 3973, 3974a, 4159, 4249, 5811b	
106.	488-69-7	*D*-Fructose, 1,6-bis(dihydrogen phosphate)		429b, 4249, 4720	
107.	70954-04-0	*D*-Fructose, 1-[(1-carboxy-2-hydroxypropyl)amino]-1-deoxy-, [R-(R*,S*)]-		434, 1351, 3555, 3973, 3974a	
108.	34393-27-6	*D*-Fructose, 1-[(3-amino-1-carboxy-3-oxopropyl)amino]-1-deoxy-, (S)-		1351, 2337, 4362	
109.	10003-63-1	*D*-Fructose, 1-[(3-carboxypropyl)amino]-1-deoxy-		1351, 2337, 3639, 3923, 3973, 3974a, 5811b	
110.	70906-15-9	*D*-Fructose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		4159	
111.	643-13-0	*D*-Fructose, 6-(dihydrogen phosphate)		429b, 4249, 4670	
112.	36119-15-0	*D*-Fructose, mono(dihydrogen phosphate)		429b, 4249, 4960	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
113.	2438-80-4	Fucose 		3075, 5811b	
114.	9037-55-2	*D*-Galactan		2939, 3797, 3974a, 4249	
115.	9051-94-9	β-(1→4)-*D*-Galactan		5811, 5811b	
116.	526-99-8	Galactaric acid $HOOC\text{-}(CHOH)_4\text{-}COOH$		1263, 1971, 4249, 5079	
117.		Galactitol, 2,3-di-*O*-methyl- $HOH_2C\text{-}[CH(OCH_3]_2\text{-}(CHOH)_2\text{-}CH_2OH$		3669	
118.		Galactitol, 2,4-di-*O*-methyl- $HOH_2C\text{-}CH(OCH_3)\text{-}CHOH\text{-}CH(OCH_3)\text{-}CHOH\text{-}CH_2OH$		3669	
119.		Galactitol, 2,6-di-*O*-methyl- $HOH_2C\text{-}CH(OCH_3)\text{-}(CHOH)_3\text{-}CH_2OCH_3$		3669	
120.		Galactitol, 2-*O*-methyl-		3669	
121.		Galactitol, 3-*O*-methyl-		3669	
122.		Galactitol, 2,3,4,6-tetra-*O*-methyl-		3669	
123.		Galactitol, 2,3,4-tri-*O*-methyl-		3669	
124.		Galactitol, 2,3,6-tri-*O*-methyl-		3669	
125.		Galactitol, 2,4,6-tri-*O*-methyl-		3669	
126.	9036-66-2	*D*-Galacto-*L*-arabinan	4249, 4751a	429b, 2939, 3797, 4249	
127.	33818-21-2	α-*D*-Galactofuranose, 1,6-anhydro-	2321, 4249, 5811b		
128.	107389-81-1	Galactoglucomannan		5811b	
129.	9040-29-3	*D*-Galacto-*D*-gluco-*D*-mannan		429b, 4249, 4583	
130.	644-76-8	β-*D*-Galactopyranose, 1,6-anhydro-	2321, 4249, 5811b		
131.	6118-79-2	2-*O*-α-*D*-Galactopyranuronosyl-*L*-mannose, 6-deoxy-		5811, 5811b	
132.	26656-33-7	*D*-Galactopyranuronic acid, homopolymer		4249	
133.	1948-54-5	Galactose, 2-amino-2-deoxy-		3797, 3974a, 4249	
134.	35381-83-0	Galactose, diether with 1,2,3-propanetriol (1:2)		908, 4249, 4640, 8A09	
135.	59-23-4	*D*-Galactose	3266, 4249, 5580	120, 158, 344a, 933, 1053, 1263, 2070, 2270, 2338, 2939, 3075, 3266, 3555, 3797, 3973, 3974a, 4249, 4411, 5079, 5114, 5768, 5785, 5811b	
136.	7535-00-4	*D*-Galactose, 2-amino-2-deoxy- {galactosamine}		3973, 4224, 4226, 4422, 5811b	
137.	1949-89-9	*D*-Galactose, 2-deoxy-		3075	
138.	97234-09-8	*D*-Galactoside, [(1-oxohexadecatrienyl)oxy] [(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249	
139.	97234-10-1	*D*-Galactoside, [(1-oxohexadecyl)oxy] [(1-oxooctadecatrienyl)oxy]propyl, (*Z,Z,Z*)-		4249	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

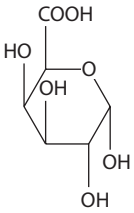
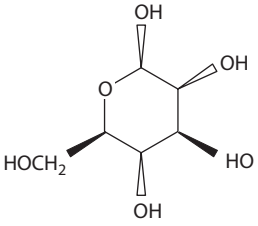
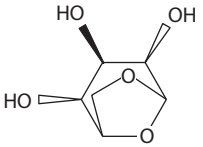
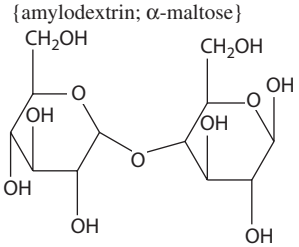
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
140.	97276-55-6	*D*-Galactoside, [(1-oxooctadecadienyl)oxy] [(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249	
141.	97232-94-5	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy] propyl *O*-*D*-galactosyl-, (all-*Z*)-		4249, 4570	
142.	97170-15-5	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl, (all-*Z*)-		4249, 4570	
143.	97233-43-7	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy] propyl *O*-*D*-galactosyl-, (all-*Z*)-		4249, 4570	
144.	97170-14-4	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249, 4570	
145.	97275-71-3	*D*-Galactoside, 2,3-dihydroxypropyl, 2′(or 3′)-hexadecanoate 3′(or 2′)-octadecadienoate, (*Z*,*Z*)-		4249	
146.	100092-00-0	Galactoxyloglucan {amyloid}		5811, 5811b	
147.	14982-50-4	Galacturonic acid 	2321, 4249	120, 344a, 722, 1263, 2079, 2939, 3107, 3555, 3797, 3973, 3974a, 4249, 5079, 5114, 5189, 5306	
148.	25990-10-7	Galacturonic acid, homopolymer		1051a, 1971, 4249, 5079, 5114	
149.	685-73-4	*D*-Galacturonic acid	2321, 4249	344a, 722, 2070, 2270, 2939, 3797, 4249, 5811b	
150.	34150-36-2	*D*-Galacturonic acid, anhydro-		4249, 4933	
151.	25249-06-3	*D*-Galacturonic acid, homopolymer		1051a, 1334e, 1971, 4249	
152.	9037-91-6	Glucan		842, 1102	
153.	9051-97-2	β-*D*-Glucan, (1→3)-		842, 1102, 4249	
154.	9012-72-0	β-(1,3)-*D*-Glucan {glucan}		5811	
155.	7425-74-3	β-*D*-Glucofuranose, 1,6-anhydro-	1883, 2939, 4249, 5811b	429b, 5811b	2466, 3402, 3405, 4249
156.	4451-30-3	β-*D*-Glucofuranose, 1,5:3,6-dianhydro-	5811, 5811a, 5811b	5811, 5811a, 5811b	
157.	66537-22-2	Glucometasaccharinic acid, γ-lactone	2493, 5811b	4249	
158.	492-62-6	α-*D*-Glucopyranose 		2079, 3667, 4249	
159.	492-61-5	β-*D*-Glucopyranose	5811b	2079, 3667, 4249	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
160.		α-*D*-Glucopyranose, 1-acetate 2,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
161.	28977-67-5	β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylvalerate) β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylpentanoate)	1352, 1373, 3251, 3278, 3286, 3302, 4249, 5811b	1352, 1373, 2338, 3185, 3215, 3473, 3535, 3542, 3560, 3561, 3607, 4249, 4575, 4990	
162.	60517-74-0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)		5811b	
163.	25545-13-5	*D*-Glucopyranose, 4-(4-hydroxybenzoate)		4249, 4915	
164.	23445-11-6	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)		4249, 4915	
165.	41682-52-4	β-*D*-Glucopyranose, 1-(3-phenyl-2-propenoate)		429b, 4249, 4915	
166.	59-56-3	α-*D*-Glucopyranose, 1-(dihydrogen phosphate)		120	
167.	498-07-7	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan} 	277, 568b, 1089a, 1351, 1354, 1364, 1371, 1375a, 1377, 1378, 1586, 1887a, 1971, 2170, 2270, 2493, 2524a, 2601a, 2607, 2761, 2762, 2765–2767, 2777, 2850, 2939, 3302, 3308, 3462, 3553, 3557, 3653, 3797, 3963, 4199, 4200, 4202, 4249, 5079, 5811b	568b, 2607, 3430, 3973, 4249, 5079, 5811b	1354, 1375a, 1377, 1378, 3402, 3405, 4249
168.	61891-55-2	β-*D*-Glucopyranose, 1,6-anhydro-, monoacetate	568b, 3553, 4249, 5811b		
169.	10139-18-1	α-*D*-Glucopyranose, 1,6-bis(dihydrogen phosphate)		429b	
170.	21056-52-0	β-*D*-Glucopyranose, 1-benzoate		4249, 4915	
171.	69-79-4 4482-75-1 9005-84-9	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin; α-maltose} 		120, 429b, 1063–1066, 1068–1074, 1835b, 2079, 2270, 2283, 3018, 3075, 3555, 3667, 3974a, 4249, 4411, 4841a, 5079, 5189, 5344, 5449, 5768, 5819	
172.		α-*D*-Glucopyranose, 1,2,3,4,5-penta((+)-3-methylbutanoate)		3556	
173.	133-99-3	β-*D*-Glucopyranose, 4-*O*-β-*D*-glucopyranosyl- {β-maltose}		429b, 2079, 3555, 3667, 3974a, 4249	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

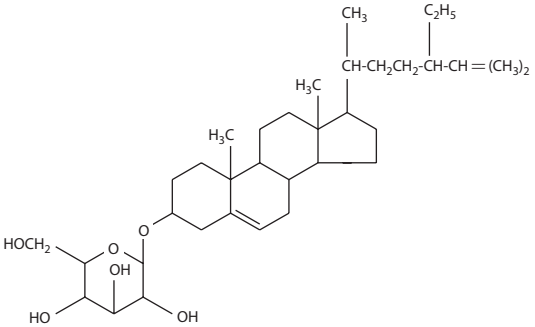
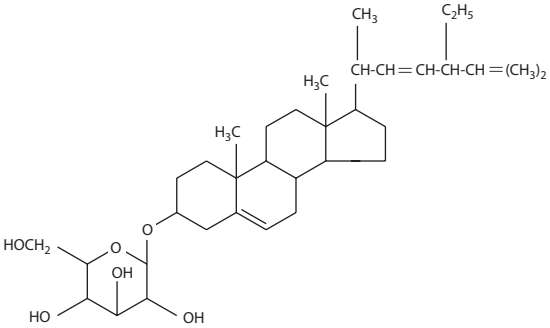
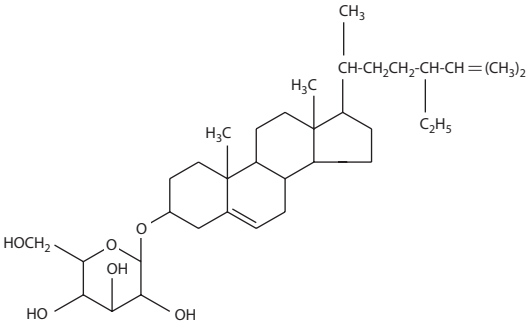
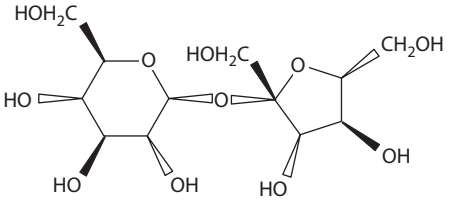
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
174.	64461-84-3	β-*D*-Glucopyranose, 6-(3-phenyl-2-propenoate)		3367a, 4249, 4915	
175.		α-*D*-Glucopyranose, 1,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
176.		α-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
177.		β-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
178.	7724-09-6	β-*D*-Glucopyranoside, (2-hydroxyphenyl)methyl-		4249, 4790	
179.	7073-61-2	β-*D*-Glucopyranoside, (3β)-cholest-5-en-3-yl {cholesteryl glucoside}	648, 1434, 4249, 4534	390, 4249	
180.	32214-82-7	β-*D*-Glucopyranoside, (3β)-ergost-5-en-3-yl- {campesteryl glucoside}	648, 2018, 2019, 2079, 3308, 3667, 4249	2019, 2018, 2019, 4249, 5777	
181.		β-*D*-Glucopyranoside, 3-hexen-1-yl- {3-hexen-1-yl glucoside; leaf acid glucoside}		740	
182.	474-58-8 20431-48-5	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl- {β-sitosteryl glucoside} 	648, 2018, 2019, 2939, 3296, 3302, 3308, 4249	1079, 2018, 2019, 2270, 2939, 3296, 3302, 3346, 3349, 4249	
183.	19716-26-8	β-*D*-Glucopyranoside, (3β,22E)-stigmasta-5,22-dien-3-yl- {stigmasteryl glucoside} 	648, 908, 2018, 2019, 2939, 3296, 3302, 3308, 4249, 4534	908, 2019, 2018, 2019, 3302, 3346, 3349, 4249	
184.	51064-38-1	β-*D*-Glucopyranoside, (3β,24S)-stigmast-5-en-3-yl- {γ-sitosteryl glucoside} 	2018	120, 2087, 3346, 4249	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
185.	57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose} 	1264, 1265, 1361, 4249, 5811b	71, 120, 172c, 248, 321b, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1264, 1265, 1289, 1361, 1933a, 1958, 1960, 1971, 2070, 2079, 2270, 2283, 2313a, 2337, 2532, 2818, 2911c, 2939, 2947c, 3059, 3075, 3266, 3370, 3398, 3409, 3449, 3461, 3462, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3973, 3974a, 3974b, 4249, 4411, 4990, 5079, 5108, 5109, 5126, 5189, 5449, 5562, 5679, 5692, 5748, 5768, 5811b, 5819, 5836, 5896	
186.	126-14-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate		1053, 3266	
187.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-		4990	
188.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-3′-acetyl-		4990	
189.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-4′-acetyl-		4990	
190.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-		4990	
191.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′-*O*-acetyl-		4990	
192.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-4′-*O*-acetyl-		4990	
193.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′,4′-*O*-diacetyl-		4990	
194.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-1′,3′,4′-*O*-triacetyl-		4990	
195.	470-55-3	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)-*O*-α-*D*-galactopyranosyl-(1→6)-		429b, 1971, 3797, 4249, 5811b	
196.	512-69-6	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)- {raffinose}		3075, 1971, 3797, 4249, 5768, 5811b	
197.	13101-54-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→4)- {erlose}		429b, 3667, 4249	
198.	25954-44-3	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-β-*D*-glucopyranosyl-(1→6)-		429b, 4249, 4460	
199.	98913-58-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 3-methylpentanoate		4249, 5811b	
200.	154063-13-5	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(2-methylbutanoate)		3606	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

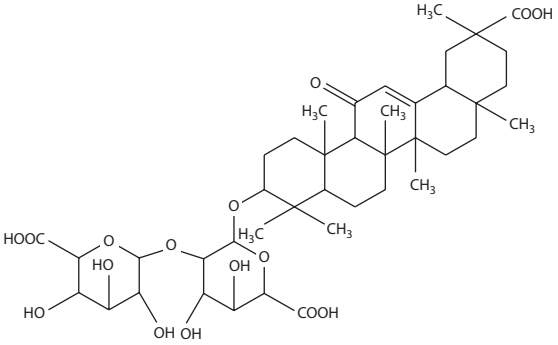
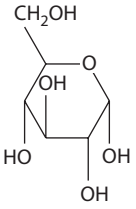
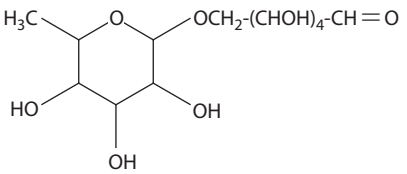
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
201.	97614-61-4	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(3-methylpentanoate)		3606, 5811b	
202.	106033-38-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, 6-acetate 2,3,4-tris(3-methylpentanoate), [2(S),3(S),4(S)]-		4249, 5811b	
203.	41055-68-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl, labeled with ^{13}C		4249, 4720	
204.	21291-36-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→6)-		429b, 3667, 4249	
205.	88848-61-7	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl 2-*O*-β-*D*-glucopyranosyl-, [1S-(1α,2β,3α,7β)]-		4249, 4716, 4717, 5811b	
206.	99499-89-5	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl *O*-6-deoxy-α-*L*-mannopyranosyl-(1→4)-*O*-β-*D*-glucopyranosyl-(1→4)-, [1S-(1α,2β,3α,7β)]-		4249, 5811b	
207.	138-52-3	β-*D*-Glucopyranoside, 2-(hydroxymethyl)phenyl-		4249, 4790	
208.	136448-99-2	β-*D*-Glucopyranoside, 2-[5-(acetyloxy)-1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl]-2-hydroxypropyl-, 2,3,4,6-tetraacetate, [2R-[2α(S*),5α,8β,8aα]]-		4249, 5811b	
209.	75039-16-6	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl-, mono(dihydrogen phosphate) (ester), (*E*)-		4249, 4813	
210.	62512-96-3	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)butyl-		4249	
211.	78081-83-1	β-*D*-Glucopyranoside, 3-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-1-methyl-2-propenyl-		4249, 4713	
212.	63648-83-9	α-*D*-Glucopyranoside, 3-*O*-acetyl-β-*D*-fructofuranosyl-		4249	
213.	470-57-5	α-*D*-Glucopyranoside, *O*-α-*D*-galactopyranosyl-(1→6)-β-*D*-fructofuranosyl- {theanderose}		3667, 4249	
214.	1464-44-4	β-*D*-Glucopyranoside, phenyl-		689a, 2527, 4249	
215.	1405-86-3	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid; glycyrrhizin} 		74e, 242, 743, 1356, 1361, 1671, 2313a, 3390, 3555, 4623, 5019, 5811b	
216.	53596-04-0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated 3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated; glycyrrhizin ammoniated}		172a, 174b, 1053, 3266	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
217.	50-99-7 26655-34-5	α-*D*-Glucose 	1264, 1265, 1352, 1360, 1361, 1371, 1375a, 1883, 1944, 2145, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	72, 120, 172c, 174b, 248, 321b, 480, 727, 840, 924, 933, 1053, 1063–1066, 1068–1074, 1077b, 1128a, 1141, 1142, 1264, 1265, 1289, 1352, 1361, 1835b, 1835d, 1863, 1916, 1933a, 1971, 2070, 2079, 2270, 2283, 2313a, 2338, 2339b, 2381, 2394a, 2532, 2704a, 2850, 2911c, 2913, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3913, 3973, 3974a, 4103, 4159, 4249, 4275, 4411, 4999, 5079, 5108, 5109, 5126, 5189, 5255, 5344, 5449, 5562, 5655, 5656, 5698, 5748, 5768, 5774, 5811b, 5819, 5831	1360, 1375a
218.	110187-42-3	Glucose, labeled with ^{13}C {Glucose- ^{13}C}		4249, 4720	
219.	9050-36-6	α-*D*-Glucose, labeled with ^{14}C {α-*D*-Glucose- ^{14}C}		1264, 1265, 5644, 25A30, 25A74	
220.	3416-24-8	*D*-Glucose, 2-deoxy-, 2-amino- {glucosamine}		1032, 1063–1066, 1068–1074, 2445a, 3705, 3797, 3973, 3974a, 4224, 4226, 4249, 4422, 5540, 5811b	
221.	1398-61-4	D-Glucose, β-(1,4)-2-acetamido-2-deoxy-		1102	
222.	90-74-4	*D*-Glucose, 6-*O*-(6-deoxy-α-*L*-mannopyranosyl)- {rutinose} 		1971. 5777, 5811	
223.	28905-12-6	β-*D*-Glucose	1354, 1360, 1375a, 2761, 2762, 2765, 2766, 2777	3667, 4275	1354, 1360, 1375a
224.	37294-28-3	Glucoxylan		4249	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

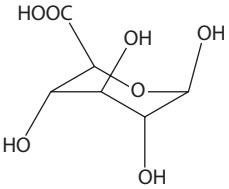
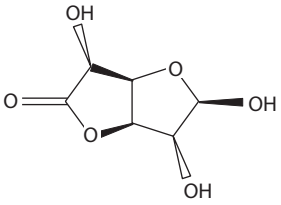
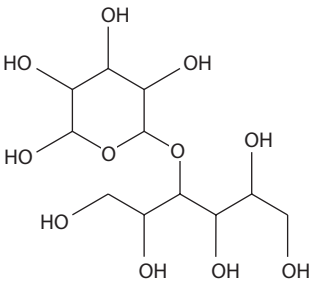
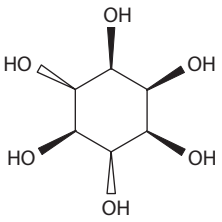
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
225.	576-37-4	Glucuronic acid 	312, 4249	120, 2070, 2939, 3973, 4249, 4360a, 5079, 5478, 5706, 5785	
226.	6556-12-3	*D*-Glucuronic acid		5811	
227.	14984-34-0	*D*-Glucuronic acid, monosodium salt		5811b	
228.	28905-07-9	α-*D*-Glucuronic acid, methyl ester		4249	
229.	66369-21-9	Glucuronoarabinoxylan		5811	
230.	32449-92-6	*D*-Glucurono-3,6-lactone 	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249		1360, 1375a
231.	62930-75-0	Glucuronomannan		2042a, 4249	
232.	77272-02-7	Glucuronomannoarabinan		4249, 4428	
233.	37317-38-7	Glucuronoxylan		5811	
234.	9034-32-6	Hemicellulose		120, 385, 385a, 842, 1838, 1887, 2056, 2154, 2283, 2850, 2939, 3059, 3372, 3665a, 3702, 3973, 4249, 5079, 5189, 5344, 5811b	
235.	63100-39-0	Hemicellulose A		120, 3973, 4249	
236.	63100-40-3	Hemicellulose B		120, 3973, 4249	
237.	65058-12-0	Hemicellulose C		3973, 4249, 4805	
238.		Heptose		5777	
239.	50-70-4	Hexane, hexahydroxy- {sorbitol; glucitol} $HOCH_2$-$(CHOH)_4$-CH_2OH	627, 1360, 1375a, 1586, 2761, 2762, 2765–2767, 2777, 2850, 5580	120, 174b, 627, 773, 933, 1221, 1971, 2079, 2195, 2705, 2939, 3075, 3163, 3264, 3266, 3667, 3797, 3973, 3974a, 5079, 5180, 5216, 5811b	1360, 1375a

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

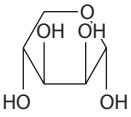
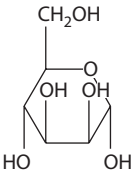
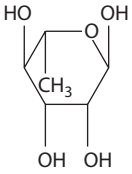
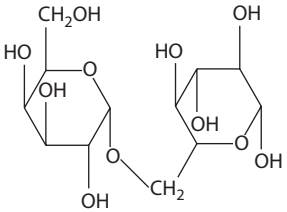
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
240.	585-88-6	Hexane, hexahydroxy-, 4-*O*-β-*D*-glucopyranosyl-{maltitol; 4-*O*-β-*D*-glucopyranosyl-*D*-glucitol} 		3163	
241.		Hexane, hexahydroxy-, 2,6-di-*O*-methyl-		3669	
242.		Hexane, hexahydroxy-, 2,3,6-tri-*O*-methyl-		3669	
243.		Hexane, hexahydroxy-, 2,3,4,6-tetra-*O*-methyl-		3669	
244.	45009-62-9	Hexoses		429b, 3430	
245.	8064-26-4	Holocellulose		3702, 3973, 4249, 4261, 4262, 4573	
246.		Hydropectin		102, 5079, 5114	
247.	6917-35-7	Inositol	966, 1354, 1360, 1375a, 2761, 2762, 2765, 2766, 2777, 2939, 3302, 3876, 4249, 5580	120, 840, 2079, 2270, 2283, 2704, 2939, 2947b, 3075, 3656, 3797, 3876, 4249, 5079, 5189, 5383, 5384, 5595, 5768, 5852	1354, 1360, 1375a
248.	87-89-8	myo-Inositol 	1572, 5811b	1572, 3667, 3974a, 4249, 4427, 5811b	
249.	71608-14-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]octadecyl hydrogen phosphate], disodium salt		429b, 1838, 4249	
250.	71608-17-8	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-1-[(2-hydroxy-1-oxopentacosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
251.	71608-15-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
252.	71608-16-7	myo-Inositol,*O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4- dihydroxy-2-[(2-hydroxy-1-oxotetracosyl) amino]octadecyl hydrogen phosphate], disodium salt		429b, 1838, 4249	
253.	71608-19-0	myo-Inositol,*O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl) amino]- 8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
254.	71608-20-3	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
255.	71608-21-4	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		429b, 1838, 4249	
256.	71608-22-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-,1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxopentacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
257.	71608-23-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxohexacosyl) amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
258.	89194-80-9	myo-Inositol, *O*-*D*-glucopyranosyl-		3667, 4249	
259.	49741-70-0	*D*-myo-Inositol, *O*-*D*-glucopyranosyl-		429b, 3667, 4249	
260.		myo-Inositol, phosphatidyl-		3973, 4249	
261.	63-42-3	Lactose		933, 1361, 1835b, 3075, 5079, 5811b	
262.	9005-53-2	Lignin		71, 120, 216, 277, 337, 385, 385a, 420, 535, 539, 598, 722, 1102, 1063–1066, 1068–1074, 1077, 1077b, 1289, 1329, 1361, 1485, 1887, 2014, 2043, 2046, 2079, 2270, 2283, 2338, 2356, 2454, 2529, 2543, 2545, 2765, 2766, 2914, 2939, 2947c, 3029, 3059, 3087, 3305, 3372, 3428, 3429a, 3430, 3449, 3450, 3462, 3468, 3476, 3702, 3797, 3974a, 3984, 4159, 4249, 4364, 4418, 5079, 5189, 5344, 5811b	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

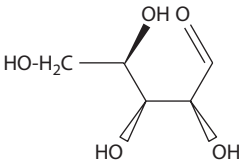
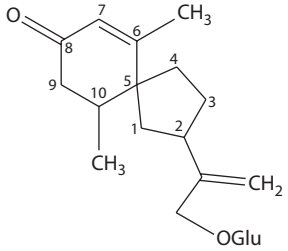
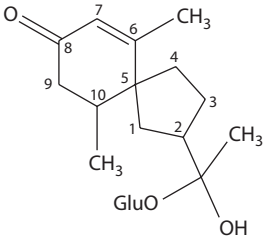
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
263.	1114-34-7	Lyxose 	5580	3075	
264.	69-65-8	*D*-Mannitol {cordycepic acid} $HOCH_2$-$(CHOH)_4$-CH_2OH	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249, 5580	312, 1360, 2761, 2777, 3075, 3555, 3973, 4249, 5811b	1360, 1375a
265.	31103-86-3	Mannose 	1587, 2761, 2762, 2765, 2766, 2777, 3266, 3555, 4249	1053, 2070, 3266, 3555, 3797, 3973, 3974a, 4249, 5768	
266.	3458-28-4	*D*-Mannose {seminose}	1360, 1375a, 2765, 2766, 4249	3797, 4249, 5811b	1360, 1375a
267.	14307-02-9	*D*-Mannose, 2-amino-2-deoxy-		1063–1066, 1068–1074, 1370, 4249, 4422, 5811b	
268.	3615-41-6	*L*-Mannose, 6-deoxy- {α-rhamnose} 	3555, 5580	71, 120, 158, 344a, 2070, 2079, 2270, 2338, 2704a, 2939, 3075, 3555, 3655b, 3797, 3973, 3974a, 4249, 5079, 5698, 5768, 5811b, 5831	
269.	585-99-9	Melibiose 		3075	
270.	105300-09-2	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 1a-[(β-*D*-glucopyranosyloxy)methyl]octahydro-5,7b-dimethyl-		4249, 5811b	
271.	125537-96-4	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 3-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,3β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
272.	125537-95-3	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 4-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-,[1aS-(1aα,2β,4β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
273.	105300-10-5	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 5-[(β-*D*-glucopyranosyloxy)methyl]octahydro-1a,7b-dimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

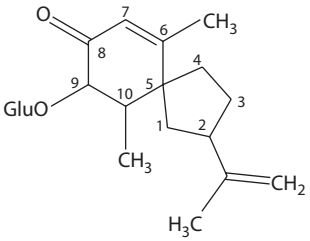
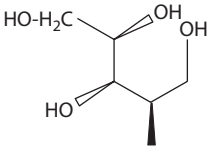
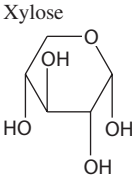
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
274.	88848-60-6	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 6-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy] octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,6β,7aα,7bα)]-		4249, 4717, 5811b	
275.	9046-40-6	Pectic acid		120, 925, 2270, 2947c, 3492, 3973, 4249, 5079, 5114, 5189, 5306, 5419	
276.		Pectic acid, labeled with ^{14}C {pectic acid-^{14}C}		2764	
277.		Pectic acid, calcium magnesium salt		1971, 5777	
278.	65028-58-2	Pectic acid, magnesium salt		1971, 2939, 4249	
279.	9000-69-5	Pectin		120, 172, 174b, 176, 248, 344a, 385, 385a, 535, 722, 1063–1074, 1077, 1263, 1289, 1361, 1435a, 1887, 1933a, 2070, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2851, 2939, 2947c, 3029, 3042, 3059, 3266, 3305, 3372, 3429, 3450, 3468, 3551, 3651, 3665a, 3702, 3767, 3797, 3871, 3973, 3974a, 3974b, 4151, 4249, 4279, 4396, 4999, 5079, 5114, 5189, 5234, 5306, 5344, 5811b, 5831	
280.		Pectin, labeled with ^{14}C {pectin-^{14}C}		2874	
281.	9047-18-1	Pectinic acid		120, 344a, 925, 1263, 2270, 2337, 2338, 3702, 3973, 3974b, 5079	
282.	116001-96-8	Pentosan		2154, 2947c, 5079. 5194, 5234	
283.		Pentose		1971, 5079, 5189, 5306, 5344, 5777	
284.	533-67-5	*D*-erythro-Pentose, 2-deoxy- {deoxyribose}		1351, 3079, 3973, 3974a, 4249, 5811b	
285.	5962-29-8	*D*-erythro-2-Pentulose {xylulose} = *D*-ribulose 488-84-6 $HOCH_2$-CO-$(CHOH)_2$-CH_2OH		429b, 4249, 4712a	
286.	24218-00-6	*D*-erythro-2-Pentulose, 1,5-bis(dihydrogen phosphate)		4249	
287.	62137-28-4	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-,*trans*-		4249, 4429	
288.	62137-29-5	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-		4249, 4429	
289.	551-68-8	*D*-Psicose $HOCH_2$-CO-$(CHOH)_3$-CH_2OH		3667, 4249	

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
290.	56159-42-3	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-		4249, 4603	
291.	38477-23-5	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-		4249, 4603	
292.	54538-20-4	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-		4249, 4620	
293.	90-80-2	2*H*-Pyran-2-one, tetrahydro-6-hydroxymethyl, 3,4,5-trihydroxy {gluconic acid, δ-lactone}	1360, 4249		
294.	5328-43-8	Rhamnitol $H_3C\text{-}(CHOH)_4\text{-}CH_2OH$		3669	
295.		Rhamnitol, 2,4-di-*O*-methyl-		3669	
296.		Rhamnitol, 3,4-di-*O*-methyl-		3669	
297.		Rhamnitol, 3-*O*-methyl-		3669	
298.		Rhamnitol, 2,3,4-tri-*O*-methyl-		3669	
299.	39280-21-2	(1→2)-*L*-Rhamno-(1→4)-α-*D*-galacturonan		5811, 5811b	
300.	3615-55-2	Ribose, 5-(dihydrogen phosphate)		429b, 4249, 4670	
301.	50-69-1	*D*-Ribose  	5580	120, 344a, 2939, 3075, 3254, 3797, 3973, 3974a, 4249, 5811b	
302.	24259-59-4	*L*-Ribose		3075	
303.	62574-27-0	Spiro[4.5]dec-6-en-8-one, 2-[1-[(β-*D*-glucopyranosyloxy) methyl]ethenyl]-6,10-dimethyl-  		77, 1156, 4090, 4249	
304.	62574-29-2	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-  		77, 1156, 4090, 4249	
305.	62623-87-4	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-		77, 1156, 4090, 4249	

(*continued*)

TABLE 8.3 (continued)
Carbohydrates in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
306.	62574-25-8	Spiro[4.5]dec-6-en-8-one, 9-(β-*D*-glucopyranosyloxy)-6,10-dimethyl-2- (1-methylethenyl)-, [5S-[5α(S*),9α,10β]]- 		77, 1156, 4090, 4249	
307.	9005-25-8	Starch	5811b	69, 120, 248, 385, 385a, 420, 535, 677b, 722, 963, 1063–1066, 1068–1074, 1266, 1267, 1289, 1329, 1330, 1333, 1933a, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2394a, 2395, 2529, 2543, 2545, 2688, 2761, 2762, 2764–2766, 2914, 2939, 2947c, 3059, 3087, 3334, 3372, 3450, 3551, 3592, 3797, 3871, 3973, 3974a, 3974b, 4249, 4261, 4262, 4275, 5079, 5108, 5109, 5126, 5189, 5194, 5298, 5344, 5449, 5468, 5767, 5811b, 5831, 5843, 5866, 5896	
308.	39341-47-4	Starch, labeled with ^{13}C {starch-^{13}C}		976a, 4249, 4720	
309.	70226-57-2	Starch, labeled with ^{14}C {starch-^{14}C}		2764	
310.	99-20-7	Trehalose		3075	
311.	9014-63-5	Xylan		842, 2070, 2850, 2939, 3371, 3666, 3797, 3973, 3974a, 4249, 5811b	
312.		Xylan, 4′-*O*-methylglucuronyloxy)-		4249, 4584	
313.	87-99-0	Xylitol 	5580	3075	
314.	25990-60-7	Xylose 	2145, 2939, 3302, 4249, 5580, 5811, 5811a, 5811b	120, 2070, 2270, 3079, 3797, 3973, 3974a, 4249, 5768, 5785, 5811, 5811a, 5811b	
315.	31178-70-8	α-*D*-Xylose		3075, 3667, 3973, 3974a, 4249	
316.	31178-71-9	β-*D*-Xylose		3667, 3973, 3974a, 4249	

detail the 1979 findings of Mizusaki et al. (2568) on the effect of the cigarette smoke condensate (CSC) from high-sugar tobacco (20%–30%) *vs.* the CSC from low-sugar tobacco (5%) in the Ames test (*Salmonella typhimurium* strain TA1538). The high-sugar tobacco CSC was much less mutagenic than the low-sugar tobacco CSC. DeMarini (933) also summarized the results of a study by Sato et al. (8A05) in which various sugars were added to the tobacco in high-"tar" and low-"tar" cigarettes, the CSCs collected, and tested for mutagenicity in the Ames test with *S. typhimurium* TA98 and TA100, with and without activation. The sugars tested included glucose, fructose, galactose, lactose, sucrose, and sorbitol. The mutagenicity of the CSC from the sugar-treated high-"tar" cigarettes was reduced 35% from the mutagenicity observed for the CSC from the untreated tobacco cigarette. The mutagenicity of the CSC from the low-"tar" cigarettes was reduced 36% from mutagenicity of the CSC from the untreated tobacco cigarette.

In the National Cancer Institute study of the third set of cigarettes, Gori (1332) reported the effect of adding invert sugar at a level approximating that used commercially to the Standard Experimental Blend III (SEB III) [see Table 8, p. 99, cigarette 81 in (1332)] on the per cigarette MSS yields of numerous smoke components, including formaldehyde, acetaldehyde, and acrolein [see Table 8, p. 59 in (1332)]. The multiple samples of SEB III yielded an average of 33.8 µg/cig of formaldehyde, 1212 µg/cig of acetaldehyde, and 110 µg/cig of acrolein. Cigarette 81, fabricated from SEB III with added invert sugar, yielded 32.3 µg/cig of formaldehyde, 1090 µg/cig of acetaldehyde, and 113 µg/cig of acrolein. Dermal assays were initiated with 100 ICR Swiss female mice in each group. Multiple samples of CSC from SEB III at 12.5 and 25.0 mg doses produced 27 and 47 tumor-bearing animals (TBA), respectively [see Table 2, p. 86 in (1332)], whereas the CSC from the invert sugar-treated SEB III at 12.5 and 25.0 mg doses produced 19 and 41 TBA, respectively [see Table 3, p. 87, cigarette 81 in (1332)]. However, the CSCs studied would be devoid of formaldehyde, acetaldehyde, and acrolein because of their vaporization during the collection, solution preparation, and administration of the CSCs.

Table 8.3 lists the carbohydrates and their derivatives identified to date in tobacco, tobacco smoke, and tobacco substitute smoke. Of the 316 identified carbohydrates listed, most of them are tobacco components: 310 have been identified in tobacco *vs.* only 44 in smoke; 38 have been identified in both tobacco and tobacco smoke.

9 Phenols and Quinones

9.1 PHENOLS

Examination of the extensive literature on the composition of tobacco smoke reveals that considerable effort was expended in the early 1960s in defining the nature of the phenolic components of tobacco smoke. Subsequently, even though the identity of many phenols in tobacco smoke is now known, research has indicated their identified number in tobacco smoke is much fewer than the number of identified polycyclic aromatic hydrocarbons (PAHs).

With the tremendous effort expended on the identification of PAHs and some of their nitrogen analogs in tobacco smoke, what series of events triggered the interest in and the emphasis on phenols in tobacco smoke in the early 1960s?

The reports by Wynder et al. (4306a, 4306c) in the early 1950s that cigarette smoke "tar" or cigarette smoke condensate (CSC) was tumorigenic to mouse skin prompted an intense search for the responsible component(s). Initially, the PAHs were selected for investigation because of the wealth of chemical and biological data generated on a great number of them following the synthesis of dibenz[*a,h*]anthracene (DB[*a,h*]A) in 1929 (760, 1184), the isolation of benzo[*a*]pyrene (B[*a*]P) from coal tar in 1932 (796a, 797), and the demonstration of the potent tumorigenicity of both of them to mouse skin (194, 2078). Almost immediately after the report by Wynder et al. (4306a) of the mouse-skin-painting results with tobacco "tar," the PAHs were proposed by some investigators to be the major tumor initiators in CSC. Because of its level in CSC and its potency in mouse-skin tumorigenesis, B[*a*]P was defined as the most significant of the PAHs in tobacco smoke.

However, it was soon recognized that neither the B[*a*]P content nor its tumorigenicity could explain the biological response observed in the mouse-skin-painting bioassay. Similarly, neither the total content of the PAHs tumorigenic to mouse skin nor their summed tumorigenicities could explain the observed biological response. In fact, it was pointed out repeatedly over the next several decades that the levels of B[*a*]P and other tumorigenic PAHs in CSC accounted for less than 3% of the observed tumorigenicity [Wynder and Wright (4353, 4354), Wynder and Hoffmann (4307, 4308, 4312, 4317, 4319, 4332, 4342) Druckrey (1056), Roe (3310, 3311), USPHS (3999, 4005, 4009, 4010) Lazar et al. (2320), Stedman (3797), Selikoff et al. (3584a), Coultson (830)].

As early as the mid-1950s, Wynder and Wright (4353) noted that the concentration of B[*a*]P in cigarette tar was insufficient to account for its observed carcinogenicity to mouse epidermis: "The concentration in which benzo[*a*]pyrene seems to be in cigarette tar is insufficient to account for the observed carcinogenic activity to mouse epidermis."

At the 1957 Blatnik Committee hearings, Wynder reported Wright's opinion (4282a) on the subject as well as his own (4296). Wynder noted that much attention had been directed at the PAH B[*a*]P. So much in fact that, as Wynder stated, B[*a*]P had become an issue in itself because it was one of the known tumorigenic substances and everyone tried to blame everything on it alone. During his testimony, he also noted that his Sloan Kettering group had repeatedly stated that the amount of B[*a*]P in tobacco "tar" was insufficient to explain the animal results published by his group. He added that cigarette "tar" contained numerous other B[*a*]P-related compounds much more active than B[*a*]P and they most likely accounted for the majority of the activity, and it was more or less academic whether it was B[*a*]P or a dibenzopyrene or a dibenzanthracene or a substituted B[*a*]P because they were all formed in the same manner during the tobacco smoking process. That same year, Wynder and Wright (4354) wrote that, to that date, no carcinogens had been identified in large enough quantities in tobacco "tar" or its fractions to account for the observed activity in mouse-skin-painting studies:

> We have demonstrated experimentally … that 0.0001 per cent or even 0.0005 per cent benzopyrene in acetone will not produce any tumors in the present experimental mouse or rabbit groups. Thus, there is conclusive proof that the animal results cannot be solely due to the benzopyrene content of tobacco [sic].
>
> The benzpyrene content of the total tar as well as the active fractions is far too low to account alone for the positive results [in laboratory animal]. So far, no carcinogens have been identified in large enough quantity in tobacco tar or its fractions to account for the observed activity.

These Wynder–Wright results led to an intensive but unsuccessful 18-month search for a "supercarcinogenic" PAH by Wright. The absence of such a PAH was subsequently confirmed by the USDA group at Athens, GA [Snook (3732), Snook et al. (3756–3758)], by their identification of over 500 PAHs in the PAH fraction from cigarette mainstream smoke (MSS), an identification procedure that completely accounted for the fraction in the cigarette smoke studied.

In 1959, unable to explain the bioassay (mouse-skin-painting) results with CSC on the basis of either its B[*a*]P content (less than 2% explainable) or its total tumorigenic PAH content (less than 3% explainable), Wynder and Hoffmann (4307) added the concept of promotion by low-molecular-weight phenols to the concept of tumor initiation by PAHs in an attempt (unsuccessful) to explain the bioassay results:

A similar comment that the amount of tumorigenic PAHs found in CSC could not by themselves account for the total biological activity observed was included in a more detailed publication (4307). They also stated (4308) that the higher PAHs played an important role in the carcinogenicity of CSC but when the various known

concentrations of the carcinogenic PAHs, as estimated in CSC, were summed, it was obvious that they could not account for the established carcinogenicity of the CSC nor of its isolated PAH fraction:

> Several carcinogenic higher aromatic polycyclic hydrocarbons [are] present in tobacco smoke condensate. They include benzo[*a*]pyrene …, benzo[*e*]pyrene …, chrysene …, benz[*a*]anthracene …, dibenz[*a,h*]anthracene …, and dibenzo[*a,i*]pyrene… From the amount in which these materials have been found in tobacco smoke condensate it was evident that these, by themselves, could not account for the total biological activity observed.

In 1960, Van Duuren et al. (4027) reported the identification of several aza-arenes (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, dibenzo[*c,g*]carbazole) not only structurally similar to some of the known tumorigenic PAHs in CSC but also tumorigenic under certain conditions to mouse skin. Adding this class of tumorigenic cigarette smoke components to the assessment of the tumorigenicity of CSC failed to account for more than a few percent of the observed response.

However, it should be noted that Candeli et al. (587) could not confirm the findings of Van Duuren et al. on the presence of these three aza-arenes in cigarette MSS. During the next three decades, other research groups, as shown in Table 9.1, in Germany, Japan, and the United States were also unable to confirm the presence in cigarette MSS of dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and dibenzo[*c,g*]carbazole.

Wynder and Hoffmann (4312) wrote that the PAHs in CSC accounted for not more than 3% of the total biological activity observed in mouse-skin bioassays:

> The polynuclear aromatic hydrocarbons are mainly formed during the combustion of tobacco. The tobacco of our standard cigarettes contains only very minute quantities of benzo(a)pyrene (0.02 ppm). A bioassay indicates that these polycyclic hydrocarbons of the condensate by themselves, however, can account for not more than 3 per cent of the total biological activity.

They also wrote (4313) that the established carcinogenicity of CSC to mouse epidermis could to a great extent be accounted for on the basis of initiating carcinogens, largely PAHs, and promoting substances, a major group of which was the phenols. This statement was not true in 1961, nor is it true now.

Wynder and Hoffmann (4314), unable to explain the mouse-skin-painting bioassay results with CSC on the basis of its content of tumorigenic PAHs and aza-arenes, promoting and/or cocarcinogenic phenols, and promoting and/or cocarcinogenic nontumorigenic PAHs, added the concept of ciliastasis in an attempt (unsuccessful) to explain cigarette smoke tumorigenicity in smokers' lungs.

In their lengthy 1964 review of tobacco carcinogenesis, Wynder and Hoffmann (4319) stated that no one could deny that tobacco products were tumorigenic even though no single component in tobacco smoke could by itself or jointly with other components account for the observed tumorigenic activity of such tobacco products to the skin of laboratory animals:

> It is furthermore true that none of the agents is carcinogenic in the concentrations in which they are present in tobacco products.

Wynder and Hoffmann (4332) expressed similar views on the tumorigenicity of tobacco smoke components in their

TABLE 9.1
Dibenz[*a,h*]acridine (I), Dibenz[*a,j*]acridine (II), and 7*H*-Dibenzo[*c,g*]carbazole (III) in Nicotine Pyrolysates (Pyr) and Mainstream CSC

	Dibenz[*a,h*]acridine		Dibenz[*a,j*]acridine		7*H*-Dibenzo[*c,g*]carbazole	
Investigators	**Pyr**	**CSC**	**Pyr**	**CSC**	**Pyr**	**CSC**
Van Duuren et al. (4027)	Yes	Yes	Yes	Yes	No	Yes
Candeli et al. (587); Wynder and Hoffmann (4319, 4332)	NE	No	NE	Yes	NE	NE
Kaburaki et al. (2006)	No	NE	No	NE	NE	NE
Schmeltz et al. (3499)	No	NE	No	NE	No	NE
Schmeltz et al. (3512)	No	No	No	No	No	No
Snook (3733)	NE	No	NE	No	NE	No
Snook et al. (3750)	NE	No	NE	No	NE	No
Grimmer et al. (1409)	NE	No	NE	No	NE	No
Kamata et al. (2021)	NE	No	NE	No	NE	NE
Sasaki and Moldoveanu (3414)	NE	No	NE	No	NE	NE
Rustemeier et al. (3370)	NE	No	NE	Yes	NE	NE

Yes, compound identified; No, compound not found or identified; NE, substrate not examined for compound in question.

Examination of these results indicates that Van Duuren et al. (4027) reported the identification of the three *N*-heterocyclic compounds (I, II, and III) in MS CSC and two of them (I and II) in a nicotine pyrolysate, whereas Candeli et al. (587) failed to identify I but did identify II in MS CSC. The 1963 Candeli et al. findings on II in MS CSC were not confirmed in 1979 by investigators (3512) from the same laboratory: Hoffmann was a participant in both the 1963 and 1979 studies. Two studies (3499, 3512) confirmed the 1960 report by Van Duuren et al. that 7*H*-dibenzo[c,g]carbazole (III) was not present in a nicotine pyrolysate.

1967 book, but they continued to maintain that the PAHs in cigarette smoke were important as tumor initiators:

> While BaP and other carcinogenic PAH can by themselves account for only a small portion of the total tumorigenic activity of cigarette smoke condensate, probably less than 2%, they are, nevertheless, of obligatory importance as tumor initiators.

The next year, Wynder and Hoffmann (4342) wrote: "Carcinogenic polynuclear hydrocarbons in the concentrations present in tobacco 'tar' clearly do not, by themselves, account for the observed carcinogenicity."

On several occasions, the U.S. Surgeon General in his periodic reports on smoking and health discussed the relationship between the levels of PAHs in cigarette smoke, their tumorigenic potency to mouse skin, and the observed biological response with CSC in mouse-skin-painting bioassays:

> The results of a number of such assays [mouse skin-painting] present a puzzling anomaly: the total tar from cigarettes has about 40 times the carcinogenic potency of the benzo(a)pyrene present in the tar. The other carcinogens known to be present in tobacco smoke are, with the exception of dibenzo(a,i) pyrene, much less potent than benzo(a)pyrene and they are present in smaller amounts. Apparently, therefore, the whole is greater than the sum of the known parts. [see p. 58 in (3999)]
>
> Benzo(a)pyrene is present in much larger concentrations than is any other carcinogenic polycyclic hydrocarbon. The inability to account for the carcinogenicity of the tobacco products, except to a very minor degree, by the amount of benzo(a)pyrene present was unanticipated. Both Druckrey (1056) and Wynder (4300) emphasized that the benzo(a) pyrene concentration of various tobacco and smoke preparations is only sufficient to account for a very small part of the carcinogenicity of these materials. [see pp. 144–145 in (3999)]
>
> PAH alone, however, account for only a small portion of the carcinogenicity of tobacco 'tar'… The levels of carcinogenic PAH in tobacco smoke are well below their practical threshold as complete mouse skin carcinogens… (see 4005)
>
> The contribution of BaP or PAH in general to mouse skin carcinogenesis by cigarette smoke condensate cannot be fully measured at this time. Wynder and Hoffmann [1967] found a correlation between BaP levels and carcinogenicity of smoke condensates from several types of cigarettes. A much larger series of experimental cigarettes was studied in the smoking and health program of the National Cancer Institute. No significant dependence of carcinogenic potency on BaP content was observed [Gori (1329, 1330, 1332, 1333), NCI (2683)]. (see 4009)

The carcinogenic activity of the particulate matter of tobacco smoke in epithelial tissues of laboratory animals is greater than the sum of the effects of the known carcinogens present [(see 4010); cf. the comment in the 1964 Advisory Committee Report to the Surgeon General]. Apparently, therefore, the whole is greater than the sum of the known parts (3999).

In 1980, Coultson (830) commented on the decades of attention on B[*a*]P in cigarette MSS and its supposed relevance in cigarette smoke-induced cancers:

> Whether it's benzo[*a*]pyrene or not, nobody really knows. More work has been done on benzo[*a*]pyrene to prove it to be the causative agent in cigarette smoking than I think on any other chemical for any disease that I know. And yet the point is, you can't prove it.

The failure of PAHs to explain no more than a few percent of the tumorigenicity of CSC led to the inclusion of the concept of promotion in the overall equation. As noted previously, Wynder and Hoffmann (4313) asserted that the established carcinogenicity of CSC on mouse epidermis could to a great extent be accounted for on the basis of initiating carcinogens, largely PAHs, and promoting substances, a major group of which was the phenols. Their assertion was incorrect in 1961, and it is incorrect today.

In his listing of reported identified tobacco smoke components (Table 9.2), Kosak (2170) listed published reports on two simple phenols, the early reports on phenol by Wenusch (4202) and Ikeda (1857) and on catechol (1,2-benzenediol) by Kissling (2107) and Wenusch (4202), but he questioned the identification of phenol. Kosak also cited earlier reports by Thoms (3912) and McNally (2524) who mentioned the presence of "phenols" in tobacco smoke and Roffo (3324) who mentioned the presence of phenolic acids. However, it should be remembered that Roffo's 1939 studies dealt with a destructive distillate from tobacco, not with tobacco smoke generated in a tobacco smoking process simulating that used by human smokers.

Table 9.3 summarizes 1954 listing by Kosak of phenolic components reported in tobacco smoke, the year of the report, the investigators involved.

However, critical examination of the chronology of the pre-1954 investigations of phenolic compounds in tobacco smoke reveals that Kosak's 1954 publication suffers from several deficiencies with regard to reports on this class of tobacco smoke components. The examination indicates that his manuscript was submitted to the journal *Experientia* in September 1953, accepted for publication shortly thereafter, and appeared in a February 1954 issue of the journal. One of the significant omissions was the report by Rayburn and his colleagues at the Research Department of the American Tobacco Company: At the *6th Tobacco Chemists' Research Conference* (TCRC) in December 1952, Rayburn (3089) described the unequivocal identification of four low-molecular-weight phenols in the MSSs from a series of cigarettes, each member of the series fabricated from one of the four major tobacco types (flue-cured, burley, Maryland, Oriental). The phenols identified were phenol, guaiacol (2-methoxyphenol), *o*-cresol (2-methylphenol), and *m*-cresol (3-methylphenol). The next year, these results were published by Rayburn et al. in the journal *Analytical Chemistry* (3090).

In Table 9.4 literature references are listed for phenolic components in tobacco smoke cited by Kosak (2170) plus several pertinent references not included in his publication.

The report of the possible presence of phenol-like compounds in Oriental tobacco by Jones and Latimer (1980) at RJRT R&D eventually prompted a research project to synthesize a series of phenols in an attempt to find one or more which would impart a pleasant leatherlike aroma to cigarette smoke (3235a, 3240a). Some 20 phenols were synthesized. However, none was ever used commercially as a tobacco

TABLE 9.2
Tobacco Smoke Components Listed by Kosak (2170)

Class	Component	Class	Component	Class	Component
Hydrocarbons	Hentriacontane (?)	Ketones	3-Pentanone	Acids	Formic acid
	Acetylene		4-Heptanone		Acetic acid
	"Unsaturated hydrocarbons"		17-Tritriacontanone (?)		Butyric acid
	Azulene		2,3-Butanedione		Valeric acid
	Phenanthrene (?)		"Higher" ketones (?)		Caproic acid
	Anthracene (?)				C_7 and C_8 aliphaticacids (?)
	Benzopyrene (?)				Succinic acid (?)
	"Condensed aromatics" (?)				Fumaric acid (?)
					Citric acid (?)
					Benzoic acid (?)
					Phenolic acids (?)
Alcohols and phenols	Methanol	Alkaloids	Nicotine	Miscellaneous components	Levoglucosan[c]
	Glycerol Diethylene glycol[a]		Pyridyl ethyl ketone		"Phytosterol" (?)
	Ethylene glycol[a]		Myosmine		$C_{10}H_{14}O$ (a furan ?)
	Phenol (?)		Nicotyrine		"Resins" (?)
	Catechol (?)		α-Socratine[b]		"Resin acids" (?)
			β-Socratine[b]		
			γ-Socratine[b]		
			Obelin[b]		
			Lohitam[b]		
			Anodmin[b]		
			Lathraein[b]		
			Poikiline[b]		
			Gudham[b]		
Aldehydes	Formaldehyde	Other *N*-containing components	Pyrrole (?)	Inorganic components	Ammonia
	Acetaldehyde		"Pyrroles" (?)		Carbon monoxide
	Butyraldehyde		"*N*-Methyl-Pyrrolidines" (?)		Carbon dioxide
	Acrolein (?)				Hydrogen cyanide
	Benzaldehyde		Pyridine		Hydrogen sulfide
	2-Furaldehyde (?)[d]		"Picoline" (?)		Thiocyanic acid (?)
			"Lutidine" (?)		Oxygen
			"Collidine" (?)		Arsenic[e]
			"Pyridine bases" (?)		"Acetates" (?)
			Methylamine (?)		"Chlorides" (?)
			"Chlorophyll degradation products" (?)		"Cyanides" (?)
					"Nitrates" (?)
			"Uric acids" (?)		

[a] In smoke because of transfer of an humectant added to tobacco.
[b] Subsequent study demonstrated this component was not a well-defined compound but an artifact, a mixture, or an ammonium salt [see discussion by Johnstone and Plimmer (1971)].
[c] 1,6-Anhydro-β-*D*-glucopyranose.
[d] The question mark indicates that Kosak did not consider the evidence in the literature to be definitive proof of the identity of the component.
[e] Probably present as As_2O_3.

flavorant nor in any extensive in-house panel tests for the following reasons:

During the course of his initial research project (3235a, 3240a) at RJRT R&D, Rodgman suggested the possibility of the conversion of several of the phenols to a quinone during the smoking process. This suggestion, coupled with the reports by Takizawa (3865a) that several simple quinones such as *p*-benzoquinone (2,5-cyclohexadiene-4-dione), 1,2-naphthoquinone (1,2-naphthalenedione), and 1,4-naphthoquinone (1,4-naphthalenedione) were tumorigenic to mouse skin, raised serious questions about the addition of phenols to the tobacco blend. The biological findings on *p*-benzoquinone were subsequently confirmed by Tiedemann (3916a). Takizawa (3865a) reported that neither of the higher molecular weight quinones 9,10-anthraquinone (9,10-anthracenedione) or 9,10-phenanthrenequinone (9,10-phenanthrenedione) was tumorigenic to mouse skin.

Rodgman also communicated to management the substance of the early reports by Boutwell et al. (414), subsequently amplified by Boutwell and Bosch (414), that when certain low-molecular-weight phenols were applied to mouse skin in sequence with a level of a tumorigenic PAH such as B[*a*]P either insufficient

TABLE 9.3
Phenolic Components of Tobacco Smoke Listed by Kosak (2170)

Year	Investigator	Component
1904	Thoms (3912)	"Phenols"
1919	Kissling (2107)	Catechol
1932	McNally (2524)	"Phenols"
1939	Roffo (3324)	Phenolic acids
1939	Wenusch (4202)	Catechol
1939	Wenusch (4202)	Phenol
1947	Ikeda (1857)	Phenol

TABLE 9.4
Studies of Phenolic Components of Tobacco Smoke Omitted from the 1954 Listing by Kosak (2170)

Year	Investigator	Component
1871	Vohl and Eulenberg (4065)	Phenol
1876	Ludwig (2408)	Phenol
1904	**Thoms (3912)**	**"Phenols"**
1919	**Kissling (2107)**	**1,2-Dihydroxybenzene (catechol)**
1932	**McNally (2524)**	**"Phenols"**
1939	**Roffo (3324)**	**Phenolic acids**
1939	**Wenusch (4202)**	**Phenol, 1,2-dihydroxybenzene (catechol)**
1947	**Ikeda (1857)**	**Phenol**
1950	Molinari (2605)	Phenol, 1,2-dihydroxybenzene (catechol)
1952	Rayburn (3089)	Phenol, 2-methoxyphenol (guaiacol), 2-methylphenol (*o*-cresol), 3-methylphenol (*m*-cresol)
1953	Rayburn et al. (3090)	Phenol, 2-methoxyphenol (guaiacol), 2-methylphenol (*o*-cresol), 3-methylphenol (*m*-cresol)
1954	**Kosak (2170)**	**List of tobacco smoke components**

Note: Entries in bold refer to items included by Kosak (2170).

to induce tumors or sufficient to induce tumors in only a small percentage of the treated animals, the phenols enhanced (or promoted) the tumorigenic effect of the PAH, i.e., the % tumor-bearing animals (% TBA) was much higher than that anticipated on the basis of the PAH dose administered.

The effectiveness of the promotion of the tumorigenicity of a tumorigenic PAH by a phenol is dependent on the substituents R_2 and R_6 on the C_2 and C_6 carbons, the carbon atoms adjacent to the carbon to which the hydroxyl group is attached (Figure 9.1). If $R_2 = H$ or $R_6 = H$ or if $R_2 = R_6 = H$, then the phenol will exert a promoting effect, the effect being greatest when both substituents $R_2 = R_6 = H$. If neither R_2 nor R_6 is hydrogen, i.e., when $R_2 \neq H$ and $R_6 \neq H$, no promoting effect is observed.

The coupling of the findings reported by Boutwell et al. (414) on the promoting effects of low-molecular-weight phenols on PAHs in the mouse-skin-painting bioassay with the failure to explain the tumorigenicity of CSC on the basis of its PAH content subsequently triggered extensive research both

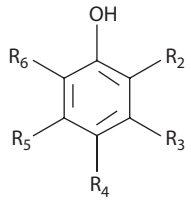


FIGURE 9.1 A substituted phenol.

within and outside of the tobacco industry on several aspects of the phenols in tobacco smoke:

1. Identification and quantitation of phenols in cigarette MSS: To date, the number of phenols identified in tobacco smoke exceeds 400 (see Table 9.22). While the number of phenols identified is significantly fewer than the number of PAHs identified in cigarette MSS, the number of identified tobacco smoke phenols is much greater than that identified in any other consumer product such as tea, coffee, or cocoa, again a reflection of the intense scrutiny directed at tobacco smoke *vs*. that directed at any other consumer product.
2. Bioassays to determine contribution of phenols to CSC tumorigenicity: Determination of the biological relationship, if any, between the phenol fraction from cigarette MSS or its individual components and the PAH fraction from cigarette MSS or its individual components needed to be conducted. Was the biological relationship between phenol and the tumorigenic PAHs one of promotion, cocarcinogenesis, inhibition, or anticarcinogenesis?
3. Determination of the nature of the precursors in tobacco of the phenols in cigarette MSS: The studies in the mid-1960s to identify the major precursors in tobacco of the phenols in tobacco smoke paralleled the studies in the late 1950s and early 1960s on the precursors in tobacco of the PAHs in tobacco smoke.
4. The effect of cigarette design parameters on delivery of MSS phenols: Determinations of which cigarette design parameters enabled significant control of the levels of phenols in MSS needed to be conducted.

In the following paragraphs, each of the previously listed topics is discussed in considerable detail with an attempt to put in perspective the relationships between isolation/identification, precursor definition, bioassay results, and delivery control pertinent to the phenols in cigarette MSS.

9.1.1 Identification and Quantitation of Phenols in Cigarette MSS

In their reviews of phenolic components of tobacco smoke, Wynder and Hoffmann (4319, 4332) concluded their report on the first successful isolation of phenols from tobacco smoke by Vohl and Eulenberg (4065) and Ludwig (2408) with the comment: "Since that time, publications have dealt sporadically with smoke phenols."

From the early 1950s through 1967, over 110 reports dealing with phenols in smoke were presented at scientific

meetings and/or published in peer-reviewed journals. Such a number can hardly be considered as sporadic!

Many of the studies in the 1950s dealt with the identification and quantitation of various low-molecular-weight phenols in cigarette MSS [cf. the studies on phenol, the methylphenols (the cresols), 2-methoxyphenol (guaiacol), the dimethylphenols (the xylenols) by Rayburn (3089), Rayburn et al. (3090), Commins and Lindsey (786–789, 789a), Izawa et al. (1906), and on scopoletin by Yang et al. (4373–4375)].

Not only was a variety of separation techniques employed to obtain the phenols but also a variety of analytical techniques was employed for the quantitation. Examples of these methods follow:

Diazotization with *p*-nitroaniline, paper chromatography, UV absorption spectrophotometry	Rayburn et al. (3090)
Methylation, paper chromatography, UV absorption spectrophotometry	Commins and Lindsey (786)
Formation of 2,4-dinitrobenzoates	Izawa et al. (1906)
Formation of phenylazobenzene sulfonic acid derivatives	Izawa et al. (1906)
Methylation, gas chromatography	Carruthers and Johnstone (615)
Gas chromatography, internal standard addition	Hoffmann and Wynder (1789), Crouse et al. (851), Spears (3764)
Gas chromatography	Oakley et al. (2820)
4-Aminoantipyrine treatment, colorimetry	Lorentzen and Neurath (2397)
Glass capillary gas chromatography	Smith and King (3716)
Diazotization with *p*-nitroaniline, colorimetry	Smith and King (3717, 3718)
Thin-layer chromatography	Smith and Sullivan (3719)
Derivatization, colorimetry	Knoop and Rosene (2142a)

In 1959, Johnstone and Plimmer (1971) cataloged the 16 tobacco smoke phenols listed in Table 9.5.

Examination of the chronology of the published reports on phenols in tobacco smoke reveals the escalation (see Table 9.6) of the scientific publications/presentations between 1952 and 1964, the year of the Advisory Committee's Report on Smoking and Health to the U.S. Surgeon General (3999). This escalation was similar to but not as extensive as the increase from 1953 to 1964 in the number of presentations/publications pertinent to PAH in tobacco smoke.

In January 1964, the Advisory Committee on Smoking and Health submitted its report to the U.S. Surgeon General (3999). Because of the widespread dissemination of the contents of this report, its January 1964 publication provides an appropriate point in time to assess the situation with regard to prior research publications on phenolic compounds in tobacco smoke. Table 9.6 summarizes chronologically some of the various reports issued between 1952 and 1964 on tobacco smoke phenols. Of the 82 reports cited in Table 9.6 from 1952 through 1964, 80 were issued from 1955 through 1964. If, because of the early 1964 issuance of the Advisory Committee's Report, the publications on tobacco smoke phenols in 1964 are omitted from the listing, the number from 1953 through 1963 becomes 65. As noted previously in the discussion of the early studies of PAHs, a similar assessment of publications on PAHs in tobacco smoke indicated that some 213 reports were issued from 1953 through 1964. If the publications on tobacco smoke PAHs in 1964 are omitted, the number from 1953 through 1963 becomes 200.

During the first decade of research on tobacco smoke, effort was divided between the identifications of the various

TABLE 9.5
Tobacco Smoke Phenols Cataloged by Johnstone and Plimmer (1971)

Phenol	References
1,2-Benzenediol {catechol}	Molinari (2605, 2607), Bonnet and Neukomm (396), Carruthers and Johnstone (615)
1,3-Benzenediol {resorcinol}	Commins and Lindsey (789, 789a)
1,4-Benzenediol {hydroquinone}	Bonnet and Neukomm (396)
2*H*-Benzopyran-6-one, 7-hydroxy-6-methoxy- {scopoletin}	Yang et al. (4373–4375)
Ethanone, 1-(3-hydroxyphenyl)- {3′-hydroxyacetophenone}	Carruthers and Johnstone (615)
Ethanone, 1-(4-hydroxyphenyl)- {4′-hydroxyacetophenone}	Carruthers and Johnstone (615)
1-Naphthalenol {1-naphthol}	Commins and Lindsey (789, 789a)
2-Naphthalenol {2-naphthol}	Commins and Lindsey (789, 789a)
Phenol	Vohl and Eulenberg (4065), Ludwig (2408), Rayburn (3089), Rayburn et al. (3090), Commins and Lindsey (789, 789a), Bonnet and Neukomm (396), Carruthers and Johnstone (615)
Phenol, 2,4-dimethyl- {2,4-xylenol}	Wynder and Wright (4354)
Phenol, 3,5-dimethyl- {3,5-xylenol}	Carruthers et al. (616), Clemo {765)
Phenol, 2-dimethoxy- {guaiacol}	Rayburn (3089), Rayburn et al. (3090);
Phenol, 2-methyl- {*o*-cresol}	Rayburn (3089), Rayburn et al. (3090), Commins and Lindsey (789, 789a), Carruthers and Johnstone (615)
Phenol, 3-methyl- {*m*-cresol}	Rayburn et al. (3089), Commins and Lindsey (789, 789a), Carruthers and Johnstone (615)
Phenol, 4-methyl- {*p*-cresol}	Commins and Lindsey (789, 789a), Carruthers and Johnstone (615)
Phenol, 2,4,6-trimethyl- {mesitol}	Bonnet and Neukomm (396)

TABLE 9.6
Publications/Presentations (1952–1964) Pertinent to Identification of Phenolic Components of Tobacco Smoke

	Number		
Year	In Year	Accumulated	Investigator(s)
1952	1	1	Rayburn (3089)
1953	1	2	Rayburn et al. (3090)
1955	1	3	Wright and Wynder (4353)
1956	5	8	Commins and Lindsey (786–789, 789a)
1957	3	11	Bonnet and Neukomm (396), Landahl and Tracewell (2261), Wynder and Wright (4354)
1958	11	22	Bonnet (392), Carruthers et al. (616), Clemo (765), Rowland (3347), Weaving (4156), Wender et al. (4164), Yang et al. (4373–4375)
1959	8	29	Dieterman et al. (969), Doll (1025), Izawa et al. (1906), Onishi (2858), Reid (3096), Rodgman and Cook (3271), Roe et al. (3314)
1960	3	33	Carruthers and Johnstone (615), Rodgman and Cook (3280, 3286), Weaving (4158), Yang et al. (4376)
1961	8	41	Cundiff (859), Herrmann (1625), Hoffmann and Wynder (1789), Latimer (2274), Rodgman and Cook (3286), Wynder and Hoffmann (4311–4313)
1962	7	48	Kato and Shibayama (2044), P. Lorillard Co. R&D (2399), Rodgman and Cook (3286), Schmeltz et al. (3488), Wynder and Hoffmann (4314), Yang and Wender (4377, 4378)
1963	17	65	Crouse et al. (851), Hoffmann et al. (1766),Hoffmann and Wynder (1791), Kato et al. (2045), Laurene (2295, 2295a), Laurene et al. (2311, 2312), Lorentzen and Neurath (2397), Osman et al. (2876), Rodgman and Cook (3286), Rodgman and Mims (3305), Spears (3764, 3765), Unghvary et al. (3995), Wender and Yang (4163), Wynder and Hoffmann (4317)
1964	17	82	Ehmke and Neurath (1115), Elmenhorst (1129), Esterle and Campbell (1164), Knoop and Rosene (2142a), Mann et al. (2451), Oakley et al. (2820), Pyriki and Moldenauer (3043), Rodgman and Cook (3286), Seehofer et al. (3574), Smith and King (3716, 3717)

phenolic compounds and improvements of their quantitation in cigarette MSS.

Less than a decade after the Johnstone and Plimmer 1959 review, Stedman (3797) tabulated the reports in which the identifications of 54 phenols in tobacco smoke were described (Table 9.7).

In their 1980 review, Ishiguro and Sugawara (1884) listed over 150 phenolic compounds that had been identified as tobacco smoke components.

By the mid-1990s, over 270 completely identified phenolic compounds were reported as tobacco smoke components (Table 9.22). It should be noted that, despite repeated criticisms of the publication policy of the R.J. Reynolds Tobacco Company on tobacco smoke composition, 70 of the phenolic compounds listed in Table 9.22 were first reported as tobacco smoke components by R.J. Reynolds Tobacco Company R&D personnel and the identities of an additional 25 phenolic smoke components reported by others were confirmed.

As shown by the citations included in Table 9.8, the TCRC over the years has been a significant forum for the dissemination of new and meaningful information pertinent to phenolic components in tobacco smoke.

While the nature and levels of the low-molecular-weight phenols in tobacco smoke were being defined in the late 1950s and early 1960s, additional research permitted the identification of several more complex phenolic components of tobacco smoke, e.g., the naphthalenols by Commins and Lindsey (789, 789a), hydroxybenzopyranones such as scopoletin by Yang et al. (4373–4375) and Wender et al. (4164), esculetin by Dietermann et al. (969), α-tocopherol by Rodgman and Cook (3271), hydroxycinnamic acids by Yang and Wender (4376), hydroxyphenylacetic acids by Yang and Wender (4377) and Wender and Yang (4163), and several hydroxybenzaldehydes by Yang and Wender (4379). In contrast to the low-molecular-weight phenols, many of these more complex phenols are also present at more than trace amounts in tobacco. A series of low-molecular-weight, volatile phenols were identified in the tobacco type Latakia by Irvine and Saxby (1876, 1877a) at much greater levels than volatile phenols found in other tobacco types such as flue-cured and burley.

Eventually, several hydroxyphenyl alcohols and hydroxybenzyl alcohols were identified in tobacco and tobacco smoke by Hecht et al. (1561). These identifications were soon followed by the identification of a series of phenolic acids from tobacco by Snook et al. (3749, 3751). Table 9.5 had summarized the studies on phenols in tobacco smoke up to 1964. In Table 9.9, studies on phenols in tobacco smoke from 1964 to date are summarized.

9.1.2 Bioassays to Determine the Contribution of Phenols to Cigarette Smoke Condensate Tumorigenicity

At several scientific meetings in the mid-1950s, Boutwell et al. (414) described their preliminary findings on the promoting effect of phenol on the specific tumorigenicity of 7,12-dimethylbenz[*a*]anthracene (DMB[*a*]A) when the application of the PAH to mouse skin was followed by an

TABLE 9.7
Tobacco Smoke Phenols Cataloged by Stedman (3797)

No.	CAS Nomenclature	Common Name
1.	Acetic acid, 2-hydroxyphenyl-	
2.	Acetic acid, 3-hydroxyphenyl-	
3.	Acetic acid, 4-hydroxyphenyl-	
4.	Benzaldehyde, 3,4-dihydroxy-	Protocatechualdehyde
5.	Benzaldehyde, 3,5-dimethoxy-4-hydroxy-	Syringaldehyde
6.	Benzaldehyde, 2-hydroxy-	Salicaldehyde
7.	Benzaldehyde, 3-hydroxy-	
8.	Benzaldehyde, 4-hydroxy-	
9.	Benzaldehyde, 4-hydroxy-3-methoxy-	Vanillin
10.	1,2-Benzenediol	Catechol
11.	1,3-Benzenediol	Resorcinol
12.	1,4-Benzenediol	Hydroquinone
13.	Benzoic acid, 3,4-dihydroxy-	Protocatechuic acid
14.	Benzoic acid, 3,5-dimethoxy-4-hydroxy-	Syringic acid
15.	Benzoic acid, 2-hydroxy-	Salicylic acid
16.	Benzoic acid, 3-hydroxy-	
17	Benzoic acid, 4-hydroxy-	
18.	Benzoic acid, 3-hydroxy-4-methoxy-	Isovanillic acid
19.	Benzoic acid, 4-hydroxy-3-methoxy-	Vanillic acid
20.	2*H*-1-Benzopyran-6-one, 6,7-dihydroxy-	Esculetin
21.	2*H*-1-Benzopyran-6-one, 7-hydroxy-6-methoxy-	Scopoletin
22.	Cinnamic acid, 3,4-dihydroxy-	Caffeic acid
23.	Cinnamic acid, 3,4-dihydroxy-, 3-ester with 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid	Chlorogenic acid
24.	Cinnamic acid, 3,4-dihydroxy-, 5-ester with 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid	Neochlorogenic acid
25.	Cinnamic acid, 3,5-dimethoxy-4-hydroxy-	Sinapic acid
26.	Cinnamic acid, 4-hydroxy-	Coumaric acid
27.	Cinnamic acid, 4-hydroxy-3-methoxy-	Ferulic acid
28.	Ethanone, 1-(2-hydroxyphenyl)-	Acetophenone, 2′-hydroxy-
29.	Ethanone, 1-(3-hydroxyphenyl)-	Acetophenone, 3′-hydroxy-
30.	Ethanone, 1-(4-hydroxyphenyl)-	Acetophenone, 4′-hydroxy-
31.	1-Naphthalenol	1-Naphthol
32.	2-Naphthalenol	2-Naphthol
33.	Phenol	
34.	Phenol, 2,6-dimethoxy-	
35.	Phenol, 2,3-dimethyl-	2,3-Xylenol
36.	Phenol, 2,4-dimethyl-	2,4-Xylenol
37.	Phenol, 2,5-dimethyl-	2,5-Xylenol
38.	Phenol, 2,6-dimethyl-	2,6-Xylenol
39.	Phenol, 3,4-dimethyl-	3,4-Xylenol
40.	Phenol, 3,5-dimethyl-	3,5-Xylenol
41.	Phenol, 2-ethyl-	
42.	Phenol, 3-ethyl-	
43.	Phenol, 4-ethyl-	
44.	Phenol, 2-methoxy-	Guaiacol
45.	Phenol, 2-methoxy-	
46.	Phenol, 4-methoxy-	
47.	Phenol, 2-methoxy-4-(1-propenyl)-	Isoeugenol
48.	Phenol, 2-methoxy-4-(2-propenyl)-	Eugenol
49.	Phenol, 2-methyl-	*o*-Cresol
50.	Phenol, 3-methyl-	*m*-Cresol
51.	Phenol, 4-methyl-	*p*-Cresol
52.	Phenol, 5-methyl-2-(1-methylethyl)-	Thymol
53.	Phenol, 2,4,6-trimethyl-	Mesitol
54.	Propanoic acid, 3-hydroxyphenyl-	
55.	Propanoic acid, 4-hydroxyphenyl-	

TABLE 9.8
Presentations at TCRC and TSRC on Phenolic Components of Tobacco Products

TCRC	Investigator(s)	TCRC	Investigator(s)
Isolation, identification, and quantitation of phenols in tobacco products			
6th	Rayburn (3089)	34th	Carmella et al. (600)
12th	Rowland (3347)	34th	Schlotzhauer et al. (3462)
16th	Davis and George (911a)	35th	Carmella et al. (598)
16th	Schmeltz et al. (3488)	36th	Lee et al. (2329)
17th	Burdick et al. (526)	36th	Snook and Chortyk (3737)
18th	Ayres and Thornton (127)	37th	Carmella et al. (599)
18th	Esterle and Campbell (1164)	39th	Adams et al. (30)
18th	Knoop and Rosene (2142a)	40th	McWilliams et al. (2526)
18th	Mann et al. (2451)	42nd	Nanni et al. (2681a)
18th	Rodgman and Cook (3280)	42nd	Risner and Cash (3172)
19th	Ayres and Thornton (128)	42nd	Snook et al. (3754)
19th	Spears et al. (3767)	43rd	Risner and Cash (3174)
20th	Kallianos et al. (2016)	45th	Lee et al. (2330a)
20th	Schlotzhauer et al. (3468)	46th	Prakasch and Ireland (2983)
21st	Kallianos et al. (2017)	46th	Risner (3166)
22nd	Benner et al. (276)	48th	Wilson (4268)
22nd	Leach and Alford (2321)	50th	Green and Rodgman (1373)
23rd	Benner et al. (275)	50th	Risner (3170)
24th	Miller et al. (2554)	51st	Risner and Nelson (3170)
25th	Singer and Hoffmann (3674)	51st	Zhangyu et al. (4412)
27th	Thacker and Martin (3894)	52nd	Risner and Cash (3174)
28th	Guerin et al. (1450)	53rd	Forehand et al. (1213)
29th	Newell et al. (2769)	54th	Wooten et al. (4279)
29th	Roberts and Watts (3228)	55th	Li et al. (2361)
29th	Schumacher et al. (3553)	55th	Purkis et al. (3007)
30th	Chamberlain et al. (664)	56th	Honglin et al. (1825)
30th	Kallianos (2614)	56th	Reffick et al. (3093)
31st	Hecht et al. (1561)	57th	Volgger et al. (4067)
31st	Schlotzhauer et al. (3474)	57th	Warren (4137)
32nd	Cornell et al. (828)	58th	Hwang et al. (1854)
32nd	Heckman and Best (1587)	58th	Little et al. (2379)
32nd	Snook et al. (3744)	58th	Loureau et al. (2400a)
32nd	Snook et al. (3746)	58th	Sheng et al. (3646)
33rd	Snook et al. (3751)	59th	Hwang et al. (1853a)
Precursor, biological, and other studies on phenols in tobacco products			
19th	Chortyk et al. (725a)	28th	Hecht et al. (1582)
19th	Spears et al. (3767)	29th	Brunnemann et al. (496)
22nd	Bell et al. (246)	31st	Hardy and Hobbs (1501)
23rd	Benner et al. (275)	37th	Brunnemann et al. (499)
23rd	Burton et al. (539)	48th	Wilson (4268)
23rd	Colucci et al. (783b)	50th	Hu (1840a)
23rd	Lakritz et al. (2253)	52nd	Leffingwell and Alford (2339)
25th	Rathkamp et al. (3087)	54th	Doolittle et al. (1051)
26th	Artho et al. (105)	59th	Dyakonov et al. (1077a)
28th	Baggett and Morie (156)	59th	Hwang et al. (1853a)

TCRC, Tobacco Chemists' Research Conference; TSRC, Tobacco Science Research Conference.

TABLE 9.9
Reports of Research Pertinent to Phenolic Compounds in Tobacco and Tobacco Smoke, 1964–2005

Year	Investigator(s)
1964	Ehmke and Neurath (1115), Elmenhorst (1129), Esterle and Campbell (1164), Knoop and Rosene (2142a), Mann et al. (2451), Oakley et al. (2820), Pyriki and Moldenauer (3043), Rodgman (3251), Rodgman and Cook (3286), Seehofer et al. (3574), Smith and King (3716, 3717), Smith and Sullivan (3719), Testa et al. (3890), USPHS (3999), Wynder and Hoffmann (4319)
1965	Bock et al. (358), Chortyk et al. (725a), Cuzin et al. (884), Kaburaki et al. (1996, 1997), Kato et al. (2043, 2046), LeRoux (2351), Lipp (2374, 2376, 2377), Rodgman and Cook (3286), SEITA (3602), Smith and King (3718), Spears et al. (3767), Steck and Wender (3792), Steck et al. (3793), Testa et al. (3891), Waltz and Häusermann (4121), Waltz et al. (4123, 4124), Wynder and Hoffmann (4330)
1966	Bell et al. (248), Chortyk et al. (726), Kallianos et al. (2016), Mokhnachev and Latayeva (2577), Mold et al. (2594), Müller and Moldenhauer (2653), Schlotzhauer et al. (3468), Shamberger (3625), Touey and Kiefer (3937), Van Duuren et al. (4037)
1967	Hoffmann and Wynder (1797), Kallianos et al. (2017), Lyerly and Gilleland (2413a), Mokhnachev and Latayeva (2578), Müller and Moldenhauer (2653), Schlotzhauer et al. (3468), Schmeltz et al. (3486), Wynder and Hoffmann (4332)
1968	Avetyam et al. (125), Bell et al. (246), Benner et al. (274), Chamberlain and Stedman (666), Colucci and Sizemore (783a), Dalhamn (891a), Hoffmann and Wynder (1798), Irvine and Saxby (1876), Kaburaki et al. (1994, 1995), Kallianos et al. (2016), Leach and Alford (2321), Schmeltz and Schlotzhauer (3497), Stedman (3797), Van Duuren et al. (4036), Wynder and Hoffmann (4342, 4346)
1969	Benner et al. (275, 276), Burton et al. (539), Colucci et al. (783b), Georgiev (1284a), Green et al. (1377, 1378), Grob and Völlmin (1427), Irvine and Saxby (1877a), Lakritz et al. (2253), Leach et al. (2322), Wynder and Hoffmann (4344, 4346)
1970	Green et al. (1377), Grob and Völlmin (1426), Kaburaki et al. (2006), Kushnir et al. (2245), Laurene et al. (2306), Martin and Thacker (2478), Miller et al. (2554), Reynolds (3111), Testa (3884), Viart (4050), Wynder and Hoffmann (4346a)
1971	Green and Schumacher (1375), Hoffmann and Wynder (1800), Kaburaki et al. (2005), Miller et al. (2554), Rathkamp et al. (3087), Royal College of Physicians (3363), Shigematsu et al. (3650), Singer and Hoffmann (3674), Van Duuren et al. (4035)
1972	Artho et al. (105), Bock (352), Elmenhorst (1132), Hoffmann and Wynder (1802, 1803), Klimisch and Reese (2125), Schmeltz et al. (3499), Schumacher et al. (3557), USPHS (4003)
1973	Baggett and Morie (155), Benner et al. (278), Derreux et al. (952), Diffee (970), Morie and Sloan (2635), Rathkamp et al. (3088), Thacker and Martin (3894), Van Duuren et al. (4029)
1974	Akin and Chamberlain (39a), Baggett and Morie (156), Green and Best (1356), Guerin et al. (1449), Hecht et al. (1582), Heckman (1586), Klus and Kuhn (2137), Lloyd and Miller (2387, 2388), Newell et al. (2767), Schmeltz et al. (3484), Schumacher et al. (3553)
1975	Baggett and Morie (156), Brunnemann et al. (496), Hecht et al. (1583), Malaterre et al. (2447), Newell et al. (2769, 2777), Roberts and Watts (3228), Schmeltz et al. (3484), Schumacher et al. (3553)
1976	Best et al. (312), Brunnemann et al. (497), Chamberlain et al. (664), Green et al. (1375b), Hoffmann et al. (1780), Ishiguro et al. (1878a, 1879, 1886), Kallianos (2014), Kensler (2082), Mauldin (2506), Miller et al. (2543), Moates (2570), Newell et al. (2761, 2762, 2765, 2766), Patterson et al. (2904), Sakuma et al. (3395), Testa and Hys (3892), Van Duuren and Goldschmidt (4028)
1977	Brunnemann et al. (514), Hardy and Hobbs (1501), Harrell (1530), Hecht et al. (1561), Schlotzhauer et al. (3474), Schmeltz and Hoffmann (3491), Schmeltz et al. (3512), Schumacher et al. (3553), Walters (4113)
1978	Chamberlain et al. (663), Cornell et al. (828), Green et al. (1371), Hecht et al. (1561), Heckman and Best (1587), Ishiguro and Sugawara (1881–1883), Newell et al. (2769), Schlotzhauer (3447), Schlotzhauer et al. (3474), Snook et al. (3744, 3746,3753), Van Duuren et al. (4038)
1979	Chamberlain et al. (652), Green et al. (1367), Schmeltz et al. (3512), Snook and Fortson (3745), Snook et al. (3751), USPHS (4005)
1980	Ishiguro and Sugawara (1884), Martin and Gilleland (2476), Mokhnachev and Mironenko (2579), Sakuma et al. (3402), Schlotzhauer et al. (3452), Snook et al. (3747), Van Duuren (4026), Wattenberg et al. (4149c)
1981	Hecht et al. (1562), Heckman and Best (1587), Morée-Testa (2615), Schlotzhauer and Chortyk (3453), Shelar and Colby (3641–3643), Snook et al. (3748, 3749), USPHS (4009)
1982	Hwang et al. (1854a), Sakuma et al. (3400), Schlotzhauer et al. (3462), Snook and Chortyk (3737, 3738), USPHS (4010)
1983	Brunnemann et al. (499), Hoffmann et al. (1736), Yoshida and Fukuhara (4386)
1984	Adams et al. (28), Jeanty et al. (1984)
1985	Adams et al. (30), Eaker and Hutcherson (1091), Eble et al. (1105), Sakuma et al. (3392), Snook et al. (3743)
1986	Grimmer et al. (1409), IARC (1871), LaVoie et al. (2314a, 2314b), McWilliams et al. (2526), Risner (3159)
1987	Adams et al. (31), Grimmer et al. (1409), Melikian et al. (2527f)
1988	Nanni et al. (2681), Risner (3161), Risner and Cash (3171, 3172)
1989	Melikian et al. (2527c, 2527d), Risner and Cash (3173, 3174), Schmidt and Hecker (3519a), Snook et al. (3754)
1990	Martin et al. (2480), Melikian et al. (2527g), Nanni et al. (2681), Risner and Cash (3173)
1991	Risner (3165)
1992	Prakash and Ireland (2983), Risner (3166), Zhao and Zhou (4414)
1994	Risner et al. (3168), Wilson (4268)
1996	Green and Rodgman (1373), Hu (1840a), Risner (3170)
1997	Borgerding et al. (420), Risner and Nelson (1970), Zhangyu et al. (4412)
1998	Hecht et al. (1572), Hoffmann and Hoffmann (1741), Leffingwell (2339), Nelson et al. (2691)
1999	Baker (172), Forehand et al. (1213), Hirose et al. (1656a), Leffingwell (2338), Omori et al. (2857)

TABLE 9.9 (continued)
Reports of Research Pertinent to Phenolic Compounds in Tobacco and Tobacco Smoke, 1964–2005

Year	Investigator(s)
2000	Fowles et al. (1217), Hajaligol and Fisher (1485), Wooten et al. (4279)
2001	Hoffmann and Hoffmann (1743), Li et al. (2361), Wooten et al. (4277)
2002	Carmines (603), Lauterbach (2313a), Reddick et al. (3093), Smith et al. (3712)
2003	Chen and Moldoveanu (688), Dagnon and Edreva (890), Volgger et al. (4067), Warren (4137)
2004	Gregg et al. (1386), Hwang et al. (1854), Little et al. (2379), Loureau et al. (2400a), Zha and Moldoveanu (4407)
2005	Little et al. (2379a), Uchii and Sato (3990a)
2006	Larkins (2262a)
2007	Kim and Kim (4702), Moldoveanu (4796), Williams and Watts (4965), Zawadzki and Ergle (4986)
2008	Dyakonov et al. (4999), Watts and Wilson (5031), Vaughan et al. (5879a)
2009	Wu and Rickert (5093)
2010	Fisher-Jones et al. (5500), Mao et al. (5532), Renfro (5555), Steach and Fisher-Jones (5564), Uwano and Yoshida (5576), Zhou et al. (5588)
2011	Dagnon et al. (5643a)

application of phenol. Subsequently, Boutwell and Bosch (414) reported that phenol and many substituted phenols enhanced or promoted the specific tumorigenicity of PAHs. However, they reported that 1,2-benzenediol (catechol) exhibited no tumor-promoting activity. Later, 1,2-benzenediol (catechol) was found to be the most plentiful low-molecular-weight phenol in cigarette MSS [Kallianos et al. (2016), Schlotzhauer et al. (3462), Schlotzhauer and Chortyk (3453), Morée-Testa (2615), Risner and Cash (3171–3174), Risner (3165)] and was reported [Van Duuren et al. (4029)] to be a cocarcinogen for PAHs, not a promoter.

Coincident with the phenol studies of Boutwell et al. (414) and during the time that much effort was being expended to resolve the question about the presence of PAHs in tobacco smoke, Gwynn and Salaman (1463b) reported the promoting effect of CSC.

Two years later, Gellhorn (1281) reported that whole CSC acted as a promoting agent for several tumorigenic PAHs applied to mouse skin.

The next year, Roe et al. (3314) reported that the phenolic fraction from CSC exerted a significant promoting effect on the specific tumorigenicity of PAHs. They theorized:

> Cigarette smoke condensate may be richer in tumour-promoting substances than in tumour-initiating substances. Phenolic compounds may be responsible for much of its promoting activity.

As noted previously, Wynder and Hoffmann (4307), unable to explain the bioassay (skin painting) results with CSC on the basis of either its B[*a*]P content (less than 2% TBA explainable) or its total tumorigenic PAH content (less than 3% TBA explainable), added the concept of promotion, particularly that attributed to low-molecular-weight phenols, in an attempt (unsuccessful) to explain the bioassay results in laboratory animals. They amplified their theory in a more detailed publication (4307). They also stated (4308) that the higher molecular weight PAHs played an important role in the carcinogenicity to mouse skin of CSC but when the various known concentrations of the carcinogenic PAHs as estimated in CSC were summed, it was obvious that these smoke components acting either individually or in concert could not account for the established carcinogenicity to mouse skin of the CSC nor of its isolated PAH fraction.

Because of the inability to explain the mouse-skin-painting bioassay results with CSC on the basis of its PAH content and because of the presumed biological relationship between the phenol fraction and/or its individual components and the PAH fraction and/or its individual components, the findings reported by Boutwell et al. (414), Gwynn and Salaman (1463b), Gellhorn (1281), and Roe et al. (3314) stimulated extensive research on the nature and levels of the phenols in cigarette MSS in the late 1950s to early 1960s. Over the next few years, the results from different laboratories of the bioassays involving tobacco smoke phenols varied considerably. The variations raised the question as to whether the relationship between the tobacco smoke phenols and PAHs was one of promotion, cocarcinogenesis, inhibition, or anticarcinogenesis.

From the results of their studies on the administration of B[*a*]P plus phenol and the administration of DMB[*a*]A plus phenol, Wynder and Hoffmann (4313) concluded:

> [Our results] show that promoting substances present in tobacco smoke can increase and accelerate the tumor yield of carcinogenic polynuclear hydrocarbons that by themselves are not present in sufficient concentration to yield any tumors or yield them only after a prolonged latent period.

In 1958, Wynder et al. (4355) proposed the use of the level of B[*a*]P in CSC as an "indicator" or "marker" of the specific tumorigenicity (mouse skin) of CSC as well as an "indicator" or "marker" of its levels of tumorigenic PAHs with four or more rings. When the low-molecular-weight phenols in tobacco smoke attracted considerable attention because of their claimed contribution to the specific tumorigenicity of CSC, Hoffmann et al. (1766) and Wynder and Hoffmann (4317) extended the "indicator" concept to phenol, designating it as an "indicator" or "marker" for the promoting

low-molecular-weight, volatile phenols in cigarette MSS. Just as the concept of B[*a*]P as an "indicator" or "marker" of CSC-specific tumorigenicity and tumorigenic higher PAHs content was subsequently shown to be incorrect, so was the concept of phenol as an "indicator" or "marker" of phenol-induced promoting activity of CSC and promoting phenols content shown to be incorrect. The phenol "indicator" situation is discussed in the following.

Table 9.10 summarizes some of the diversity observed in the bioassay results on the properties pertinent to the tumorigenicity of PAHs of several phenol components of tobacco smoke (phenol, catechol, α-tocopherol), the phenolic fraction from CSC, and CSC itself.

Although much attention and effort were devoted to the supposed deleterious effects of various tobacco smoke components such as the PAHs, the aza-arenes, and the low-molecular-weight phenols, very little was reported about the tobacco smoke components with properties that offset the supposed tumorigenicity or promoting effects of the compound classes mentioned. One of the first examples of cigarette MSS components inhibiting the action of a "tumorigen" was described by Wynder and Hoffmann (4311). This finding was an outgrowth of their studies on the effect of organic solvent extraction of tobacco on the PAH content of the extracted tobacco smoke. Lam (2255) and Wynder (4294) in the mid-1950s proposed that the precursors in tobacco of PAHs in cigarette MSS were the saturated aliphatic hydrocarbons; Wright (4282a) and Wynder et al. (4355, 4356) proposed the phytosterols as the PAH precursors, and Wright (4282) also proposed the terpenoid compounds as major PAH precursors. These compounds are removable almost totally or to a substantial degree by extraction of tobacco with organic solvents such as hexane or pentane. Cigarettes fabricated from the extracted tobacco yielded lower quantities in MSS of PAHs such as B[*a*]P that were known under certain laboratory conditions to produce tumors on the shaved backs of susceptible strains of mice. Skin-painting studies with mainstream CSC collected by smoking cigarettes made with the control and extracted tobaccos gave a lower percentage of TBA in the extracted tobacco CSC group. However, the decrease in % TBA was much less than the percent decrease in the level in the CSC of tumorigenic PAHs such as B[*a*]P (4282, 4294, 4307, 4355, 4356).

One explanation for this difference was that the solvent extraction removed nearly all the aliphatic saturated hydrocarbons from the tobacco, and thus, they were either absent from the MSS from the extracted tobacco cigarettes or present at extremely low levels. Wynder and Hoffmann [see pp. 330–331 in (4319) and pp. 370–371 in (4332)] reported that this aliphatic saturated hydrocarbon fraction (constituting about 3% of the mainstream CSC) inhibited the activity of tumorigenic PAHs, including B[*a*]P. The components in the aliphatic hydrocarbon fraction ranged from pentadecane (C_{15}) to pentatriacontane (C_{35}). Each hydrocarbon was present as the *normal*, *iso*, and *anteiso* isomers. The C_{27}–C_{33} hydrocarbons constituted about 80% of the saturated hydrocarbon fraction; with C_{31} (*n*-hentriacontane) and C_{33} (*n*-tritriacontane) hydrocarbons usually being the most plentiful components in the fraction. Subsequent study with improved analytical methodology demonstrated the presence of trace amounts of additional isomeric aliphatic saturated hydrocarbons with as many as 40 carbons.

TABLE 9.10
Variation in Bioassay Results with Phenols or Phenol-Containing Materials

	Effect on Specific Tumorigenicity of PAHs		
Phenol	**Promotion**	**Cocarcinogenicity**	**Inhibition or Anticarcinogenesis**
CSC	Yes: Gwynn and Salaman, (1463b), Gellhorn (1281)		
Phenolic fraction from CSC	Yes: Roe et al. (3314)		
Phenols	Yes: Boutwell et al. (414)		
Phenol	Yes: Wynder and Hoffmann, (4313, 4317), Hoffmann and Wynder (1791), Hoffmann et al. (1736)	No: Van Duuren et al. (4029)	Yes: Van Duuren et al. (4029, 4035)
1,2-Benzenediol {catechol}	No: Van Duuren and Goldschmitt (4028)	Yes: Van Duuren et al. (4029), Van Duuren and Goldschmitt (4028), Hecht et al. (1562), Hoffmann et al. (1736)	
1*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-{α-tocopherol}			Yes: Shamberger (3625), Slaga and Bracken (3684), Viaje et al. (4049a), Shklar (3655a), Weerapradist and Shklar, (4159a), Toth and Patil (3927a), Mirvish (2559b)

CSC, cigarette smoke condensate.

Studies with B[*a*]P and the C_{31} and C_{35} saturated hydrocarbons (SHC), where the SHC to B[*a*]P ratio was 200:1 and 100:1, showed that both saturated hydrocarbons exerted a significant inhibiting effect at both levels on the specific tumorigenicity of B[*a*]P in mouse-skin-painting experiments [4311, 4314, see also pp. 330–331 in (4319) and pp. 370–371 in (4332)].

When the saturated hydrocarbon content (normally about 3% of the particulate phase) of mainstream CSC was increased from 3% to 4% (an overall 33% increase) by addition of the saturated hydrocarbon fraction isolated from CSC, the specific tumorigenicity of the CSC decreased, and the % TBA decreased from 40% to 24%. The MSS of a cigarette delivering 20 mg of CSC contains about 0.6 mg (600,000 ng) of this saturated hydrocarbon fraction and 10 ng of B[*a*]P, a SHC to B[*a*]P ratio of 60,000:1, far in excess of the 200:1 or 100:1 SHC to B[*a*]P ratio that produced the significant inhibition of the specific tumorigenicity of B[*a*]P reported in the mouse-skin-painting bioassay (4314, 4319, 4332).

Other MSS components may have also influenced the PAH and mouse-skin-painting results obtained with control tobacco CSC *vs*. the CSC from organic solvent-extracted tobacco. The extraction of tobacco with a solvent such as hexane not only removed the saturated aliphatic hydrocarbon inhibitors from the tobacco, thus making impossible their transfer to MSS when such tobacco is smoked, but also removed other components such as β-sitosterol (4356), α-tocopherol (vitamin E) (3271, 3347), indole 3279), and α- and β-4,8,13-duvane-1,3-diol (3221, 3361, 3389), thus preventing their transfer to MSS during the smoking process. Subsequently, these tobacco components, now known to transfer from the tobacco rod to MSS during the smoking process and presumably to sidestream smoke (SSS) during cigarette smolder, have been shown to behave as anticarcinogens for several of the reported tobacco smoke "tumorigens" such as the PAHs, the *N*-nitrosamines, and ethyl carbamate. Neither the presence of several of these tobacco and MSS components nor their anticarcinogenic or inhibitory activity *vs*. known tumorigens was known in the late 1950s/early 1960s.

Despite the emphasis on the contribution of CSC components to its specific tumorigenicity when administered to laboratory animals via skin painting, the inhibition of tumorigenesis by CSC and several of its components was not completely ignored during the 1960s. In addition to the role of saturated aliphatic hydrocarbons in the inhibition of the specific tumorigenicity of CSC reported by Wynder and Hoffmann [4311, 4314, see also pp. 330–331 in (4319) and pp. 370–371 in (4332)], other studies pertinent to the antitumorigenicity of tobacco smoke included an earlier one in 1958 by Hoffman and Griffin (1672a) plus later ones in the mid-1960s by Homburger and his colleagues (1823, 1823b, 1824) as well as one reported in the late 1970s by Chamberlain et al. (663) at the USDA.

Comparison of the list of the 6000 or so identified components in tobacco smoke with extensive lists presented by Fay et al. (1177a) and Slaga and DiGiovanni (3685) of compounds and elements reported to possess inhibitory or anticarcinogenic action in carcinogenesis-type experiments in laboratory animals reveals not only that tobacco smoke contains numerous anticarcinogens but also that the levels in tobacco smoke of many of them far exceed those of the levels of the reported tobacco smoke "tumorigens" (3255a). The levels of many of the anticarcinogens in tobacco smoke *vs*. those of the reported smoke "tumorigens" are far in excess of the ratio needed for the anticarcinogenicity to be effective. Table 9.11, adapted from Rodgman (3255a), lists tobacco smoke components reported to be inhibitory or anticarcinogenic to several of the "tumorigens" reported to be present in tobacco smoke.

TABLE 9.11
Inhibitors and Anticarcinogens in Tobacco Smoke

Tobacco Smoke Component Class (Examples)	Tumorigen Suppressed
Hydrocarbons, saturated (e.g., $C_{31}H_{64}$, $C_{35}H_{72}$)	B[*a*]P
Hydrocarbons, unsaturated (*D*-limonene)	NNK, dibenzo[*a,i*]pyrene
Hydrocarbons, monocyclic aromatic (benzene)	B[*a*]P, DB[*a,h*]A
Hydrocarbons, aromatic, polycyclic (naphthalene, anthracene, phenanthrene, fluoranthene, pyrene, benzo[*e*]pyrene, benzo[*b*]triphenylene)	B[*a*]P, DB[*a,h*]A, DMB[*a*]A
Lactones (coumarin, α-angelica lactone)	B[*a*]P, DMB[*a*]A
Alcohols (ethanol, *n*-butanol, *tert*-butanol, cholesterol, β-sitosterol, α- and β-4,8,13-duvane-1,3-diol	NNN, DMB[*a*]A
Purines (caffeine, theobromine)	Ethyl carbamate, *N*-nitrosamines, DMB[*a*]A
Indoles (indole, indole-3-acetonitrile)	B[*a*]P
Miscellaneous components (maleic anhydride, aconitic acid, selenium, carbon disulfide)	B[*a*]P, DMB[*a*]A, 1,2-dimethylhydrazine
Phenols (phenol, caffeic acid, ferulic acid, gallic acid; 2-hydroxycinnamic acid; 4-methoxyphenol; α-tocopherol) (see Table 9.9)	B[*a*]P, *N*-nitrosamines, 1,2-dimethylhydrazine, DMB[*a*]A, 1,2-dihydro-3-methylbenz[*e*]aceanthrylene (3-methylcholanthrene)

NNK, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone; NNN, *N*′-nitrosonornicotine.

Hoffmann et al. (1766) reported that the results from their study of the levels of several selected components in the MSSs from different tobacco products gave suggestive support to the hypothesis that B[*a*]P and phenol may serve as "indicators" of the specific tumorigenic activities (initiation, promotion) of tobacco "tars." During the next decade, the hypothesis that phenol was an "indicator" of the low-molecular-weight, promoting phenols was reiterated numerous times by Wynder and Hoffmann (4319, 4330, 4332, 4342, 4344, 4346, 4346a). However, as research on the biological effects of phenols in tobacco smoke escalated, it became obvious that the promoting effect of the low-molecular-weight phenols on the specific tumorigenicity of PAHs in tobacco smoke was not as definitive as Wynder and Hoffmann and other investigators asserted. The discovery that a large percentage of the volatile phenols are removed from MSS by the plasticized filter tip led to differences of opinion on the promoting action of the volatile phenols.

Numerous statements in Hoffmann–Wynder presentations and publications described their conclusions with respect to volatile phenols removal *vs*. tumorigenicity of the phenol-depleted CSC. Examples of Wynder–Hoffmann statements follow:

In their 1967 book, Wynder and Hoffmann [(4340), see p. 626 in (4332)] stated:

> It should be noted, however, that a reduction of phenols in tobacco smoke condensate has not led to a concomitant reduction of tumorigenicity in the corresponding "tars."

In 1968, Wynder and Hoffmann (4342) again discussed phenols as promoters:

> Volatile phenols represent one type of tumor promoter in tobacco smoke. In mouse-skin carcinogenesis, however, they evidently do not play an essential role as such, since a significant reduction of phenols in the smoke condensate is not accompanied by a similar reduction in carcinogenic activity of the "tar" [4332].

A year later, Wynder and Hoffmann [see p. 298 in (4344)] wrote:

> The only known group of promoters in tobacco smoke are the volatile phenols. Their reduction of up to 80% by selective filtration, however, did not lead to a reduction of tumor promoting activity.

In the same article, they added [p. 299 in (4344)]:

> A reduction of phenol in tobacco smoke through the use of filters, however, does not alter the complete tumorigenic activity of "tar" obtained from such cigarettes. This infers that a selected reduction of volatile phenols will not reduce the tumor-promoting activity of such "tar."

In the written introduction to their presentation at the 28th TCRC in 1974, Hecht et al. (1582) stated the following and cited Wynder and Hoffmann (4332) as their source:

> Phenol and some substituted phenols are weak promoters, but they alone contribute only a small part of the promoting activity, since selective filtration of phenol does not change significantly the biological activity of the resulting condensate.

In their discussion of tumor promoters and the complexity of CSC, Van Duuren et al. (4035) reported:

> Phenol, which is a weak tumor-promoting agent, is indeed an inhibitor of tumorigenesis when applied simultaneously with benzo[*a*]pyrene.

Van Duuren et al. also noted that rutin, a tobacco component, also inhibited B[*a*]P carcinogenesis in the mouse-skin-painting bioassay. From the results of their biological experiments on cocarcinogenesis [simultaneous and repeated application of an agent, in this case 1,2-benzenediol (catechol)], with B[*a*]P, Van Duuren et al. (4029) deduced that 1,2-benzenediol (catechol) showed remarkable cocarcinogenic activity with B[*a*]P. They reported:

> Phenol has been regarded as an important 'tumor promoter' in cigarette smoke condensate…[but our] work indicates it is inactive in cocarcinogenesis and, indeed, has a slightly inhibitory effect on benzo[*a*]pyrene carcinogenesis.

Later, Van Duuren and Goldschmidt (4028) demonstrated the cocarcinogenicity of 1,2-benzenediol (catechol) when applied as a 2% solution to mouse skin three times weekly with a solution of 0.005% B[*a*]P. They contrasted the remarkable cocarcinogenic activity of 1,2-benzenediol (catechol) with its inactivity as a tumor promoter for B[*a*]P.

Hecht et al. (1562) described the importance of 1,2-benzenediol (catechol) as a tobacco smoke cocarcinogen. They also noted that the levels of 1,2-benzenediol (catechol) in MSS were reduced by prior extraction of the tobacco with hexane–ethanol or by inclusion of reconstituted tobacco sheet (RTS) in the tobacco blend.

While Wynder and Hoffmann wrote at length about the promoting effect of low-molecular-weight phenols and the phenol fraction of CSC on PAH tumorigenicity, it is interesting to note their change in emphasis in 1986. In a 1986 article (1808), the Hoffmann–Wynder discussion dealt primarily with the nature of tumor initiators (PAHs) and cocarcinogens (catechols), with no mention of the phenolic promoters they had discussed repeatedly for more than two decades since the early 1960s! In that same year, the IARC published its monograph on tobacco smoking to which Wynder and Hoffmann had contributed substantial information on tobacco smoke chemistry. In its monograph, IARC defined the phenols as a major group of promoting agents in tobacco smoke (1870), but IARC made no mention of the Wynder–Hoffmann observation of a lack of effect on specific tumorigenicity of the almost complete removal of the phenols from MSS.

Although much was written during the 1950s, 1960s, and 1970s about the supposed adverse effect, i.e., the promoting effect of phenolic compounds in tobacco smoke on its specific tumorigenicity in laboratory animals, significant properties, e.g., their anticarcinogenicity and/or antipromoting

TABLE 9.12
Tobacco Smoke Phenols with AC or AP Properties

Phenolic Smoke Component	Reference to Identification in Tobacco Smoke	Reference to AC or AP
Benzoic acid, 3,4,5-trihydroxy- {gallic acid}	Kröller (2195)	(AC) Mirvish et al. (2559c)
1*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)- {α-tocopherol}	Rodgman and Cook (3271, 3286), Rodgman (3251)	(AC) Shamberger (3625), Slaga and Bracken (3684), Viaje et al. (4049a), Shklar (3655a), Weerapradist and Shklar, (4159a), Toth and Patil (3927a), Mirvish (2559b)
Phenol	Vohl and Eulenberg (4065), Ludwig (2408), Ikeda (1857)	(AP) Van Duuren et al. (4035)
Phenol, 4-methoxy-	Spears (3764)	(AC) Wattenberg et al. (4149c)
2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, *cis*- {*cis*-caffeic acid}	Yang et al. (4376), Yang and Wender (4377), Wender and Yang (4163)	(AC) Wattenberg et al. (4149c); Wattenberg (4149b)
2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, *trans*- {*trans*-caffeic acid}	Yang et al. (4376), Yang and Wender (4377), Wender and Yang (4163)	(AC) Wattenberg et al. (4149c); Wattenberg (4149b)
2-Propenoic acid, 3-hydroxy-4-methoxyphenyl)-, *trans*- {ferulic acid}	Yang and Wender (4377)	(AC) Wattenberg (4149b)

AC, Anticarcinogenesis; AP, Antipromotion.

effects, of several specific tobacco smoke phenols have generally been overlooked. Phenolic compounds in tobacco smoke known to possess either of these properties are listed in Table 9.12.

In addition to the known antitumorigenic and anti-promoting effects of CSC and several specific components in it, it has also been shown by Lee et al. (2327a, 2327b, 2337c) that cigarette MSS possess antimutagenic properties that offset the mutagenicity in the Ames test (*Salmonella typhimurium*)of several *N*-nitrosamines and several of the *N*-heterocyclic amines defined as "cooked food" mutagens.

9.1.3 Determination of the Nature of the Precursors in Tobacco of the Phenols in Mainstream Smoke

Resolution of the question of the presence of tetracyclic and higher PAHs, particularly B[*a*]P, in tobacco smoke was followed chronologically by studies to determine the source of the PAHs in tobacco smoke. When the PAH-containing environmental pollutants from lighting sources (matches, hydrocarbon-fueled cigarette lighters, etc.) were discarded in the early 1950s as significant contributors to the PAHs in tobacco smoke, particularly cigarette MSS, the contribution of tobacco itself to the PAHs in smoke was questioned: What were the components in tobacco that, during the smoking process, could act as significant precursors of the PAHs in its smoke? The investigation sequence was essentially the same with the reported tumorigenic aza-arenes in tobacco smoke: Initially, the identifications of the aza-arenes were resolved. Subsequently, studies were conducted to define the precursors in tobacco of the aza-arenes identified in tobacco smoke. As noted previously, however (see Table 9.1 and accompanying text), the results reported on numerous studies between 1963 and 1992 have raised other serious questions concerning the presence of the aza-arenes dibenz[*a,h*]acridine, dibenz[*a,j*] acridine, and 7*H*-dibenzo[*c,g*]carbazole in tobacco smoke and their supposed generation from nicotine.

The difference in the levels of simple phenols in tobacco smoke *vs*. their levels in the major tobacco types (flue-cured, burley, Maryland tobaccos), which collectively constitute the major proportion of American cigarette tobacco blends, suggested that the simple phenols in cigarette MSS were present not as a result of their significant direct transfer per se from the tobacco but as a result of their pyrosynthesis from precursors comprising one or more tobacco components. Long before the concern expressed that the simple phenols possessed promoting activity that enhanced the tumorigenicity of tumorigenic PAHs (414) and the concern expressed by Roe et al. (3314) and Wynder and Hoffmann (4307) about the presence of the simple phenols in tobacco smoke, Wenusch (4202) had suggested that the major sources in tobacco of the tobacco smoke phenols were its lignin and complex carbohydrate and polyphenol components.

In contrast to flue-cured, burley, and Maryland tobaccos, highly aromatic tobaccos such as Latakia were reported to contain significant levels of free simple phenols (1876, 1877a). As the complexity of the phenols increased, the likelihood of their presence in tobacco increased and many were found in smoke as a result of direct transfer, e.g., the high-molecular-weight phenol 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-1*H*-1-benzopyran-6-ol (α-tocopherol), first identified as a tobacco component by Rowland (3347) and as a tobacco smoke component by Rodgman and Cook (3271), and 6,7-dihydroxy-2*H*-1-benzopyran-6-one (esculetin), identified in tobacco and its smoke by Dieterman et al. (969). In the early 1960s, Herrmann (1625, 1626) reviewed

various studies on the phenols, phenolic acids, and related compounds identified in tobacco and tobacco smoke.

Examination of the chronology of the investigation of phenolic components of tobacco smoke reveals an interesting situation. In the early 1960s, substantial research was conducted on the phenols in tobacco smoke, their identification, their quantitation, and their major precursors in tobacco. When the promoting effect of the low-molecular-weight monohydric phenols was seriously questioned, the effort on phenols waned for some years but accelerated again when the claims on the cocarcinogenicity of the dihydric phenols, particularly 1,2-benzenediol (catechol), surfaced. This situation triggered examination of the levels of the benzenediols in tobacco smoke and their possible precursors in tobacco. Table 9.13 summarizes some of the studies conducted to define the nature of the major precursors in tobacco of the phenolic components of tobacco smoke.

Zane and Wender (4403) described their pyrolysis (pyrolysis temperature that of a Bunsen burner flame) of the tobacco components rutin, quercetin, and chlorogenic acid. In addition to nonphenolic compounds, each pyrolysate was reported to contain 1,2-benzenediol (catechol) with lesser amounts of 4-methyl-1,2-benzenediol, 1,3-benzenediol (resorcinol).

The amounts of phenol and 4-methylphenol (*p*-cresol) in the pyrolysates obtained under various conditions from several major tobacco components (cellulose, pectin, and lignin), a tobacco additive (invert sugar), several individual tobacco types (flue-cured tobacco, cased burley tobacco, Maryland tobacco), and a tobacco substitute (spinach) were reported by Rodgman and Mims (3305) and Rodgman and Cook (3286). Table 9.14 summarizes the results.

Spears et al. (3767) and Bell et al. (248) determined the generation of phenol when flue-cured and burley tobaccos and various tobacco components (glucose, sucrose, starch, cellulose, and pectin) were pyrolyzed at various temperatures in an air or nitrogen atmosphere. In each instance, phenol was generated.

In their study of tobacco lignin as a phenols precursor, Kato et al. (2043) examined the residue resulting from heating tobacco stalk lignin at 450°C–500°C for 2 h. They identified the following phenols: phenol, 2-methoxyphenol (guaiacol), 2-methylphenol (*o*-cresol), 3-methylphenol (*m*-cresol), and 4-methylphenol (*p*-cresol). Kato et al. (2046) also conducted a comparative thermal analysis of tobacco stalk-derived cellulose, holocellulose, and lignin subjected to similar heating.

In a continuation of the pyrolysis study by Chortyk et al. (725a, 726) on the possible contribution of the tobacco pigment to the PAH content of tobacco smoke composition, Schlotzhauer et al. (3468) examined the pyrogenesis of phenols from high-molecular-weight components of tobacco, specifically the tobacco pigment and the biopolymers lignin, cellulose, and pectin. Schlotzhauer et al. (3468) reported that the phenol amounts [phenol, 3- and 4-methylphenol (*m*- and *p*-cresol)] found in the pyrolysates from Oriental tobacco and the high-molecular-weight tobacco components (pigment, lignin, pectin, cellulose) pyrolyzed at 700°C/nitrogen atmosphere were generated in the following sequence:

Oriental tobacco > pigment > lignin ≥ pectin >> cellulose

In a study of the effect of steady state pyrolysis of tobacco *vs.* pulsed pyrolysis simulating the puffing sequence in a smoked cigarette, Patterson et al. (2904) reported that the pulsed pyrolysis procedure gave much higher levels of the low-molecular-weight phenols [phenol, 2-, 3-, and 4-methylphenol (*o*-, *m*-, and *p*-cresol), 2-, 3- and 4-ethylphenol, 2,4- and 2,5-dimethylphenol (2,4- and 2,5-xylenol), 2-methoxyphenol (guaiacol)] in the pyrolysate than did the steady state pyrolysis.

The report of the significant cocarcinogenicity of 1,2-benzenediol (catechol) by Van Duuren and Goldschmidt (4028) and the subsequent confirmation of its cocarcinogenicity by Hecht et al. (1562) triggered considerable interest in the source in tobacco of 1,2-benzenediol (catechol) in tobacco smoke.

In the early 1980s, Schlotzhauer et al. (3462) and Schlotzhauer and Chortyk (3453) at the USDA in their study of the precursors in tobacco of phenols in tobacco smoke investigated the pyrolysis of various solvent-extracted fractions from tobacco plus the tobacco residue after extraction. The extracted tobacco residue, the ethanol extract, and the methanol extract were the major sources of benzenediols (catechol, resorcinol, hydroquinone). From these results, it was proposed that chlorogenic acid in tobacco was a major precursor of the benzenediols, particularly 1,2-benzenediol (catechol), in tobacco smoke. The extracted tobacco residue was also reported as the major source of the monohydric phenols (phenol, cresols, xylenols, guaiacols).

Figure 9.2 illustrates the possible relationship between 1,2-benzenediol (catechol) and several complex tobacco phenols subsequently studied as its precursor.

In a continuation of their study of the conversion of various tobacco components to catechol, Schlotzhauer et al. (3462) examined the phenols formed during the pyrolysis of a variety of tobacco components, including chlorogenic and caffeic acids, rutin and quercetin, cellulose and lignin, and fructose and sucrose (Table 9.15). They reported that chlorogenic acid, usually the most abundant polyphenol in tobacco, produced the highest levels of 1,2-benzenediol (catechol) and 4-ethyl-1,2-benzenediol (4-ethylcatechol) during pyrolysis. In addition, the tobacco biopolymer lignin was also reported to be a significant source of 1,2-benzenediol (catechol). Their examination of the phenols generation by pyrolysis of several different flue-cured and burley tobaccos indicated that the flue-cured tobaccos produced significantly higher levels of the phenols than did the burley tobaccos. A similar situation is obtained when the MSS phenols from cigarettes fabricated from all flue-cured and all burley tobaccos are compared on a per milligram of phenol per milligram of CSC basis [Wynder and Hoffmann (4317), cf. Wynder and Hoffmann (4332)].

Because they considered 1,2-benzenediol (catechol) a "major constituent of tobacco smoke," a component they considered an important contributor to the biological properties of smoke, Hoffmann and his colleagues at the American Health

TABLE 9.13
Precursors in Tobacco of Phenols in Tobacco Smoke

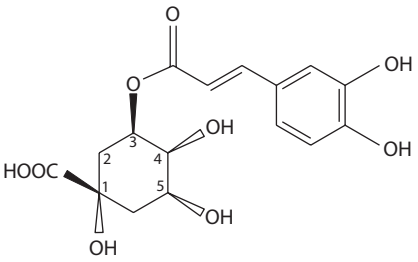
Tobacco Smoke Phenol	Tobacco Leaf Precursor	References
Phenol, Methylphenols {cresols}, Dimethylphenols {xylenols}, Benzenediols {catechol, resorcinol, hydroquinone}	Lignin	Rodgman and Mims (3305), Kato et al. (2043, 2046), Schlotzhauer et al. (3456, 3462, 3468), Higman et al. (1647), Carmella et al. (598)
	Sugars	Spears et al. (3767), Bell et al. (248), Higman et al. (1647), Carmella et al. (598, 602), Schlotzhauer et al. (3462)
	Polysaccharides (cellulose, starch, pectin)	Kato et al. (2043, 2046), Spears et al. (3767), Bell et al. (248), Schlotzhauer et al. (3456, 3462, 3468), Higman et al. (1647), Brunnemann et al. (496, 497), 1975, 1976, Carmella et al. (598, 601, 602)
	Protein	Higman et al. (1647)
	Amino acids	Higman et al. (1647)
	Extracted tobacco	Rodgman and Cook (3277), Rodgman and Mims (3305), Severson et al. (3616), Carmella et al. (600), Schlotzhauer et al. (3453, 3462)
	Tobacco pigment	Schlotzhauer et al. (3468)
	Tobacco extracts	Schlotzhauer et al. (3456), Severson et al. (3616)
	Rutin	Zane and Wender (4403), Spears et al. (3767), Bell et al. (248), Brunnemann et al. (496, 497), Carmella et al. (598), Schlotzhauer et al. (3462)
	Quinic acid[a]	Ayres and Thornton (127a)
	Chlorogenic acid[b]	Zane and Wender (4403); Brunnemann et al. (496, 497), Carmella et al. (598, 600, 602); Schlotzhauer et al. (3462)

[a] Quinic acid = 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid.
[b] Chlorogenic acid = 3-(3,4-dihydroxyphenyl)-2-propenoic acid, 3-ester with 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid.

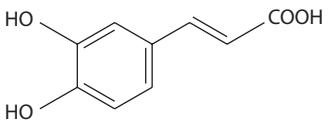
Foundation conducted an extensive study in the early 1980s on the pyrosynthesis of 1,2-benzenediol (catechol) during the tobacco smoking process. The goal of the study was to determine the major precursor(s) in tobacco of the 1,2-benzenediol (catechol) in MSS. Initial experiments by Carmella et al. (600) involved the sequential extraction of tobacco with hexane, chloroform, benzene, and methanol, followed by pyrolysis of the material extracted by each solvent and determination of the 1,2-benzenediol (catechol) in the pyrolysate. Only the pyrolysates from the methanol extract and the residual extracted tobacco indicated the presence of 1,2-benzenediol (catechol) precursors.

TABLE 9.14
Pyrolysis of Tobacco, Tobacco Components, and Spinach: Phenol Content of Pyrolysate

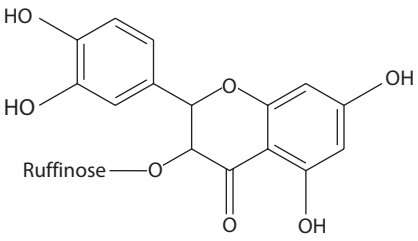
			Phenol, µg/g Pyrolyzed	
Material Pyrolyzed	**Atmosphere**	***T*, °C**	**Phenol**	**4-Methylphenol (*p*-Cresol)**
Individual component				
Cellulose	Nitrogen	550	460	215
Cellulose	Nitrogen	650	350	110
Pectin	Nitrogen	550	310	130
Lignin	Nitrogen	550	2370	2330
Lignin	Air	550	440	460
Invert sugar	Nitrogen	550	140	50
Tobaccos and spinach				
Flue-cured	Nitrogen	550	730	310
Burley, cased	Nitrogen	550	620	390
Maryland	Nitrogen	550	470	150
Spinach	Nitrogen	550	360	280



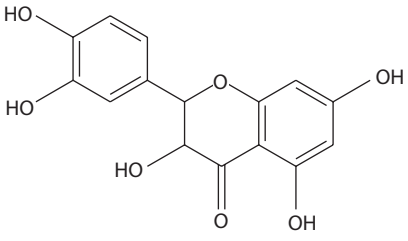
Chlorogenic acid;
3-*O*-caffeoylquinic acid
CAS No. 327-97-9
Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-\



trans-Caffeic acid
CAS No. 4361-87-9
2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-



Rutin
CAS No. 153-18-4
4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-



Quercetin
CAS No. 117-39-5
4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-

FIGURE 9.2 Potential precursors in tobacco of 1,2-benzenediol (catechol) in tobacco smoke.

TABLE 9.15
Pyrolysis of Tobacco Components: Generation of Phenols

	Tobacco Component Pyrolyzed							
Phenol	**Chlorogenic**	**Caffeic Acid**	**Rutin**	**Quercetin**	**Lignin**	**Cellulose**	**Fructose**	**Sucrose**
Phenol	x	—	—	—	x	—	—	—
Phenol, 2-methoxy-[a]	—	—	—	—	x	—	—	—
Phenol, 2-methoxy-4-(1-propenyl)-[b]	—	—	—	—	x	—	—	—
1,2-Benzenediol[c]	x	x	x	x	x	—	—	—
1,2-Benzenediol, 4-methyl-	—	—	x	x	x	—	—	—
1,2-Benzenediol, 4-ethyl-	x	—	x	—	—	—	—	—
1,2-Benzenediol, 4-propyl-	—	—	x	—	—	—	—	—
Furfurals[d]	x	—	...	—	—	x	x	x

[a] Guaiacol.
[b] Isoeugenol.
[c] Catechol.
[d] Furfural and/or 5-(hydroxymethyl)furfural.

From the results of a study in which Kentucky reference 1R1 cigarettes were "spiked" with increasing levels of chlorogenic acid (the 3-ester of 3,4-dihydroxycinnamic acid with 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid), smoked under standard conditions, and the MSS analyzed for 1,2-benzenediol (catechol), Carmella et al. (598) concluded that, under their experimental conditions, chlorogenic acid was not a major precursor in tobacco of 1,2-benzenediol (catechol) in tobacco smoke. This finding was the opposite of that reported by Schlotzhauer et al. (3453, 3462).

In a subsequent study by Carmella et al. (602), tobacco was extracted sequentially with hexane then aqueous methanol. The major components of the aqueous methanol extract were identified as fructose, glucose, sucrose, and chlorogenic acid. Contributions of each of these tobacco components plus the contributions of the tobacco components cellulose and rutin to the 1,2-benzenediol (catechol) level in cigarette MSS were determined in a "spiking" experiment in which cigarettes were "spiked" with each of the components mentioned, two of which were radiolabeled (fructose and cellulose). The minimum contributions of these components to the 1,2-benzenediol (catechol) level in MSS were as follows: cellulose, 7%–12%; total of the sugars, glucose, fructose, and sucrose, 4%; chlorogenic acid, 13%; and rutin, less than 1%. Carmella et al. considered that a significant portion of the unaccounted for 1,2-benzenediol (catechol) was formed from the other biopolymers, pectin, starch, and hemicellulose. It would appear that these 1984 results on the involvement of chlorogenic acid as a 1,2-benzenediol (catechol) precursor differed from those presented previously by the same investigators [Carmella et al. (602) *vs.* Carmella et al. (598) who earlier stated in 1981:

> The results under these experimental conditions [a "spiking" experiment] suggest that chlorogenic acid is not a major precursor of catechol in cigarette smoke.

Carmella et al. (601) reported that cellulose in tobacco was a major precursor of 1,2-benzenediol (catechol) in tobacco smoke. Comparison of the pyrogenesis of 1,2-benzenediol (catechol) from cellulose and carboxymethylcellulose suggested that the 1,2-benzenediol (catechol) level in tobacco smoke might be reduced by modification of the tobacco cellulose. Subsequently, Carmella et al. (599) reported that carboxymethylation of the cellulose in tobacco reduced the1,2-benzenediol (catechol) in the MSS from 252 to 162 µg/cig, a 36% reduction.

In addition to investigations of the possible precursors in tobacco of phenols in cigarette MSS, the contribution of several tobacco additives to phenols in MSS was studied. Many years before the advent of the use of expanded tobacco and filter-tip perforations in the design of low- to medium-"tar" cigarettes, Kato and Shibayama (2044) reported that vanillin (4-hydroxy-3-methoxybenzaldehyde) incorporated in the tobacco blend as a flavorant by many cigarette was converted to phenol during the smoking process and therefore should not be used as a cigarette tobacco flavorant. Contradictory results were reported in a subsequent study by Eble et al. (1105). They reported that no radiolabeled phenol was detected in the cigarette MSS and concluded that vanillin did not generate phenol during the smoking process. The difference between the Kato and Shibayama 1962 results and the Eble et al. 1985 results was readily explained by the difference in the experimental conditions used in the two studies: Kato and Shibayama (2044) used continuous draw in their smoking regime, i.e., no alternating puff and smoldering period, whereas Eble et al. (1105) used the intermittent-puff regime and smoking procedure defined by in the U.S. FTC "tar" and nicotine procedure (35 mL puff volume, 2 s puff duration, 1 puff/min 25°C, 60% relative humidity, etc.).

Many flavoring materials have been proposed for use as flavoring materials in tobacco smoking products. Leffingwell et al. (2341) reported that these range from

individual chemical compounds to a variety of natural herbs, essential oils, and extracts. Many of the proposed flavoring additives for tobacco smoking products have been included in commercial products, but many have not. Among the naturally occurring mixtures used historically were deer tongue, tonka bean, and vanilla extract (2341). In the early 1970s, Higman et al. (1649) investigated the pyrolysis of these three historically used tobacco additives to determine their possible contributions to the composition of cigarette smoke. In addition to numerous monocyclic and PAHs and their monocyclic and polycyclic nitrogen analogs, all three pyrolysates contained phenol, cresols, and xylenols. The deer tongue and tonka bean pyrolysates also contained naphthols and coumarin. With regard to the use of these three materials as tobacco additives, the authors noted:

> The contribution of such additives [tonka bean, deer tongue, vanilla extract] to the chemical and biological effects of cigarette smoke would be in proportion to the amounts of such additives used and also to the pyrolytic-distillation pattern to which the additive is subjected in the thermal flow environment of the burning cigarette.

The report by Gori (1332) and the NCI (2683) on the results obtained in the NCI Smoking and Health Program on "less hazardous" cigarettes (1329, 1330, 1332, 1333, 2683) led to an initial concern about the contribution of cocoa added to tobacco to the chemical and biological properties of the smoke from cigarettes containing cocoa-treated tobacco. Subsequent examination of the biological data indicated that the initial concern was unfounded. Schlotzhauer (3447) at the USDA Athens, GA, research center reported the results of his analysis of the pyrolysis of cocoa powder and its possible contribution to the phenol content of smoke from cigarettes made with cocoa-treated tobacco. Pyrolysis of cocoa at various temperatures (350°, 450°, 550°, 650°, 750°C) yielded phenol, the three dimethylphenols (*o*-, *m*-, and *p*-cresol), several dimethylphenols (xylenols), and 1,2-benzenediol (catechol). From his results, Schlotzhauer concluded:

> Addition of cocoa powder to tobacco products in the quantities normally utilized for flavoring purposes would not… be expected to significantly enhance the phenolic content of tobacco smoke.
>
> Results of the study indicate that the levels of phenols derived from pyrolysis of cocoa should not significantly enhance the phenol content of tobacco smoke…

As shown in Table 9.16, comparison of the MSS phenol data from the NCI study on cocoa-free (Sample Code 83) *vs.* cocoa-treated (Sample Code 82) (1332, 2683) confirms the view expressed by Schlotzhauer (3447):

Over a decade later in 1990, Roemer and Hackenberg (3314a) reported the results of mouse-skin-painting bioassay in which the CSCs from cigarettes containing various levels of cocoa were tested. The CSCs from cigarettes containing different levels of cocoa (0%, 1%, and 3%) were studied for their specific tumorigenicity. Their results contradicted those reported by Gori (1332) for the NCI less hazardous cigarette study. The 1% and 3% addition levels of cocoa were equivalent to and three times, respectively, the level of cocoa usually added to commercial cigarettes. Roemer and Hackenberg noted:

> We found no evidence for indicating an enhancement of the biological activity of cigarette smoke condensates derived from cigarettes to which 1 and 3% cocoa was added.

Additional details pertinent to cocoa are summarized by Rodgman (3264).

TABLE 9.16
Smoke Chemistry Data: NCI Study of Cocoa Addition (1332)

Code No.	Filler	Relative to "Dry" Condensate, µg/g		
		Phenol	*o*-Cresol	*m*- and *p*-Cresol
83	SEB III	4.33	0.68	1.98
82	SEB III + 1% cocoa	4.46	0.75	2.02

9.1.4 Effect of Cigarette Design Parameters on Yield of MSS Phenols

Despite the controversy over the biological properties of the phenols in tobacco smoke, i.e., were they promoters of the tumorigenicity of the PAHs in the mouse-skin-painting bioassay, or were they cocarcinogens for the PAHs in that bioassay, or were they noncontributors or minor contributors to the bioassay results, the next step after identification, refinement of quantitation procedures, and resolution of the question of precursors was the determination of which cigarette design parameters would permit control of the levels of phenols in MSS.

Of course, the first method discovered to control the MSS levels of phenols was their selective filtration by the plasticized cellulose acetate filter tip.

The extensive research on phenols in tobacco smoke eventually led to the resolution of the question whether selective filtration of a particular component or class of components in cigarette MSS was possible. Despite listing effective filtration as an important means to reduce cigarette MSS particulate matter, Wynder and Hoffmann in 1961 (4311) categorized "selective filtration" of a particular component or class of components in cigarette MSS as an impossibility. However, the next year, because of their findings with low-molecular-weight phenols in the MSS of filter-tipped cigarettes, Wynder and Hoffmann (4314) reversed their previously expressed assertion on the impossibility of "selective filtration." They reported that the levels of MSS low-molecular-weight phenols were significantly reduced (75%–90%) by the plasticized cellulose acetate filter tip.

It was determined by numerous investigators within and outside the tobacco industry that highly volatile, low-molecular-weight phenols such as phenol and the isomeric methylphenols (the cresols) were selectively filtered from cigarette MSS. That the filter-tip plasticizer (usually triacetin) played a significant role in the selective filtration was demonstrated in the early 1960s by Lorillard (2399), Laurene (2295, 2295a, 2298), Laurene et al. (2311, 2312), Spears (3765), and Hoffmann and Wynder (1791). Brown and Williamson patented the use of Carbowax® as an alternative filter-tip additive for selective filtration of low-molecular-weight phenols. Low-molecular-weight phenol levels in MSS were reduced 75%–90% by the selective filtration of triacetin- or Carbowax-treated cellulose acetate. Because of the volatility of the low-molecular-weight phenols, an equilibrium exists between these components of the tobacco smoke aerosol vapor phase and of the tobacco smoke aerosol particulate phase. Thus, these components are substantially partitioned between the particulate phase and vapor phase of cigarette MSS aerosol. The selective filtration (75%–90%) occurs by removal from the smoke stream of significant amounts of low-molecular-weight phenols in the aerosol vapor phase. During the brief time of the MSS transit through the plasticized filter tip, removal of the phenols from the vapor phase results in vaporization of the phenols from the particles in an attempt to reestablish the original particulate-phase and vapor-phase equilibrium.

Subsequently, it was determined by Fredrickson (1236) in the mid-1960s and by Morie and Sloan (2635) and Brunnemann et al. (514) in the 1970s that similar selective filtration occurred with volatile *N*-nitrosamines such as *N*-dimethylnitrosamine and *N*-diethylnitrosamine with 70%–80% of the volatile *N*-nitrosamines being removed from MSS by a plasticized cellulose acetate filter tip.

The discovery in the early 1960s of the selective filtration of the low-molecular-weight phenols from cigarette MSS was subsequently confirmed by numerous investigators throughout the world. As shown by the citations in Table 9.17, the selective filtration of phenols from cigarette MSS was extensively studied from the early 1960s to the mid-1970s. A few additional studies have been described from the mid-1970s to date.

From these studies, it was also reported by Laurene et al. (2311, 2312) that the effectiveness of the selective filtration of plasticized filter-tip cigarettes decreased during the shelf life of the cigarette.

Discovery of the extensive partitioning of low-molecular-weight phenols between the particulate and vapor phase of cigarette MSS necessitated modifications in their determination. While several low-molecular-weight PAHs such as naphthalene (mol. wt. 128) and its alkyl derivatives also show some partitioning between the particulate and vapor phases, the high-molecular-weight PAHs [anthracene and phenanthrene (mol. wt. 178),

TABLE 9.17
Studies on the Selective Filtration of Phenolic Compounds in Cigarette MSS

Year	Investigator(s)	Year	Investigator(s)
1962	Davis and George (911a)	1967	George and Keith (1284)
	Lorillard (2399)		Müller and Moldenhauer (2653)
			Waltz et al. (4122)
1963	Hoffmann and Wynder (1791)		
	Laurene (2295, 2295a)	1968	George (1283)
	Laurene et al. (2311, 2312)		Kallianos et al. (2016)
	Spears (3765)		
	Waltz and Häusermann (4118)	1969	Georgiev (1284a, 1284b)
1964	Esterle and Campbell (1164)		
	Pyriki and Moldenhauer, 1964	1970	Reynolds (3111)
	Seehofer et al. (3574)		
	Testa et al. (3890)	1972	Artho et al. (105)
1965	Cuzin et al. (884)	1974	Baggett and Morie (156)
	George (1282a)		
	Kaburaki et al. (1996)	1975	Baggett and Morie (156)
	Laurene (2298)		Brunnemann et al. (496)
	LeRoux (2351)		
	Lipp (2376, 2377)	1976	Brunnemann et al. (497)
	SEITA (3602)		Kensler (2082)
	Waltz and Häusermann (4121)		
		1980	Mokhnachev and Mironenko (2579)
1966	Kallianos et al. (2016)		
	Müller and Moldenhauer (2653)	1994	Wilson (4268)
	Touey and Kiefer (3937)		

B[*a*]A (mol. wt. 228), DB[*a,h*]A (mol. wt. 278), B[*a*]P (mol. wt. 252)] exist almost exclusively in the particulate phase. Before the extent of this partitioning and the selective filtration of low-molecular-weight phenols had been determined, most early studies dealt with analysis for the per cigarette yield of the low-molecular-weight phenols in the particulate phase. Thus, the relationships between the per cigarette levels of the tumorigenic PAHs and these phenols in mainstream CSC and the proposed promotion of the specific tumorigenicity of the PAHs by the phenols required reassessment.

This research observation-based comment raises the question about the repeated assertion of the importance of the promoting activity of phenol and other low-molecular-weight phenols, particularly in their supposed enhancement of the specific tumorigenicity of PAHs: What kind of tobacco smoke promoter is it that exerts so little effect that, in its absence, the specific tumorigenicity in the mouse-skin-painting bioassay of the CSC remains essentially unaltered?

Table 9.18 illustrates the effect of several tobacco expansion procedures and inclusion of the expanded tobacco in the cigarette blend on the MSS phenol yield.

Brunnemann et al. (496, 497) confirmed the previous finding of Waltz et al. (4123) that that 1,2-benzenediol (catechol) was the phenol usually present at the highest yield in cigarette MSS. Brunnemann et al. determined that the level of 1,2-benzenediol (catechol) in the MSS of a nonfiltered cigarette varied from 160 to 500 µg/cig. The level of 1,2-benzenediol (catechol) in the MSS from a filter-tipped cigarette varied from 60 to 200 µg/cig. They also reported that 1,2-benzenediol (catechol) and its derivatives were not selectively reduced by commercial cigarette filter tips as were many low-molecular-weight monohydric (one hydroxyl group) phenols.

In 1953, when RTS was introduced into its cigarette products by R.J. Reynolds Tobacco Company as a cigarette design technology, little was known about either the nature or yields of phenols in cigarette MSS (see Table 9.4). Also, the promoting activity of low-molecular-weight phenols to the specific tumorigenicity of PAHs had not been reported

TABLE 9.18
Effect of Tobacco Expansion on Levels of MSS Phenols

RJRT-Expanded Tobacco Study (3254)

Tobacco Blend Composition		MSS Level	
% Control Blend[a]	% RJRT-Expanded Blend	µg/cig	mg/g WTPM
100	0	117	3.36
90	10	106 (9)[b]	3.73 (−11)
75	25	95 (19)	3.36 (0)
50	50	72 (38)	2.76 (18)
0	100	45 (62)	2.16 (36)
% Flue-Cured	% RJRT-Expanded Flue-Cured		
100	0	126	3.09
0	100	70 (44)[c]	2.99 (3)

NCI "Less Hazardous" Cigarette Study (1330, 2683)

		MSS Level, mg/g WTPM		
Tobacco	Code No.	Phenol	*o*-Cresol	*m*- + *p*-Cresol
SEBII[a]	42	3.83	0.62	2.04
SEBII	42	3.66	0.55	1.78
SEBII	44	3.90	0.63	1.56
SEBII	45	3.81	0.59	1.65
SEBII	Avg	3.80	0.60	1.76
RJRT-expanded SEBII	48	2.56 (33)[b]	0.36 (40)	1.10 (40)
PM-expanded SEBII	49	2.93 (23)	0.40 (33)	1.37 (26)
NCSU-freeze-dried SEBII	50	3.47 (9)	0.49 (18)	1.61 (13)

[a] WTPM, wet total particulate matter.
[b] SEBII, the Standard Experimental Blend used in the second phase of the NCI "Less Hazardous" Cigarette Study.
[c] The number in parenthesis is the % decrease of the MSS yield of phenols in the MSS from the expanded or freeze-dried SEBII *vs*. that in the MSS from the control SEBII.

by Boutwell et al. (414). Until the early to mid-1960s, the contribution of RTS to MSS composition dealt primarily with the decrease in the yields of the MSS PAHs, particularly B[*a*]P, and the decrease in the specific tumorigenicity (mouse skin) of the CSC as the % inclusion of the RTS in the blend was increased [see pp. 531–532 in (4332)].

Reports presented during the "less hazardous" cigarette workshop held at the *1967 World Conference on Smoking and Health* were published the next year as an NCI monograph edited by Wynder and Hoffmann (4343). Moshy and Halter presented data on the effect of inclusion of experimental RTS in a blend. They wrote (2647a):

> It is apparent from the data [presented] that selective reductions of up to 45% for benzo[*a*]pyrene and up to 87% for phenol were achieved with some of the experimental tobacco leaves [sic].

At the same conference, Hoffmann and Wynder (1798) also discussed the % reduction of the PAH content, specifically the B[*a*]P content, of the cigarette CSC by inclusion of RTS in the cigarette tobacco blend. Although analytical data on the decrease in TPM, B[*a*]P, and phenol yields were presented graphically, they had no comment on the significant % reduction in the phenol content of the MSS, a % reduction that exceeded that of the B[*a*]P content.

In the NCI Smoking and Health Program on the "less hazardous" cigarette, the substantially lowering of the yields of phenol and the 2-, 3-, and 4-methylphenols (*o*-, *m*-, and *p*-cresols) in the MSS from RTS (paper process) cigarettes *vs*. the tobacco blend (SEBI) was recorded (1329).

At RJRT R&D, Newell et al. (2765) reported the results of a detailed study of the effect of increasing the level of RTS (G7) on the composition of cigarette MSS. Decreased MSS yields of the PAHs, nicotine, and phenols plus increased yields in carbon monoxide, aldehydes, ketones, and low-molecular-weight acids were observed.

In 1979, the U.S. Surgeon General (4005) reported the beneficial effects of inclusion of RTS on the MSS composition (B[*a*]P, phenols, specific tumorigenicity):

> Cigarette fillers low in wax layer components, either by use of tobacco stems, reconstituted tobacco sheet, or tobacco extracted with a hexane-ethanol mixture, delivered smoke significantly reduced in catechols … Although it has not been directly established that a selective reduction in catechol leads to a significant reduction of the tumorigenic potential of cigarette smoke, it is of interest that all those tars or whole smokes of cigarettes which are low in catechol also have a significant lower tumorigenic activity [Gori (1329, 1330, 1332)].

These comments on the relationship between RTS and the 1,2-benzenediol (catechol) yield in MSS are of interest because examination of the MSS data from the four sets of experimental cigarettes [Gori (1329, 1330, 1332, 1333), NCI (2683)] reveals that no analysis for 1,2-benzenediol (catechol) was conducted on any of the cigarette samples in the study, i.e., the 100 or so experimental cigarettes or the standard SEBI, SEBII, SEBIII, or SEBIV cigarettes and the Kentucky 1R1 reference cigarette.

In the late 1950s and the 1960s, one of the methods studied to control the pyrosynthesis of PAHs from tobacco during the smoking process was the addition of various materials (inorganic or organic) to the tobacco in attempts to control its combustion and lower the per cigarette PAHs yields, particularly the B[*a*]P yield, in the tobacco smoke [Alvord and Cardon (56, 57), Lindsey et al. (2370), Rodgman (3246, 3254), Bentley and Burgan (286), Candeli et al. (589), Wynder and Hoffmann (4311, 4317, 4319, 4332), Cuzin et al. (885), deSouza and Scherbak (953), Pyriki et al. (3046), Hoffmann and Wynder (1797, 1798)].

The most effective additives in PAHs reduction were the nitrates. The following explanation of their effectiveness was offered: When heated, the nitrates generate nitric oxide (NO), an odd-electron compound, capable of "scavenging" free radicals thermally generated from tobacco components during the smoking process, thus interrupting the free radical reactions postulated as contributing to one of the mechanisms important in the generation of PAHs in tobacco smoke [see Badger and Spotswood (152), Badger (139a, 140), Badger et al. (141, 142, 147)].

However, in addition to lowering the levels of PAHs in tobacco smoke, addition of nitrates or the use of high-nitrate tobacco affected MSS yield and composition in other ways. In the 1950s and early 1960s, the reductions in the MSS yields of "tar," nicotine, and PAHs in general and B[*a*]P in particular were viewed as desirable achievements. When concern was expressed about the supposed promoting action of the low-molecular-weight phenols, the reduction of their levels in MSS by nitrate addition to the tobacco was also viewed positively. These decreases were, however, accompanied by an increase in the level of NO in the smoke. Subsequently, two reported observations did much to dampen the enthusiasm for nitrate addition to the tobacco and/or the use of high-nitrate tobaccos in the blend:

- The identification of various volatile and tobacco-specific *N*-nitrosamines in tobacco and its smoke and the positive dependence of their levels in both tobacco and smoke on the nitrate level of the tobacco [Morie and Sloan (2635), Tso et al. (3985), Brunnemann et al. (499)].
- The identification of a series of nitrophenols, many of which are known to be highly toxic, in the MSS from cigarettes fabricated with nitrate-treated tobacco and/or with high-nitrate tobaccos in the blend [Kallianos et al. (2016), Klus and Kuhn (2137)].

Table 9.19 summarizes some of the studies on the use of nitrate addition to tobacco and/or use of high-nitrate tobacco to reduce the yields of PAHs in cigarette MSS. Also noted in Table 9.19 are some of the other compositional changes observed in MSS yield and composition. In most instances, the yields of MSS PAHs in general and B[*a*]P were reduced, although an

TABLE 9.19
Studies Involving Nitrate Addition to Tobacco

Nitrate		Change in CSC			
Identity	Amount Added, %	B[*a*]P Level	Tumorigenicity	Comments	References
$Mg(NO_3)_2 \cdot 6H_2O$	5.0	Decrease			Rodgman and Cook
	2.0	Decrease			
$Al(NO_3)_3 \cdot 9H_2O$	2.0	Decrease			
KNO_3	2.0	Decrease			
	4.0	Decrease			Bentley and Burgan (286)
$Cu(NO_3)_2$	5.0	Decrease			
	2.5	Decrease			
	1.0	Decrease			
$NaNO_3$	5.0	Decrease			
$Cu(NO_3)_2 \cdot 5H_2O$	5.0	Decrease	Decrease		Wynder and Hoffmann (4312)
$Cu(NO_3)_2 \cdot 5H_2O$	5.0	Decrease	Decrease		Wynder and Hoffmann (4317)
$Cu(NO_3)_2 \cdot 5H_2O$		Decrease			Pyriki et al. (3046)
KNO_3				MSS 1,2-benzenediol (catechol) yield/cig inversely related to tobacco nitrate level, 4-nitro-1,2-benzenediol yield/cig related to tobacco nitrate level	Kallianos et al. (2016)
$NaNO_3$	8.3	Decrease	Decrease	TPM/cig decreased, phenol/cig yield decreased, phenol/mg of CSC decreased, no *N*-nitrosamines detected in nitrate-enhanced tobacco cigarettes	Hoffmann and Wynder (4332)
$NaNO_3$	3.0	Decrease	Decrease		Hoffmann and Wynder (1798)
	8.3	Decrease	Decrease		
KNO_3	2.5	Decrease	Decrease		
	0.1% *vs.* 1.66% nitrate tobacco	Decrease		Methylphenols (cresols) yields/mg TPM inversely related to tobacco nitrate level; little difference in phenol/mg TPM delivery	Benner et al. (274)
KNO_3	1.3	ND	ND	Yields of a series of nitrophenols identified in MSS from nitrate-treated and high-nitrate tobacco cigarettes directly proportional to nitrate content of filler	Klus and Kuhn (2137)
KNO_3	2.8	Increase	Decrease	Increased nitrate gave decreased phenol/mg TPM and methylphenols (cresols) levels/mg TPM, NO increased relative to TPM	Gori (1329)
	2.3	Decrease	Decrease		
NO_3 addition		Decrease	Decrease	Nitrate addition and/or use of high-nitrate tobacco classified as "only of academic interest" because of undesirable *N*-nitrosamine-nitrate relationship	Wynder and Hecht (4306d)
NO_3 addition		Decrease	Decrease	Surgeon General reiterated Wynder–Hecht (4306d) comment	USPHS (4005)
		Decrease	Decrease	Despite decreases in TPM, B[*a*]P, phenols, CSC tumorigenicity, use of low-nitrate tobacco or nitrate removal recommended because of undesirable *N*-nitrosamine–nitrate relationship	Brunnemann and Hoffmann (480, 486)
$NaNO_3$	0.7–2.5	Decrease	Decrease	MSS 1,2-benzenediol (catechol) level inversely related to nitrate content of filler; MSS volatile and tobacco-specific *N*-nitrosamine levels proportional to nitrate content of filler	Adams et al. (28)

occasional exception was observed, e.g., in the NCI Smoking and Health Program on "less hazardous" cigarettes the MSS B[*a*]P yield increased with nitrate addition but the B[*a*]A yield decreased (1329). Benner et al. (274) reported that a comparison of the low-molecular-weight phenols in the MSS from high- and low-nitrate tobaccos showed little difference in the yields of phenol/mg TPM but significant decreases in the yields of the methylphenols (the cresols)/mg TPM. Benner et al. (276, 277) also reported that treatment of tobacco with an alternative combustion modifier (3:7 boric acid–sodium tetraborate decahydrate) increased the levels of low-molecular-weight phenols in cigarette MSS, an increase that was paralleled by the increase in low-molecular-weight phenols in the pyrolysates from cellulose or lignin treated with the same boric acid–tetraborate modifier.

In the mid-1970s, Brunnemann et al. (497) described an improved method for the quantitation of 1,2-benzenediol (catechol) in tobacco smoke and a possible way to reduce its MSS level. The procedure they described involved extraction of tobacco with a hexane–ethanol azeotrope which removed from the tobacco what Brunnemann et al. defined as "waxes." They noted:

> Compared to the corresponding control cigarette, the dry TPM [from a cigarette filled with reconstituted tobacco from which the "wax" layer had been removed by hexane-ethanol azeotrope extraction] had been reduced by 44%, the nicotine by 47% and catechol by 85%. This demonstrates a strong, selective reduction of catechols in the smoke by the removal of the "wax" layer.

Additional impetus to study the level and source of 1,2-benzenediol (catechol) in tobacco smoke was provided by Hecht et al. (1562) who asserted that 1,2-benzenediol (catechol) was an important tobacco smoke cocarcinogen. They also noted that the levels of 1,2-benzenediol (catechol) in cigarette MSS were reduced by prior extraction of the tobacco with a hexane–ethanol azeotrope or by inclusion of RTS in the tobacco blend.

From the results of their study of cellulose *vs.* carboxymethylcellulose as a precursor of 1,2-benzenediol (catechol) in tobacco smoke, Carmella et al. (599, 601) reported that the carboxymethylation of tobacco cellulose significantly reduced the level of 1,2-benzenediol (catechol) in tobacco smoke.

Wynder and Hoffmann asserted that cigarette MSS yield and composition were controllable in a beneficial way by increasing the number of cuts/in for the tobacco blend filler. Results obtained in the NCI program on the "less hazardous" cigarette and reported in 1976 by Gori (1329) and 1980 by NCI (2683) were contradictory to the unpublished results obtained in 1963 by Hoffmann and Wynder and later reported by Wynder and Hoffmann [see p. 318 in (4319), pp. 529–531 in (4332), (4330)]. In the NCI study, important analytes such as B[*a*]P, B[*a*]A, phenol, and the three methylphenols (cresols) showed no consistent relationship between their MSS yields and width of cut of the cigarette tobacco filler. The mouse-skin-painting bioassay also showed no consistency between % TBA and the CSCs generated from cigarettes with fillers of different cut widths.

In their report of the results of an unpublished study by Hoffmann and Wynder of the effect of width of cut of the cigarette filler, Wynder and Hoffmann reported that increasing the number of cuts/in (decreasing the cut width) decreased the per cigarette MSS yield of TPM and B[*a*]P. They did not report on the effect of cut width on phenols delivery. However, they did report that the specific tumorigenicity of the CSCs from cigarette fabricated with tobacco at 20, 30, and 50 cuts/in decreased as the number of cuts/in increased [see p. 318 in (4319), pp. 529–531 in (4332), (4330)]. Subsequently, Wynder and Hecht (4306d) tabulated the effect on chemical and biological properties of change in cut width as follows: "insignificant" for the change in per cigarette MSS yields of carbon monoxide, "tar," nicotine, and B[*a*]P, as "insignificant" for the change in MSS ciliatoxicity, as "insignificant" for the change in specific tumorigenicity (mouse skin) of the CSC, and "unknown" for the changes in tumor-promoting effect. Their table was used essentially unchanged by the Surgeon General in his 1979 report on smoking and health (4009).

In the NCI Smoking and Health Program on "less hazardous" cigarettes [Gori (1329), NCI (2683)], the effects of cut width on cigarette smoke properties (chemical composition, biological properties) were not as pronounced as the effects reported by Hoffmann and Wynder in Wynder and Hoffmann [see p. 318 in (4319), pp. 529–531 in (4332), (4330)]. Examination of the summary of these studies in Table 9.20 reveals the lack of confirmation of the Hoffmann–Wynder results. In fact, the proposal that cut width would be a significant technology in the design of a "less hazardous" cigarette was similar to many of the proposals from the so-called cigarette design experts not associated with the tobacco industry. Of the numerous technologies proposed during the decade-long NCI study, only those eight technologies proposed by U.S. tobacco company and/or tobacco supplier R&D personnel were eventually classified as significant by the NCI (2683), Gori (1332, 1333), the U.S. Surgeon General (4005, 4009), and other anti-tobacco smoking investigators such as Hoffmann and Hoffmann (1740).

The effectiveness of the various methods proposed to control the yield of the supposed promoting low-molecular phenols may be summarized as follows:

Tobacco extraction with wax-dissolving nonpolar organic solvents (hexane, pentane) to remove PAH precursors does indeed result in reduced levels of PAHs, including B[*a*]P, in cigarette MSS. However, the solution of what was considered by some as a possible PAH problem is accompanied by the creation of two alternative problems, both of which might be criticized from a scientific point of view. For example, extractive removal of the nonpolar organic solvent-soluble material results in an increase in the percentage of the organic solvent-insoluble biopolymers (the major phenol precursors cellulose, pectins, starch, lignin) in the extracted tobacco residue. Smoking of the extracted residue in cigarette form yields higher levels of low-molecular-weight phenols in the MSS (3277, 3305). In addition, nitrates in the tobacco are not removed by solution in nonpolar organic solvents, so their percentages in the extracted tobacco residue increase. Experimental results reported by Morie and Sloan (2635), Tso et al. (3985), and Brunnemann et al. (499) indicated that smoking of this increased nitrate level extracted residue in cigarette form would yield higher levels of *N*-nitrosamines in the MSS.

TABLE 9.20
Effect of Cut Width on MSS Properties

		PAH[a], µg/g		Phenol, mg/g			
Tobacco, cuts/in.	Condensate, mg/cig	B[a]P	B[a]A	Phenol	2-Methylphenol[b]	3- and 4-Methylphenol[b]	% TBA
Hoffmann and Wynder [see p. 318 in (4319), pp. 529–531 in (4332), (4330)]							
8	29.1	1.27					
20	27.3	1.25					27
30	25.4	1.30					16
50	24.4	0.94					13
60	23.0	0.91					
Gori (1329), NCI (2683)							
20	32.6	0.91	1.40	4.35	0.78	1.85	46[c] 33[d]
32	30.2	0.72	1.20	3.95	0.72	1.83	44.6[c] 45.0[d]
60	29.6	0.86	1.31	4.17	0.63	1.92	39[c] 39[d]

[a] PAH, polycyclic aromatic hydrocarbon; B[*a*]P, benzo[*a*]pyrene; B[*a*]A, benz[*a*]anthracene; % TBA, % tumor-bearing animals.
[b] 2-Methylphenol, 3-methylphenol, 4-methylphenol = *o*-, *m*-, and *p*-cresol, respectively.
[c] Painting dose = 50 mg of cigarette smoke condensate/day.
[d] Painting dose = 25 mg of cigarette smoke condensate/day.

Tobacco extraction with a hexane–ethanol azeotrope selectively reduced the levels of 1,2-benzenediols (catechols) in the cigarette MSS. Tobacco extraction with a polar organic solvent system (aqueous ethanol or aqueous methanol) removes chlorogenic acid, a known major precursor of 1,2-benzenediol (catechol), a phenol categorized as a cocarcinogen.

Because nitrate addition to tobacco resulted in reduction of the cigarette MSS deliveries of "tar," nicotine, PAHs including B[*a*]P, and the low-molecular-weight phenols, nitrate addition and/or use of high-nitrate tobacco was considered to be the way to introduce the most effective combustion modifier. However, while apparently solving several problems concerning MSS yield and composition, nitrate addition caused several alternate problems: Once the levels of *N*-nitrosamines and nitrogen oxides (NO) in tobacco smoke were shown to be positively correlated to the nitrate content of the tobacco filler, nitrate addition and/or the use of high-nitrate tobaccos was eventually viewed as undesirable technologies. In addition, higher nitrate tobacco fillers, whether a result of nitrate addition or inclusion of high-nitrate tobaccos, generated a series of nitrophenols, many of which are known to be highly toxic.

From a comparison of the pyrogenesis of 1,2-benzenediol (catechol) from cellulose *vs.* carboxymethylcellulose, it was reported that the carboxymethylation of tobacco cellulose significantly reduced the level of 1,2-benzenediol (catechol) in tobacco smoke (599, 601).

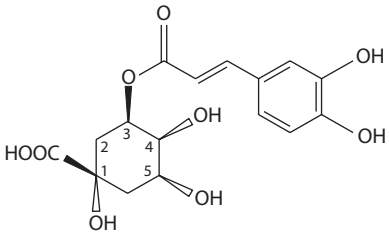
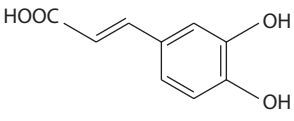
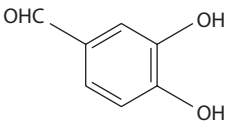
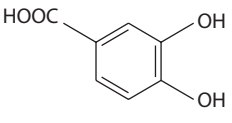
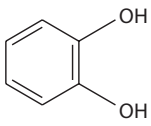
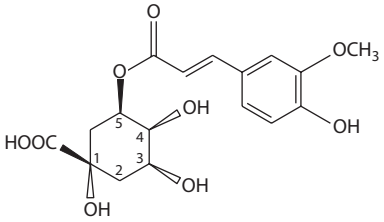
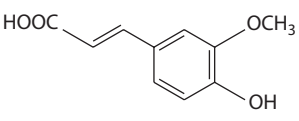
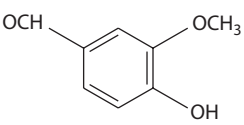
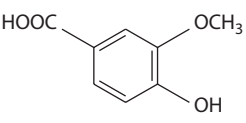
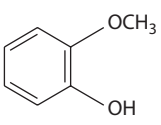
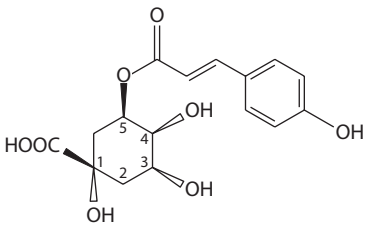
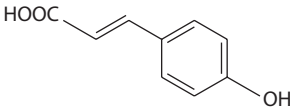
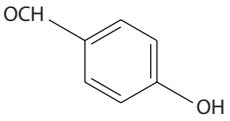
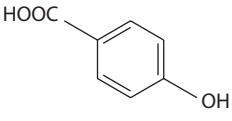
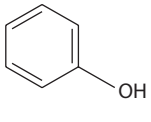
Of the various technologies proposed to control the levels of phenols in cigarette MSS, selective filtration appears to be the most effective and most efficient. A significant portion (65%–75%) of the low-molecular-weight monohydric phenols in cigarette MSS are removed from the smoke stream by a cellulose acetate filter tip plasticized with triacetin. As the cigarette ages, the plasticizer is slowly absorbed by the cellulose acetate fiber and the effectiveness of the selective filtration gradually decreases with time. The one drawback with selective filtration is that it does not occur with dihydric phenols such as 1,2-benzenediol (catechol) in the MSS, i.e., 1,2-benzenediol and its homologs are not selectively removed from MSS by a plasticized filter tip.

Many of the complex tobacco-only phenolic components have interesting structures in that they contain a cyclohexanecarboxylic acid moiety linked to one of the following: (1) a 4-hydroxyphenyl group, e.g., *p*-coumaroylquinic acid; (2) a 3,4-dihydroxyphenyl group, e.g., chlorogenic acid; or (3) a 3-methoxy-4-hydroxyphenyl group, e.g., 3-*O*-feruloylquinic acid. In each case, one can theorize that during the tobacco smoking process, the complex tobacco phenol could sequentially yield a substituted 2-propenoic acid, a substituted benzaldehyde, a substituted benzoic acid, and a simple phenol. Table 9.21 summarizes the possible sequence of the pyrogenesis of such components. Each of the compounds listed as tobacco smoke components in Table 9.21 has been identified in cigarette MSS.

A similar situation exists with a series of components in which a variously substituted 4*H*-1-benzopyranone is linked to a 4-hydroxyphenyl group, e.g., kaempferol, or a 3,4-dihydroxyphenyl group, e.g., quercetin, quercetrin, and rutin.

In Table 9.22, the various phenolic components of tobacco and tobacco smoke are listed, with appropriate references to the identifications for each. Many of the references cited

TABLE 9.21
Theoretical Relationship between Phenols in Tobacco and Several Phenols in Tobacco Smoke

Tobacco Component	Tobacco Smoke Component			
				
Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-{chlorogenic acid; 3-*O*-caffeoylquinic acid}	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*Z*)-{*trans*-caffeic acid}	Benzaldehyde, 3,4-dihydroxy-{protocatechualdehyde}	Benzoic acid, 3,4-dihydroxy-{protocatechuic acid}	1,2-Benzenediol {catechol, pyrocatechol}
327-97-9	4361-87-9	139-85-5	99-50-3	120-80-9
				
Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)-{3-*O*-feruloylquinic acid}	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)-{*trans*-ferulic acid}	Benzaldehyde, 4-hydroxy-3-methoxy-{vanillin}	Benzoic acid, 4-hydroxy-3-methoxy-{vanillic acid}	Phenol, 2-methoxy-{guaiacol}
1899-29-2	1014-83-1	121-33-5	121-34-6	90-05-1
				
Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]-,[1S-(1α,3α,4α,5β)]-{*p*-coumaroylquinic acid}	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*Z*)-{*trans*-coumaric acid}	Benzaldehyde, 4-hydroxy-	Benzoic acid, 4-hydroxy-{*p*-salicylic acid}	Phenol
1899-30-5	4501-31-9	123-08-0	99-96-7	108-95-2

contain additional references pertinent to the phenolic component in question. The many references cited in Table 9.22 include a variety of topics pertinent to the particular phenol. They cover the following topics:

1. The isolation and/or identification of the phenol from tobacco and/or smoke
2. Methods to quantitate the phenolic component in tobacco and/or smoke
3. Determination of the precursors in tobacco of the phenolic compound in smoke
4. Cigarette design technologies to decrease the per cigarette MSS yield of the phenolic compound
5. The biological properties of the phenolic compound
6. Discussions by personnel from governmental agencies, medical institutions, etc., on the biological problems pertinent to a given phenolic compound

While 607 phenolic components have been completely or partially identified in tobacco and tobacco smoke, 305 were identified in tobacco only, 468 in tobacco smoke only, and 166 were identified in both tobacco and tobacco smoke. For the tobacco smoke components partially identified, the nature and/or position of an alkyl substitute was not defined by the investigator.

TABLE 9.22
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

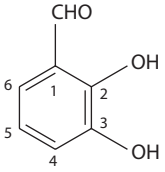
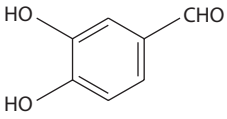
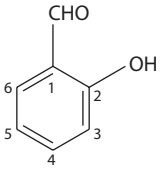
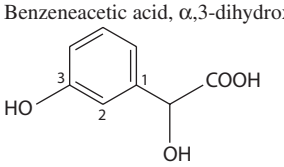
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	621-42-1	Acetamide, 3-hydroxyphenyl-		2917a	
2.	117-12-4	9,10-Anthracenedione, 1,5-dihydroxy-	5480		
3.	1620-98-0	Benzaldehyde, 3,5-di(1,1-dimethylethyl)-4-hydroxy-		2917a	
4.	33774-71-9	Benzaldehyde, dihydroxy-	4249	3748, 5811b	
5.	24677-78-9	Benzaldehyde, 2,3-dihydroxy- 	2939, 3302, 3712, 4249	3797	
6.	95-01-2	Benzaldehyde, 2,4-dihydroxy-	4249		3395, 4249
7.	1194-98-5	Benzaldehyde, 2,5-dihydroxy-	3395, 3712, 4249		3395
8.	139-85-5	Benzaldehyde, 3,4-dihydroxy- {protocatechualdehyde} 	1626, 1884, 2092, 2939, 3712, 3741, 3743, 3797, 4249, 4378, 4379, 5811b	2092, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5811b	3395
9.	134-96-3	Benzaldehyde, 3,5-dimethoxy-4-hydroxy- {syringaldehyde}	568b, 1238, 1884, 2042, 2043, 2046, 3302, 3308, 3712, 3797, 4163, 4249, 4379, 5811b	404, 568b, 3797, 3974a, 4249, 5811b	3395
10.	708-76-9	Benzaldehyde, 4,6-dimethoxy-2-hydroxy-	568b, 4249	568b, 4249	
11.	121-32-4	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}	568b, 2731, 2735, 3266, 3712, 4050, 4249, 4566	568b, 633, 1053, 2281, 2282, 2478, 2699, 3266, 3643, 3894, 4050, 4249	
12.	2539-53-9	Benzaldehyde, 4-ethoxy-3-hydroxy-		5811b	
13.		Benzaldehyde, hydroxy-	5034		
14.	90-02-8	Benzaldehyde, 2-hydroxy- {salicylaldehyde} 	414, 568b, 1238, 1378, 1586, 1626, 1789, 1884, 1906, 2088, 2327c, 2939, 3059, 3266, 3302, 3308, 3557, 3559, 3712, 3797, 4249, 4313, 4317, 4319, 4332, 5811b	120, 568b, 937, 2339a, 2862, 2939, 3059, 3266, 3973, 3974a, 4249, 5811b	1378, 3395, 3401, 3402, 3404
15.	148-53-8	Benzaldehyde, 2-hydroxy-3-methoxy-	5034	3430, 5811b	
16.	698-27-1	Benzaldehyde, 2-hydroxy-4-methyl-		172a, 174b, 1053, 3266	
17.	100-83-4	Benzaldehyde, 3-hydroxy-	568b, 1238, 1364, 1884, 2327c, 2545, 2767, 3302, 3308, 3557, 3712, 3797, 4163, 4379, 5811b	568b, 3797, 3973, 3974a	3404
18.	123-08-0	Benzaldehyde, 4-hydroxy-	568b, 1238, 2042, 2043, 3302, 3308, 3559, 3712, 3797, 4163, 4379, 5811b	568b, 3797, 3973, 3974a, 4249, 5811b	3395, 3404

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
19.	106799-60-4	Benzaldehyde, hydroxy-methoxy-		2339, 5811b	
20.	121-33-5	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}	568b, 1105, 1238, 1352, 1358, 1360, 1361, 1364, 1375, 1375a, 1375b, 1586, 2042–2044, 2327c, 2339, 2570, 2601a, 2640, 2762, 2765, 2767, 3224, 3266, 3302, 3308, 3553, 3557, 3712, 3745, 3797, 4050, 4249, 4379	172a, 174b, 404, 568b, 633, 935, 1053, 1063–1066, 1068–1074, 1105, 1352, 1379, 1590a, 1825, 2281, 2338, 2339, 2339a, 2478, 2389, 2544, 2611, 2699, 2917a, 3159, 3215, 3219, 3266, 3370, 3550, 3643, 3767a, 3797, 3973, 3974a, 4050, 4249	1360, 1375a, 3395
21.		Benzaldehyde, 4-hydroxy-3-methoxy-, labeled with ^{14}C {vanillin-^{14C}}	1105	1105	
22.		Benzaldehyde, hydroxymethyl-	1275, 2767, 4249		
23.	97122-27-5	Benzaldehyde, hydroxy-3-methyl-	3557		
24.	57295-30-4	Benzaldehyde, 3-hydroxy-4-methyl-	1375, 1375b, 4249		
25.	15174-69-3	Benzaldehyde, 4-hydroxy-3-methyl-	1375, 1375b		
26.	17119-15-2	Benzeneacetic acid, α,3-dihydroxy- 	3712, 3737, 3741, 3743, 4249		
27.	1198-84-1	Benzeneacetic acid, α,4-dihydroxy-	3712, 3737, 3741, 3743, 4249, 5811b		
28.		Benzeneacetic acid, α,?-dihydroxy-ethyl-	4249		
29.	19988-45-5	Benzeneacetic acid, 2,3-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
30.	614-82-4	Benzeneacetic acid, 2,4-dihydroxy	5811a		
31.	451-13-8	Benzeneacetic acid, 2,5-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
32.	102-32-9	Benzeneacetic acid, 3,4-dihydroxy-	3712, 3737, 3741, 3743, 5811b	52, 970, 1248, 4249, 4677	
33.	4670-09-1	Benzeneacetic acid, 3,5-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
34.	96937-42-7	Benzeneacetic acid, ar,ar-dihydroxy-ar,ar-dimethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
35.	96937-37-0	Benzeneacetic acid, ar,α-dihydroxy-ar-ethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
36.	96937-48-3	Benzeneacetic acid, ar,ar-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

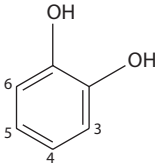
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
37.	96937-41-6	Benzeneacetic acid, 3,4-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
38.	614-75-5	Benzeneacetic acid, 2-hydroxy-	1626, 1884, 2722, 2939, 3302, 3712, 3797, 4163, 4249, 4377, 5811b	2939, 3797, 3973, 3974a, 4163, 4249, 4377, 5811b	
39.	621-37-4	Benzeneacetic acid, 3-hydroxy-	1626, 1884, 2722, 2939, 3302, 3712, 3737, 3741, 3743, 3797, 4113, 4163, 4249, 4377, 5811b	2939, 3797, 3973, 3974a, 4163, 4249, 4377, 5811b	3395
40.	156-38-7	Benzeneacetic acid, 4-hydroxy-	101, 1626, 1884, 1886, 2722, 2939, 3302, 3712, 3797, 4113, 4163, 4249, 4377, 5811b	120, 908, 2722, 2939, 3532, 3560, 3561, 3973, 3974a, 4163, 4249, 4377, 5811b	3393, 3395
41.	306-08-1	Benzeneacetic acid, 4-hydroxy-3-methoxy- {homovanillic acid}	3712, 3737, 3741, 3743, 4113, 4249, 5811b		
42.	14191-95-8	Benzeneacetonitrile, 4-hydroxy-	568b, 1375, 1375b, 1586, 2270, 3712, 3737, 3741, 3743, 4249		
43.	21850-61-3	Benzeneacetonitrile, 4-hydroxy-α-methyl-	3712		
44.		Benzenediol, C_2-alkyl-	2598, 5011		
45.		Benzenediol, C_3-alkyl-	2598		
46.	71630-70-1	Benzenediol, ethyl-nitro-	2137, 3491, 4249		
47.	80934-44-7	Benzenediol, methyl-	1367, 5034	5811b	
48.		Benzenediol, 3-methyl-	1367, 4249		
49.		Benzenediol, methyl-nitro-	1884, 2137, 3491		
50.	62726-14-1	Benzenediol, nitro- {at least four isomers detected}	1884, 2137, 3491, 4249		
51.	120-80-9	1,2-Benzenediol {catechol, pyrocatechol} 	28, 30, 31, 100, 102, 126a, 126b, 172, 174b, 174c, 190, 237, 239, 396, 402, 414, 496, 497, 568b, 596, 598–603, 636, 688, 722, 723, 789, 789a, 830a, 859, 988a, 1051, 1089a, 1099, 1132, 1158, 1217, 1284, 1285, 1332, 1333, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1427, 1437, 1442, 1445, 1448a, 1450,	100, 568b, 970, 1077b, 1102, 1825, 1877a, 2079, 2154, 2379a, 2939, 3430, 3705, 3797, 3973, 3974a, 3976, 4249, 5079, 5811b, 5856	1375a, 1377, 1378, 2210, 2387, 3395, 3402, 4249

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

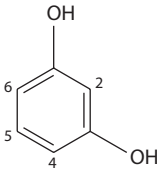
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1,2-Benzenediol {catechol, pyrocatechol} (cont.)	1562, 1582, 1586, 1626, 1673, 1674, 1741, 1743, 1744, 1749, 1751, 1781, 1798, 1808, 1810, 1842, 1870, 1871, 1879, 1882, 1883, 1884, 1887a, 1898, 1981, 2016, 2017, 2060, 2079, 2133, 2195, 2203, 2210, 2313a, 2379a, 2387, 2493, 2524a, 2527c, 2527d, 2527f, 2527g, 2545, 2570, 2594, 2598, 2601a, 2605, 2607, 2615, 2631, 2683, 2767, 2775, 2799a, 2892, 2939, 3007, 3131, 3165, 3166, 3171–3175, 3190, 3255, 3265, 3300, 3302, 3308, 3365, 3370, 3394, 3447, 3453, 3454, 3457, 3462, 3476, 3493, 3551, 3553, 3557, 3602, 3712, 3715–3719, 3737, 3741, 3743, 3746, 3747, 3753, 3754, 3797, 3844, 3879, 3891, 3952, 3992, 4005-4007, 4009–4011, 4113, 4120, 4121, 4123, 4159, 4248, 4249, 4268, 4277, 4319, 4386, 4407, 4414, 4702, 4796, 4965, 5011, 5034, 5049, 5079, 5243, 5500, 5512, 5532, 5564, 5571, 5576, 5643a, 5811b, 5835, 5836		
52.	69845-49-4	1,2-Benzenediol, dimethyl-	3474, 3737, 3741, 3743, 3744, 3745, 3753, 4249, 4897, 5811b		
53.	2785-75-3	1,2-Benzenediol, 3,5-dimethyl-	1378, 3474, 3712, 4249		1378

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
54.	2785-78-6	1,2-Benzenediol, 3,6-dimethyl-	1378, 3712, 4249		1378
55.	98-29-3	1,2-Benzenediol, 4-(1,1-dimethylethyl)-	329, 1879, 1883, 1884, 2016, 2017, 2321, 2322, 3712, 4249		
56.		1,2-Benzenediol, 3-ethenyl	1371, 3255, 4249		
57.	6053-02-7	1,2-Benzenediol, 4-ethenyl-	1089a, 1099, 1879, 1882, 1883, 1884, 1887a, 2321, 2322, 2493, 2524a, 3394, 3462, 3712, 4249, 5811b	5811b	
58.	28930-20-3	1,2-Benzenediol, ethyl-	1980, 3474, 3753, 4249		
59.	933-99-3	1,2-Benzenediol, 3-ethyl-	2016, 3712, 4249		
60.	1124-39-6	1,2-Benzenediol, 4-ethyl-	497, 723, 1089a, 1099, 1365, 1375, 1375b, 1582, 1586, 1781, 1879, 1882, 1887a, 2387, 2493, 2524a, 2601a, 255, 3394, 3462, 3557, 3712, 3753, 4010, 4011, 4249, 4702, 5811b		2387, 3395, 3402
61.	71608-02-1	1,2-Benzenediol, 5-ethyl-3-nitro-	2137, 3712, 4249		
62.	934-00-9	1,2-Benzenediol, 3-methoxy-	2767, 3712, 4249	1877a	
63.	28930-19-0	1,2-Benzenediol, methyl-	3474, 3737, 3741, 3743, 4249, 4897, 5811b		
64.	488-17-5	1,2-Benzenediol, 3-methyl-	239, 497, 1099, 1364, 1371, 1378, 1781, 1879, 1882, 2387, 2598, 3165, 3166, 3255, 3300, 3394, 3453, 3712, 3753, 4005–4007, 4009–4011, 4249, 4702, 4796, 5011		1378, 2387, 3395, 3402
65.	452-86-8	1,2-Benzenediol, 4-methyl-	239, 497, 568b, 743, 1089a, 1099, 1371, 1375, 1375b, 1378, 1582, 1586, 1781, 1879, 1882, 1884, 1887a, 2493, 2524a, 2598, 2601a, 2767, 3255, 3300, 3394, 3453, 3462, 3557, 3712, 3746, 3747, 3753, 4005–4007, 4009–4011, 4249, 4796, 5011, 5811b	568b, 1877a, 4249, 5811b	1378, 3395, 3402

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
66.	2138-48-9	1,2-Benzenediol, 3-(1-methylethyl)-	2016, 3712, 4249, 5811b		
67.	2138-43-4	1,2-Benzenediol, 4-(1-methylethyl)-	2016, 3712, 4249		
68.	102-29-4	1,2-Benzenediol, monoacetate	2601a		
69.	6665-98-1	1,2-Benzenediol, 3-nitro-	2137, 3712, 4249		
70.	3316-09-4	1,2-Benzenediol, 4-nitro-	2016, 2137, 2329, 3308, 3491, 3712, 4010, 4011, 4249, 5811b		
71.	1126-61-0	1,2-Benzenediol, 4-(2-propenyl)-	3712, 3797	120, 970, 1971, 2862, 2939, 3059, 3194, 3974a, 3974a, 4249	
72.	29031-84-3	1,2-Benzenediol, propyl-	497, 1884, 1980, 2188, 3474, 3744, 3745, 3753, 4010, 4011	1980, 4249	
73.	2896-63-1	1,2-Benzenediol, 3-propyl-	2016, 3712, 4249		
74.	2525-02-2	1,2-Benzenediol, 4-propyl-	1781, 2016, 3462, 3712, 4249		
75.	108-46-3	1,3-Benzenediol {resorcinol} 	100, 102, 174b, 174c, 174e, 396, 414, 497, 568b, 603, 688, 723, 789, 789a, 859, 1371, 1375, 1375b, 1386, 1626, 1853b, 1879, 1882, 1883, 2060, 2079, 2195, 2313a, 2379a, 2387, 2570, 2598, 2681, 2939, 3007, 3131, 3171–3175, 3190, 3300, 3302, 3308, 3370, 3394, 3457, 3474, 3557, 3712, 3716, 3717, 3753, 3797, 3992, 3999, 4005–4007, 4113, 4249, 4319, 4332, 4407, 4414, 4796, 5011, 5034, 5049, 5532, 5576, 5588, 5643a, 5811b, 5835, 5836	100, 568b, 2379a, 4249, 5811b	2387, 3395, 3402
76.	25377-27-9	1,3-Benzenediol, dimethyl-	3457, 3474, 3753, 4249, 4566		
77.	488-87-9	1,3-Benzenediol, 2,5-dimethyl-	2598, 4796, 5011		
78.	67965-47-3	1,3-Benzenediol, ethenyl-	3457, 3474, 4249		
79.		1,3-Benzenediol, ethyl-	3474, 3753		

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

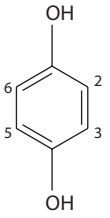
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
80.	2896-60-8	1,3-Benzenediol, 4-ethyl-	2598, 3497, 3712, 4249, 4796, 5011, 5811b		3395
81.		1,3-Benzenediol, methyl-	3474, 3744, 3745, 3753		
82.	608-25-3	1,3-Benzenediol, 2-methyl-	2598, 3497, 3712, 4249, 4796, 5011		3395, 3402
83.	504-15-4	1,3-Benzenediol, 5-methyl- {orcinol}	2598, 3497, 3712, 4249, 4796, 5011, 5811b		3395, 3402
84.		1,3-Benzenediol, (1-methylethyl)-	3753		
85.	71608-03-2	1,3-Benzenediol, 4-methyl-6-nitro-	2137, 3712, 4249		
86.		1,3-Benzenediol, monoacetate	1364		
87.	3163-07-3	1,3-Benzenediol, 4-nitro-	2137, 3712, 4249		
88.	68146-94-1	1,3-Benzenediol, propyl-	3457, 3474, 3753, 4249		
89.	123-31-9	1,4-Benzenediol {hydroquinone} 	100–102, 126a, 126b, 172, 173a, 174b, 174c, 190, 237, 239, 329, 392, 396, 402, 414, 497, 568b, 603, 663, 688, 723, 777, 778, 787, 788, 830a, 859, 1051, 1063–1066, 1068–1074, 1089a, 1099, 1158, 1235, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1386, 1437, 1445, 1582, 1586, 1626, 1674, 1751, 1879, 1882, 1884, 1887a, 1898, 2060, 2079, 2133, 2313a, 2327c, 2379a, 2387, 2493, 2524a, 2545, 2570, 2598, 2601a, 2615, 2681, 2691–2695, 2761, 2762,	100, 120, 568b, 739, 1077b, 1877a, 2379a, 3430, 3973, 4249, 4566, 4910, 5079, 5440, 5811b	1360, 1375a, 1377, 1378, 2387, 3395, 3402

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

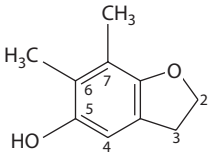
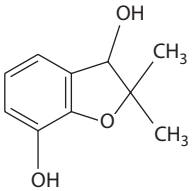
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1,4-Benzenediol {hydroquinone} (cont.)	2765–2767, 2775, 2777, 2799a, 2857, 2939, 3007, 3059, 3131, 3171–3175, 3190, 3255, 3300, 3302, 3308, 3370, 3394, 3453, 3454, 3457, 3474, 3553, 3557, 3602, 3712, 3716, 3717, 3737, 3741, 3743, 3753, 3797, 3844, 3891, 3992, 3999, 4005–4007, 4113, 4137, 4159, 4249, 4277, 4319, 4332, 4407, 4414, 4796,, 5011, 5034, 5049, 5079, 5532, 5555, 5571, 5576, 5643a, 5811b, 5835, 5836		
90.		1,4-Benzenediol, dimethyl-	3474		
91.	3233-32-7	1,4-Benzenediol, monoacetate	568b, 1364, 1365, 1884, 2545, 2767, 3553, 3557, 3712, 4249, 5811b		
92.		1,4-Benzenediol, monopropanoate	1364		
93.	608-43-5	1,4-Benzenediol, 2,3-dimethyl-	1378, 1586, 1884, 2321, 2601a, 2767, 3557, 3712, 4249, 4407, 4796, 5811b		1378
94.	615-90-7	1,4-Benzenediol, 2,5-dimethyl-	1378, 1884, 2769, 3557, 3712, 4249		1378
95.		1,4-Benzenediol, 2,6-dimethyl-	4796		
96.	2349-70-4	1,4-Benzenediol, 2-ethyl- = 1,4-benzenediol, ethyl-	1375, 1375b, 1586, 2767, 3474, 3557, 3712, 4249		
97.	72693-14-2	1,4-Benzenediol, 2-ethyl-6-methyl-	3557, 3712		
98.	497-76-7	1,4-Benzenediol, β-*D*-glucopyranoside {arbutin}		5777	
99.	824-46-4	1,4-Benzenediol, 2-methoxy-	3712		

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
100.	95-71-6	1,4-Benzenediol, 2-methyl- = 1,4-benzenediol, methyl-	101, 568b, 1099, 1375, 1375a, 1375b, 1377, 1378, 1561, 1586, 1879, 1884, 2598, 2767, 3255, 3394, 3453, 3474, 3553, 3557, 3712, 3737, 3741, 3743, 4137, 4249, 4796, 5011, 5811b	568b, 2917a, 3430, 4249, 5811b	1375a, 1377, 1378, 3395
101.	2349-71-5	1,4-Benzenediol, 2-(1-methylethyl)-		4249	
102.	4693-31-6	1,4-Benzenediol, 2-propyl-	2767, 3474, 3557, 3712		
103.	700-13-0	1,4-Benzenediol, 2,3,5-trimethyl-	1884, 2321, 3712, 4249, 4796, 5811b		
104.	13398-94-2	Benzeneethanol, 3-hydroxy-	596, 2601a, 3712, 4249	1587a, 2338, 4249	
105.	501-94-0	Benzeneethanol, 4-hydroxy-	596, 1365, 1561, 1884, 3712, 4249	1561, 4249	
106.	2380-78-1	Benzeneethanol, 4-hydroxy-3-methoxy-	596, 3712, 4249, 4897		
107.	30923-59-2	Benzenemethanol, 2-hydroxy-, α-benzoate		5811, 5811b	
108.	620-24-6	Benzenemethanol, 3-hydroxy-	1561, 3712	1561	
109.	623-05-2	Benzenemethanol, 4-hydroxy-	568b, 4249	568b, 4249	
110.	498-00-0	Benzenemethanol, 4-hydroxy-3-methoxy-	568b, 4249, 5811a	5811a	
111.	80638-48-8	Benzenepropanal, 4-hydroxy-3-methoxy-	3712	5811b	
112.	121850-61-1	Benzenepropanamide, *N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]-3,4-dihydroxy-		4249, 5811b	
113.		Benzenepropanoic acid, dihydroxy-methoxy-	3737, 3741, 3743		
114.	3714-73-6	Benzenepropanoic acid, 2,3-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		
115.	96937-38-1	Benzenepropanoic acid, 2,3-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
116.	5631-68-5	Benzenepropanoic acid, 2,4-dihydroxy-	5811a		
117.	10538-47-3	Benzenepropanoic acid, 2,5-dihydroxy-	101, 3712, 3737, 3741, 3743, 4249, 4897, 5811b	5811b	
118.	96937-34-7	Benzenepropanoic acid, 2,5-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
119.	98114-50-2	Benzenepropanoic acid, 2,6-dihydroxy-	5811a		
120.	495-78-3	Benzenepropanoic acid, 2-hydroxy-	3737, 3741, 3743, 4249, 4897, 5811b	1305b, 3973, 3974a, 4249, 5668	
121.	1078-61-1	Benzenepropanoic acid, 3,4-dihydroxy- {dihydrocaffeic acid}	101, 3712, 3737, 3741, 3743, 4113, 5811b	970, 3797, 3973, 3974a, 5811b	
122.	96961-47-6	Benzenepropanoic acid, 3,4-dihydroxy-2,5,6-trimethyl-	3712, 3737, 3741, 3743, 4249, 4897, 5811b		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
123.	96937-33-6	Benzenepropanoic acid, 3,4-dihydroxy-ar-methyl-	3737, 3741, 3743, 4249, 4897, 5811b		
124.	621-54-5 33393-93-0	Benzenepropanoic acid, 3-hydroxy-	1884, 2939, 3302, 3712, 3737, 3741, 3743, 3797, 4249, 4377, 5811b	2939, 3973, 3974a, 4249, 4377, 4951	
125.	26539-01-5	Benzenepropanoic acid, 3,5-dihydroxy	5811a		
126.	501-97-3	Benzenepropanoic acid, 4-hydroxy-	1626, 2939, 3302, 3712, 3737, 3797, 3741, 3743, 4163, 4249, 4377, 5811b	2722, 2939, 3532, 3560, 3561, 4163, 4249, 4377, 4951, 5811b	
127.	156-39-8	Benzenepropanoic acid, 4-hydroxy-α-oxo-	1871a, 3712, 4249, 5811b, 5811b		
128.	5597-50-2	Benzenepropanoic acid, 4-hydroxy-, methyl ester	568b, 1884, 3553, 3712, 4249, 5811b		
129.	1135-23-5	Benzenepropanoic acid, 4-hydroxy-3-methoxy- {hydroferulic acid}	596, 3712, 3737, 3741, 3743, 4249		
130.	96937-36-9	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methoxy-	4249, 4897, 5811b		
131.	96937-35-8	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methyl-	4249, 4897, 5811b		
132.	10210-17-0	Benzenepropanol, 4-hydroxy-	596, 3712, 4249		
133.	87-66-1	1,2,3-Benzenetriol {pyrogallol}	414, 859, 1089a, 1879, 1887a, 2195, 2203, 2210, 2524a, 3302, 3308, 3365, 3712, 4113, 4249, 4702, 5811b	2079	2210, 3395, 3402
134.	533-73-3	1,2,4-Benzenetriol {hydroxyhydroquinone}	329, 1751, 1884, 2321, 3712, 4249, 5811b	2283, 4249	3395, 3402
135.		1,2,4-Benzenetriol, methyl-	1884		3402, 4249
136.		Benzofuran, 4-hydroxy-5,6-dimethyl-	2761, 2762, 2777		
137.	60026-12-2	Benzofuran, 5-hydroxy-6,7-dimethyl- 	8, 312, 568b, 1360, 1375a, 2543, 2761, 2769, 2773, 4249	404, 568b, 1156, 2386, 2389, 2544, 3549, 3550, 4090, 4249, 5811b	1360, 1375a
138.	17781-15-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl- 		5811, 5811b	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

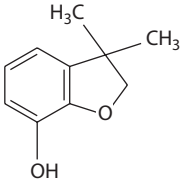
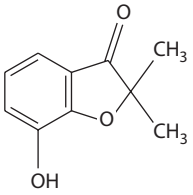
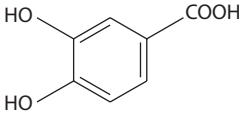
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
139.	1563-38-8	7-Benzofuranol, 2,3-dihydro-2,2-dimethyl- 		5811, 5811b	
140.	124052-02-4	3(2*H*)-Benzofuranone, 2-(3,4-dihydroxyphenyl)-2,4,6-trihydroxy-		4249	
141.	17781-16-7	3(2*H*)-Benzofuranone, 7-hydroxy-2,2-dimethyl- 		5811, 5811b	
142.	96937-46-1	Benzoic acid, dihydroxy-dimethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
143.	96937-47-2	Benzoic acid, dihydroxy-ethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
144.	96937-44-9	Benzoic acid, dimethyl-hydroxy-	3737, 3741, 3743, 4249, 4897, 5811b		
145.	96937-43-8	Benzoic acid, ethyl-hydroxy-	3737, 3741, 3743, 4249, 4897, 5811b		
146.	87323-67-9	Benzoic acid, hydroxy-methoxy-	3737, 3741, 3743, 4249, 4897, 5811b		
147.	28965-86-8	Benzoic acid, hydroxymethyl-	3737, 3741, 3743, 4249, 4897		
148.	69-72-7	Benzoic acid, 2-hydroxy- {salicylic acid}	414, 568b, 1879, 1884, 1886, 1981, 3255, 3308, 3394, 3712, 3737, 3741, 3743, 3793, 3797, 4113, 4249, 5811b	120, 568b, 1620, 2092, 2270, 2356, 2389, 2544, 2954, 3748, 3749, 3751, 4249, 5811b	
149.	2052-14-4	Benzoic acid, 2-hydroxy-, butyl ester		5811	
150.	118-61-6	Benzoic acid, 2-hydroxy-, ethyl ester {ethyl salicylate}		172a, 174b, 1053, 2386, 2995, 3266, 4249, 5811b	
151.	6259-76-3	Benzoic acid, 2-hydroxy-, hexyl ester		2339a	
152.	119-36-8	Benzoic acid, 2-hydroxy-, methyl ester {methyl salicylate}	568b, 1586, 4249	120, 172a, 174b, 568b, 908, 1053, 2094, 2389, 2544, 2611, 2862, 2939, 3059, 3266, 3370, 3547, 3973, 3974a, 3988, 4249, 5811b	
153.	87-20-7	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester		174b, 1256, 2339a, 3266, 4249	
154.	87-19-4	Benzoic acid, 2-hydroxy-, 2-methylpropyl ester {isobutyl salicylate}		1053, 3266, 3370	
155.	87-22-9	Benzoic acid, 2-hydroxy-, 2-phenylethyl ester {phenethyl salicylate}		1053, 3266	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
156.	118-58-1	Benzoic acid, 2-hydroxy-, phenylmethyl ester {benzyl salicylate}		2339a, 3266, 4249	
157.	50-85-1	Benzoic acid, 2-hydroxy-4-methyl-	3712, 4113, 4249		
158.	303-38-8	Benzoic acid, 2,3-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b	3103	
159.	3934-81-4	Benzoic acid, 2,3-dihydroxy-4-methoxy-	3712, 4113, 4249		
160.	3929-89-3	Benzoic acid, 2,3-dihydroxy-4-methyl-	3712, 4113, 4249		
161.	610-02-6	Benzoic acid, 2,3,4-trihydroxy-	3712, 4113, 4249		
162.	89-86-1	Benzoic acid, 2,4-dihydroxy- {β-resorcylic acid}	3712, 4113, 4249		
163.	490-79-9	Benzoic acid, 2,5-dihydroxy- {gentisic acid}	3737, 3741, 3743, 4249, 5811b	3103, 3748, 3749, 3751, 4249, 4914	
164.	96937-49-4	Benzoic acid, 2,5-dihydroxymethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
165.	303-07-1	Benzoic acid, 2,6-dihydroxy-	3712, 3737, 3741, 3743, 4249, 4897, 5811b	3103, 5811b	
166.	99-06-9	Benzoic acid, 3-hydroxy-	101, 568b, 1099, 1371, 1626, 1879, 1884, 1886, 2767, 2939, 3302, 3308, 3394, 3553, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	568b, 1234, 1980, 2939, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5811b	3393
167.	19438-10-9	Benzoic acid, 3-hydroxy-, methyl ester	2767, 3557, 4249		
168.	645-08-9	Benzoic acid, 3-hydroxy-4-methoxy- {isovanillic acid}	2042, 3308, 3394, 3712, 3793, 3797, 5811b		
169.	87513-63-1	Benzoic acid, 3-hydroxy-6-methoxy-, methyl ester		2917a	
170.	586-30-1	Benzoic acid, 3-hydroxy-4-methyl-	101, 3712, 3737, 3741, 3743, 4113, 4249, 5811b	3103	
171.	99-50-3	Benzoic acid, 3,4-dihydroxy- {protocatechuic acid} 	1626, 1884, 2939, 3302, 3308, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	120, 970, 1980, 2270, 2722, 2939, 3103, 3655a, 3655b, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 5079, 5811b	
172.	96937-39-2	Benzoic acid, 3,4-dihydroxy-dimethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
173.	96937-40-5	Benzoic acid, 3,4-dihydroxymethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
174.		Benzoic acid, 3,4-dihydroxy-C_4-alkyl-methyl-	3737, 3741, 3743		
175.	149-91-7	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}	1373, 1842, 2195, 3219, 3265, 3308, 3712, 4249	3655b, 5079	
176.	121-79-9	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}	3265	5811b	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

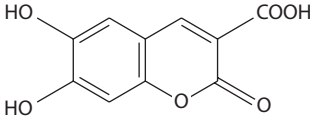
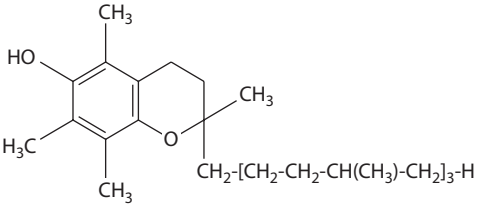
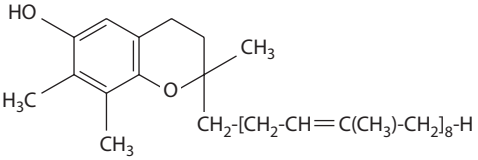
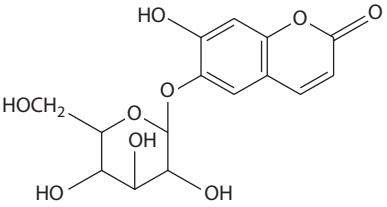
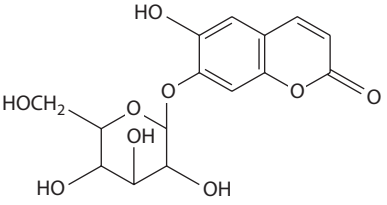
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
177.	99-10-5	Benzoic acid, 3,5-dihydroxy-	3712, 3737, 3741, 3743, 4113, 4249, 5811b		
178.	99-96-7	Benzoic acid, 4-hydroxy- {*p*-salicylic acid}	101, 414, 568b, 1626, 1879, 1884, 1886, 2042, 2043, 2939, 3302, 3308, 3394, 3553, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	568b, 908, 952, 2939, 3532, 3560, 3561, 3748, 3749, 3751, 3797, 3973, 3974a, 5811b	3393
179.	94-26-8 1322-01-6	Benzoic acid, 4-hydroxy-, butyl ester		5811, 5811b	
180.	99-76-3	Benzoic acid, 4-hydroxy-, methyl ester	1884, 2570, 2769, 3557, 3712, 4249, 5811b		
181.	94-13-3	Benzoic acid, 4-hydroxy-, propyl ester		1053, 3266, 3370, 5811b	
182.	530-57-4	Benzoic acid, 4-hydroxy-3,5-dimethoxy- {syringic acid}	1626, 1884, 2939, 3302, 3308, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 4378, 5811b	3797, 3973, 3974a	
183.	121-34-6	Benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid}	568b, 1235, 1427, 1626, 1884, 1886, 2042–2044, 2046, 2939, 3219, 3302, 3308, 3553, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	120, 568b, 908, 952, 1248, 1620, 2270, 2939, 2954, 3103, 3219, 3329, 3532, 3560, 3561, 3748, 3749, 3751, 3797, 3973, 3974a, 4092, 4249, 4677, 5811b	
184.	617-05-0	Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester		2917a	
185.	3943-74-6	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester	3712	5811b	
186.	96937-45-0	Benzoic acid, 4-hydroxymethyl-	3737, 3741, 3743, 4249, 4897, 5811b		
187.	873-62-1	Benzonitrile, 3-hydroxy-	2327c, 2570		
188.	767-00-0	Benzonitrile, 4-hydroxy-	568b, 2327c, 2767, 4249		
189.		2*H*-1-Benzopyran-3-carboxylic acid, 6,7-dihydroxy-2-oxo- 		4249, 4556	
190.	19484-74-3	2*H*-1-Benzopyran-3-carboxylic acid, 7,8-dihydroxy-2-oxo-		4249, 4752	
191.	124052-01-3	2*H*-1-Benzopyran-3,4-dione, 2-(3,4-dihydroxyphenyl)-2,5,7-trihydroxy-		4249	
192.	1406-66-2	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl {tocopherol}		5811	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
193.	59-02-9	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- {α-tocopherol} 	1360, 1373, 1375a, 1842, 1884, 2601a, 2939, 3059, 3170, 3251, 3255, 3257, 3265, 3266, 3271, 3286, 3295, 3300, 3302, 3655a, 3684, 3685, 3797, 3875, 4159c, 4249	120, 174b, 486, 557, 667, 840, 1053, 1651, 2270, 2939, 3059, 3155, 3156, 3170, 3266, 3295, 3347, 3349, 3357, 3484, 3493, 3616, 3655a, 3707, 3755, 3797, 3811, 3875, 3971, 3973, 3974a, 4098a, 4236, 4249, 5079, 5811b	1360, 1375a
194.	148-03-8	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- {β-tocopherol}	2601a, 3484, 4249	3484, 4249	
195.	7616-22-0	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-		1395a, 1971, 3611, 4249	
196.	56084-94-7	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12,16,20,24,28,32-octamethyl-3,7,11,15,19,23,27,31-tritriacontaoctaenyl)- [3*E*,7*E*,11*E*,15*E*,19*E*,23,*E*,27*E*] {solanochromene; solanachromene} 		120, 1971, 3059, 3346–3348, 3349, 3357, 3971, 3973, 3974a, 4249, 5811b	
197.	305-01-1	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}	969, 1572, 1626, 1884, 2939, 3059, 3257, 3265, 3302, 3797, 4249, 5811b	969, 970, 1626, 2939, 2954 3103, 3059, 3194, 3797, 3973, 3974a, 4249, 5711, 5811b, 5888	
198.	60091-00-1	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-		3797, 4249	
199.	531-75-9	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin} 	3257	1309, 2939, 2954, 3103, 3973, 3974a, 4249, 5711, 5811b	
200.	531-58-8	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin} 		1309, 1626, 3797, 4249, 5811b, 5838	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

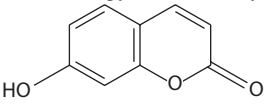
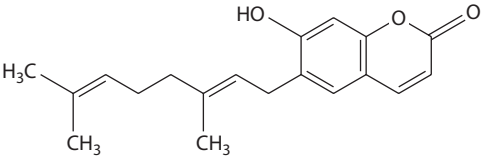
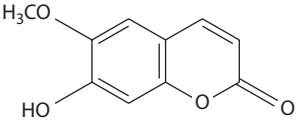
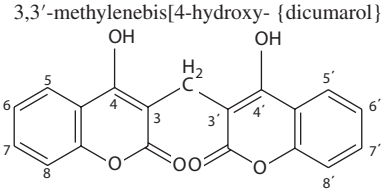
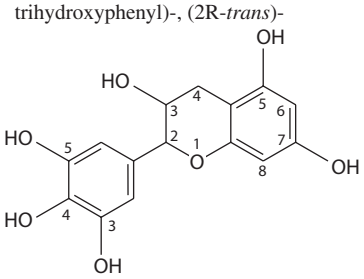
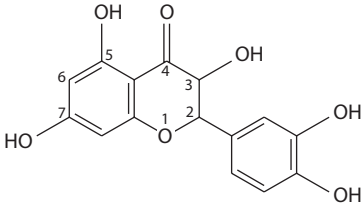
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
201.	93-35-6	2*H*-1-Benzopyran-2-one, 7-hydroxy- 		3161, 3738, 4249, 4606	
202.	148-83-4	2*H*-1-Benzopyran-2-one, 7-hydroxy-6(3,7-dimethyl-2,6-octadienyl)- {ostruthin} 		120	
203.	92-61-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin} 	419, 568b, 1284, 1373, 1626, 1842, 1884, 1898, 2377, 2524a, 2767, 2939, 3059, 3096, 3168, 3302, 3308, 3553, 3602, 3797, 3891, 3995, 4005–4007, 4119, 4121, 4123, 4124, 4164, 4249, 4319, 4373–4375, 5512, 5811b	72, 120, 254, 404, 568b, 677b, 830a, 831, 834, 835, 840, 890, 966, 1063–1066, 1068–1074, 1112, 1626, 1863, 2014, 2270, 2313a, 2338, 2361, 2389, 2531, 2544, 2557a, 2810–2812, 2914, 2939, 2954, 3059, 3103, 3109, 3161, 3194, 3219, 3329, 3631, 3641, 3646, 3705, 3738, 3794, 3797, 3973, 3974a, 3974b, 3984, 4249, 4269, 4373–4375, 5079, 5081, 5127, 5235, 5591, 5616, 5650, 5652, 5704, 5705, 5745, 5766, 5788, 5808, 5811b, 5830, 5831, 5842, 5876, 5888, 5889	
204.	90-33-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-4-methyl-		2917a	
205.	66-76-2	2*H*-1-Benzopyran-2-one, 3,3′-methylenebis[4-hydroxy- {dicumarol} 	2757, 3263, 4249 [not found in smoke from coumarin-treated tobacco]		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
206.	970-73-0	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*trans*)- 		429b	
207.	970-74-1	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*cis*)-		429b, 4249	
208.	124052-00-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,3,5,7-tetrahydroxy-		4249	
209.	21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		120, 1626, 1837a, 1971, 2023, 2270, 2939, 3059, 3194, 3555, 3667, 3794, 3797, 3973, 3974a, 4249, 5079, 5255, 5256, 5724, 5747, 5811b, 5888	
210.	117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin, 3,3a,4a,5,7-pentahydroxyflavone} 	3096, 3555, 5652, 5750, 5758, 5904,	72, 120, 970, 1077b, 1837a, 2270, 2379, 2704a, 2939, 3059, 3462, 3555, 3685, 3794, 3797, 3974a, 4036, 4403, 4999, 5079, 5255, 5641, 5652, 5750, 5758, 5811b, 5904	
211.	7215-44-3 20188-84-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-b-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy- {quercetin 3,3′-diglucoside}		4249, 5724, 5747, 5811, 5811b, 5888	
212.	1486-70-0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-methoxy-		3797, 3974a, 4249	
213.	2068-02-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5-hydroxy-3,7-dimethoxy-		3797, 3974a, 4249	
214.	491-50-9	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}		3797, 3974a, 4249	
215.	124051-99-6	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-[[2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,6-dihydroxy-3-oxo-4-benzofuranyl]oxy]-2,3-dihydro-3,5-dihydroxy-		4249	
216.	480-41-1	4*H*-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)- {naringenin}		970, 3797, 3974a, 4249	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

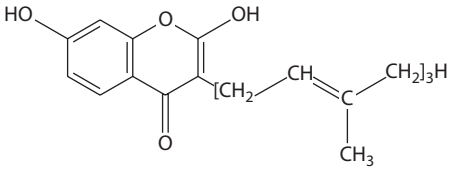
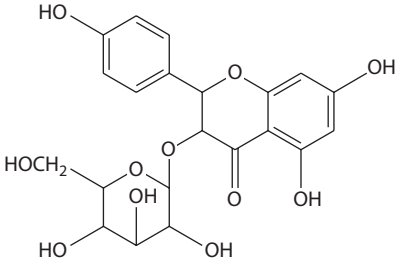
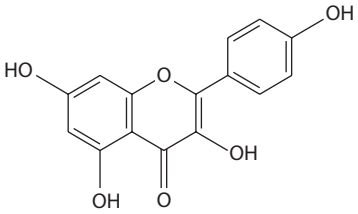
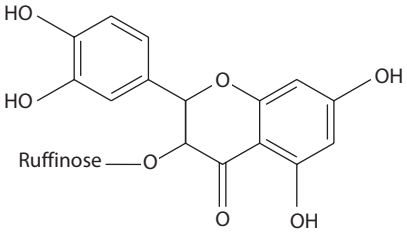
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
217.	643-572	4*H*-1-Benzopyran-4-one, 2,7-dihydroxy-3-(3,7,11-trimethyldodeca-2,6,10-trienyl- {ammoresinol} 		3763, 5079	
218.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3,4-dihydroxyphenyl)- {3a,4a,5,7-tetrahydroxy-3-methylflavone}		4147, 5776, 5888	
219.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3-methyl-4-hydroxyphenyl)- {4a,5,7-trihydroxy-3,3a-dimethylflavone}		4147, 5888	
220.		4*H*-1-Benzopyran-4-one, 3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)-{3a,4a,5-trihydroxy-3,5-dimethylflavone}		5776	
221.	480-10-4	4*H*-1-Benzopyran-4-one, 3-(b-*D*-glucopyranosyloxy)-5, 7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glucoside; 3,4a,5,7-tetrahydroxyflavone glucoside} 		120, 641, 830a, 835, 838, 840, 966, 970, 1626, 1971, 2023, 2270, 2939, 3059, 3161, 3555, 3646, 3738, 3797, 3974a, 4072a, 4249, 5079, 5724, 5753, 5758	
222.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(3,4-dihydroxyphenyl)-{3a,4a,5,7-tetrahydroxyflavone, 3-glucoside}		1625, 4147, 5353, 5724, 5834, 5888	
223.	529-44-2	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricetin}		5811, 5811b	
224.	520-18-3	4*H*-1-Benzopyran-4-one,3,5,7-trihydroxy-2-(4-hydroxyphenyl)- {kaempferol; 3,4a,5,7-tetrahydroxyflavone} 	2767, 3095a, 3555, 3794, 4249, 5652, 5758	1626, 1971, 2939, 3059, 3555, 3794, 4249, 5652, 5758, 5753, 5758, 5811b	
225.	55136-76-0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
226.	142235-82-3	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2090b	
227.	19895-95-5	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	
228.	522-12-3	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl) oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {quercetrin}	970	4036, 4249, 4573	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

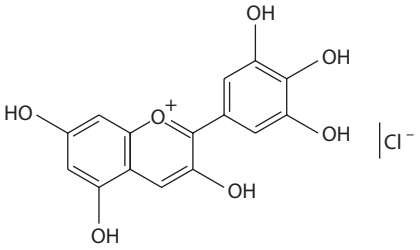
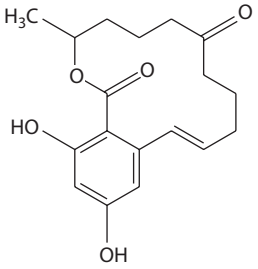
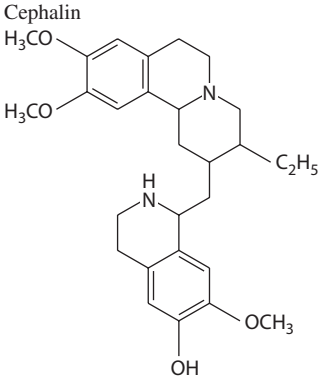
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
229.	17912-87-7	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl) oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricitrin}		5811, 5811b	
230.	55696-57-6	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-L-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-L-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-		4249	
231.	55804-74-5	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
232.	153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} 		69, 72, 120, 248, 385, 598, 828b, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1063–1066, 1068–1074, 1309, 1329, 1333, 1485, 1626, 1971, 2014, 2079, 2153a, 2270, 2313a, 2338, 2361, 2379, 2395, 2514, 2529, 2531, 2557a, 2704a, 2810–2812, 2939, 3059, 3096, 3161, 3367a, 3400, 3462, 3551, 3555, 3628, 3629, 3631, 3641, 3646, 3700, 3705, 3738, 3767, 3794, 3974a, 3974b, 3984, 3999, 4005–4007, 4036, 4156, 4157, 4249, 4403, 4999, 5079, 5110, 5156, 5157, 5189, 5204, 5217, 5304, 5305, 5310, 5576, 5591, 5596, 5641, 5652, 5661, 5681, 5697, 5698, 5724, 5747, 5750, 5780, 5788, 5808, 5809, 5811b, 5831, 5834, 5888, 5889	
233.	17650-84-9	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		1309, 4249, 5811b	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
234.	30311-61-6	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-		2023, 4147, 5777, 5811b, 5888	
235.	34336-18-0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	
236.	29859-91-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
237.	27554-19-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxy phenyl)-		1309, 4249	
238.	58934-57-9	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl)glucosyl] oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
239.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4a,5,7-trihydroxyflavone, 3-glucoside}		4147, 5888	
240.		4*H*-1-Benzopyran-4-one, 7-(β-*D*-rhamnoglucopyranosyloxy)-3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)-{3a,4a,5 -trihydroxy-3,5-dimethylflavone, 7-rhamnoglucoside}		4147, 5888	
241.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-rhamnoglucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)-{4a,5,7-trihydroxyflavone, 3-rhamnoglucoside}		3095a, 4372, 5888	
242.	520-34-3	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)- {diosmetin}		120, 4249, 4959	
243.	4382-17-6	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-methoxy-		3797, 4249	
244.		4*H*-1-Benzopyran-4-one, hydroxy-	1586, 2767, 4249		
245.	38445-24-8	4*H*-1-Benzopyran-4-one, 6-hydroxy-	1586, 2767		
246.	10236-47-2	4*H*-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}		970, 1305b, 3797, 3974a, 4249	
247.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,5′,7-pentahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2023, 4249	
248.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,7-tetrahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		4249	
249.	69453-35-6	Benzo[*a*]pyrene diol	765, 2939, 3302, 4249		
250.	63455-19-6	Benzo[*a*]pyrenol	2079, 330, 4249, 4282, 4354		
251.	37574-48-4	Benzo[*a*]pyren-4-ol	5811a		
252.	20928-82-9	Benzo[a]pyren-6-yloxy	4249, 4861		
253.	528-58-5	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride		4249, 4681	
254.	22688-80-8	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride		4249, 4681, 4710	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
255.	528-53-0	1-Benzopyrylium, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-, chloride 		2855a, 4249, 4681	
256.	18719-76-1	1-Benzopyrylium, 3-[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-, chloride		928b, 4249, 4710	
257.	33978-17-5	1-Benzopyrylium, 3-[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride		4249, 4681	
258.	17924-92-4	1*H*-2-Benzoxacyclotetradecin-1,7(8*H*)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, [S-(*E*)]- 		4249	
259.	1133-63-7	[1,1′-Biphenyl]-2,3-diol {1,1′-biphenyl, 2,3-dihydroxy-}	2601a		
260.	1322-20-9	[1,1′-Biphenyl]-ol		984	
261.	90-43-7	[1,1′-Biphenyl]-2-ol	568b, 1360, 1375a, 2761, 2762, 2765, 2766, 3753, 4249, 5811b	5811b	1360, 1375a
262.	92-69-3	[1,1′-Biphenyl]-4-ol	3457, 3753, 4249		
263.	70185-59-0	1,4-Butanediamine, *N*-[3-amino)-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy- {*p*-coumaroylspermidine}		5811, 5811b	
264.	5471-51-2	2-Butanone, 4-(4-hydroxyphenyl)-	374, 568b, 3266, 3712, 4249	172a, 174b, 568b, 1053, 3266, 3370	
265.	483-17-0	Cephalin 		5079, 5375	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

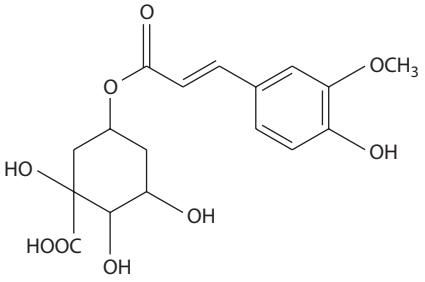
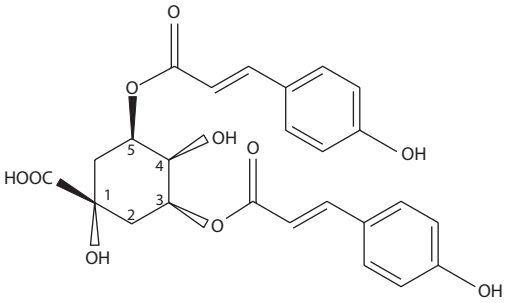
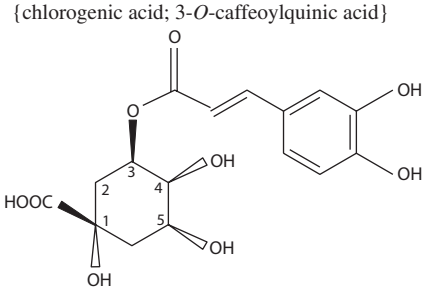
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
266.	106-34-3	2,5-Cyclohexadiene-1,4-dione, compound with 1,4-benzenediol (1:1)	1378, 2379, 2767, 4249		1378
267.	34214-77-2	Cyclohexanecarboxylic acid, 3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]trihydroxy-, (1α,3α,4α,5β)-	3302, 3792, 4249	1309, 3797, 4249, 5811b	
268.	1899-29-2 27044-07-1	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)-{3-*O*-feruloylquinic acid}  Also listed as: Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoicacid,(1α,3α,4α,5β)-		3797, 3973, 3974a, 4249, 4402, 4913, 5811b	
269.	2450-53-5	Cyclohexanecarboxylic acid, 3,5-bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4-dihydroxy-, [1R-(1α,3α,4α,5β)]- 		1309, 4249, 5705	
270.	15016-60-1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-,[1R-[1α,3β(*Z*),4α,5α]]-	3302, 3792, 4249	3797, 4249	
271.	15076-00-3	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-,[1R-[1α,3β(*E*),4α,5α]]-		4249	
272.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-{chlorogenic acid; 3-*O*-caffeoylquinic acid} 	172, 602, 1884, 3257, 3302, 3792, 3797, 4249	69, 72, 120, 254, 385, 486, 598, 602, 657, 665, 677b, 718, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1040, 1063–1066, 1068–1074, 1077b, 1309, 1329, 1333, 1352, 1485, 1625, 1626, 1923, 2014, 2056a, 2079, 2154, 2250a,	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-{chlorogenic acid; 3-*O*-caffeoylquinic acid} (cont.)		2270, 2283, 2313a, 2338, 2361, 2395, 2514, 2531, 2529, 2557a, 2810–2812, 2911c, 2911d, 2914, 2939, 2954, 3029, 3059, 3096, 3161, 3302, 3366a, 3367a, 3400, 3459–3462, 3551, 3616, 3628, 3631, 3641, 3646, 3655b, 3700, 3705, 3738, 3748, 3749, 3751, 3754, 3792, 3794, 3797, 3806, 3973, 3974a, 3974b, 3984, 3999, 4005–4007, 4156, 4221, 4249, 4275, 4279, 4372, 4402, 4403, 4421, 4999, 5079, 5189, 5200, 5246, 5353, 5389, 5576, 5592–5594, 5596, 5604, 5652, 5665, 5672, 5673, 5681, 5697. 5698, 5700, 5705, 5713, 5722, 5737, 5761, 5782, 5784, 5788, 5808–5810, 5811b, 5812, 5827, 5831, 5834, 5839, 5850, 5856, 5889, 3890, 5896, 5900, 5908	
273.	93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, (1α,3β,4α,5β)-		3973	
274.	906-33-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-,[1R-(1α,3α,4α,5β)]-{neochlorogenic acid; 5-*O*-caffeoylquinic acid} Also listed as Cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-	3302, 3792, 5811b	120, 602, 830a, 831, 834, 835, 838, 840, 890, 970, 1206a, 1626, 2557a, 2939, 3646, 3738, 3792, 3797, 3973, 3974a, 4249, 4402, 5705, 5811b, 5831	
275.	70898-22-5	Cyclohexanecarboxylic acid, 3-[[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-		4249, 4785, 4984	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

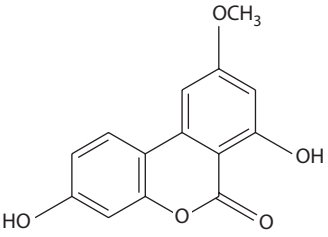
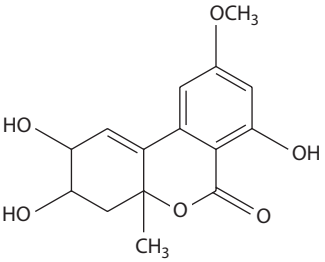
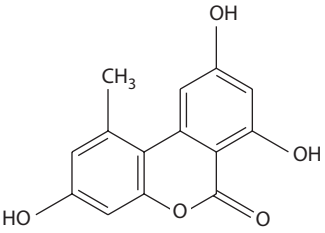
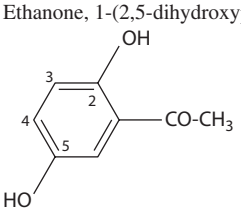
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
276.	17608-52-5	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy- {4-*O*-caffeoylquinic acid}		831, 834, 835, 838, 840, 890, 1206a, 3646, 3738, 3973, 3974a, 4249, 5705, 5811b, 5889	
277.		Cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-5-phenyl-		5705, 5749	
278.	905-99-7	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-, (1α,3α,4α,5β)-		4249, 5811b	
279.	534-61-2	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy- [1S-(1α,3β,4β,5 α)]-	5811, 5811b	5811b	
280.	6082-44-6	1-Cyclohexene-1-carboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-4,5-dihydroxy-, (3α,4α,5β)-		4249	
281.	26894-49-5	6*H*-Dibenzo[*b,d*]pyran-6-one, 3,7(3,9 or 7,9)-dihydroxy-9(7 or 3)-methoxy-1-methyl- 		4249, 4756	
282.	29752-43-0	6*H*-Dibenzo[*b,d*]pyran-6-one, 9-methoxy-4a-methyl-2,3,4,4a-tetrahydro-2,3,7-trihydroxy- (2α,3β,4aβ)- 		4249, 4756	
283.	641-38-3	6*H*-Dibenzo[*b,d*]pyran-6-one, 1-methyl-3,7,9-trihydroxy- 		4249	
284.	534-82-7	1,2-Ethanediol, 1-(4-hydroxy-3-methoxyphenyl)-		4249	
285.	711-79-5	Ethanone, 1-(1-hydroxy-2-naphthalenyl)-	4249	3430, 5811b	
286.	490-78-8	Ethanone, 1-(2,5-dihydroxyphenyl)- 	568b, 1884, 3553, 3557, 3712, 4249, 5811b		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
287.	699-83-2	Ethanone, 1-(2,6-dihydroxyphenyl)-	3712		
288.	703-98-0	Ethanone, 1-(2-hydroxy-3-methoxyphenyl)-	1375, 1375b, 3712, 4249		
289.	6921-64-8	Ethanone, 1-(2-hydroxy-4-methylphenyl)-		568b, 3547, 4249	
290.	1450-72-2	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	2601a, 4249	937, 4249	
291.	703-23-1	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-	2570, 3712		
292.		Ethanone, 1-(2-hydroxy-6-methylphenyl)-		2338	
293.	118-93-4 582-24-1	Ethanone, 1-(2-hydroxyphenyl)-	1238, 1360, 1375a, 1378, 1586, 1884, 2327c, 2387, 2767, 3557, 3712, 3797, 4036, 5811b	120, 2862, 2939, 3059, 4249, 5811b	1360, 1375a, 1378, 2387, 3395
294.	1197-09-7	Ethanone, 1-(3,4-dihydroxyphenyl)-	3712	5811b	
295.	51863-60-6	Ethanone, 1-(3,5-dihydroxyphenyl)-	4249	5811b	
296.		Ethanone, 1-(3-hydroxy-2-methoxyphenyl)-	1360, 1375a		1360, 1375a
297.	6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-	1375, 1375b, 1586, 1884, 2767, 2769, 3557, 3712		
298.	33414-49-2	Ethanone, 1-(3-hydroxy-4-methylphenyl)-	2769, 3557, 3712, 4249		
299.	121-71-1	Ethanone, 1-(3-hydroxyphenyl)-	615, 1360, 1375, 1375a, 1375b, 1378, 1586, 1884, 1971, 2178, 2767, 2939, 3059, 3302, 3557, 3712, 3797, 4036, 4249, 4319, 5811b		1360, 1375a, 1378, 3395, 4249
300.	493-33-4	Ethanone, 1-(4-hydroxy-2-methoxyphenyl)-	1360, 2327c, 2761, 2762, 3712, 4249		
301.	2478-38-8	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	3712	404, 3430, 5811b	
302.	498-02-2	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)- {acetovanillone}	568b, 1360, 1364, 1375, 1375a, 1375b, 1586, 1884, 2327c, 2765–2767, 2769, 2773, 3557, 3712, 4249, 5811b	404, 568b, 938, 2917a, 3430, 3767a, 4249	1360, 1375a
303.	99-93-4	Ethanone, 1-(4-hydroxyphenyl)-	615, 1238, 1364, 1375, 1375b, 1586, 1884, 1971, 2387, 2570, 2939, 3059, 3302, 3712, 3797, 4249, 4319, 5811b	3988, 5811b	2387, 3395
304.	70587-92-7	Ethanone, 1-(hydroxyphenyl)-	2777, 4249		642, 4249
305.	10083-24-6	Ethene, 1-(3,4-dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)- (*E*)- {*trans*-piceatannol}		4781	
306.	501-36-0	Ethene, 1-(4-hydroxyphenyl)-2-(3,5-dihydroxyphenyl)- (*E*)- {*trans*-resveratrol}		4781	
307.	61434-67-1	Ethene, 1-(4-hydroxyphenyl)-2-(3,5-dihydroxyphenyl)-, (*Z*)- {*cis*-resveratrol}		4781	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

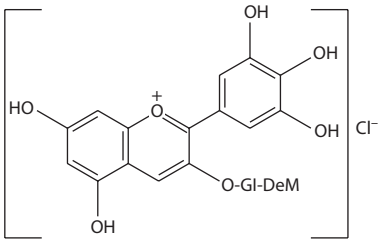
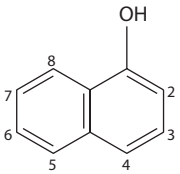
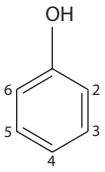
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
308.	102-61-4	Ethene, 1-(phenyl)-2-(3,5-dihydroxyphenyl)- {pinosylvin}		4781	
309.	29732-48-7	Flavylium, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride 		4249, 4527, 4710	
310.		Flavylium, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-3′,4′,5,7-tetrahydroxy-, chloride		4249, 4527**,** 4644	
311.	60517-74-0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)		5811b	
312.	25545-13-5	*D*-Glucopyranose, 4-(4-hydroxybenzoate)		4249, 4915	
313.	23445-11-6	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)		4249, 4915	
314.	7724-09-6	β-*D*-Glucopyranoside, (2-hydroxyphenyl)methyl-		4249, 4790	
315.	1415-93-6	Humic acids		2665a	
316.	56631-57-3	1*H*-Indenol [1*H*-Inden-4-ol]	1378, 1586, 1884, 2767, 3746, 3747, 5811b		1378
317.	72692-86-5	1*H*-Indenol, 2,3-dihydromethyl- [1*H*-Inden-4-ol, 2,3-dihydromethyl-]	1378		1378
318.	73850-11-0	1*H*-Indenol, dimethyl- [1*H*-Inden-4-ol, dimethyl-	1884, 3746, 3747, 5811b		
319.	73850-20-1	1*H*-Indenol, ethylmethyl- [1*H*-Inden-4-ol, ethylmethyl-]	1884, 3746, 3747, 5811b		
320.	73850-12-1	1*H*-Indenol, methyl- [1*H*-Inden-4-ol, methyl-]	1884, 3746, 3747, 5811b		
321.	73850-09-6	1*H*-Indenol, tetramethyl- [1*H*-Inden-4-ol, tetramethyl-]	1884, 3746, 3747, 5811b		
322.	73850-10-9	1*H*-Indenol, trimethyl- [1*H*-Inden-4-ol, trimethyl-]	1884, 3746, 3747, 5811b		
323.	1641-41-4	1*H*-Indenol, 2,3-dihydro-[1*H*-Inden-4-ol, 2,3-dihydro-]	661, 4249		
324.	1470-94-6	1*H*-Inden-5-ol, 2,3-dihydro-	1378, 4249		1378
325.	50-67-9	1*H*-Indol-5-ol, 3-(2-aminoethyl)-		4249, 4848	
326.	92-44-4	2,3-Naphthalenediol	278, 4249		
327.	481-39-0	1,4-Naphthalenedione, 5-hydroxy- {juglone}		3973	
328.	1321-67-1	Naphthalenol {naphthol}	5811, 5835		
329.	121198-51-4	Naphthalenol, 6,8-dimethyl-		3430, 5811b	
330.	121198-52-5	Naphthalenol, 7,8-dimethyl-		3430, 5811b	
331.	90-15-3	1-Naphthalenol {1-naphthol; α-naphthol} 	765, 786–789, 789a, 869, 1063–1066, 1068–1074, 1378, 1626, 1649, 1879, 1884, 2079, 2601a, 2767, 2939, 3059, 3263, 3302, 3474, 3557, 3616, 3746, 3747, 3797, 3999, 4248, 4249, 4319		1378, 3395
332.	40529-54-2	1-Naphthalenol, dimethyl-	1884, 3746, 3747, 4249, 5811b		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
333.	59534-35-9	1-Naphthalenol, methyl-	1884, 3746, 3747, 4249, 5811b		
334.		1-Naphthalenol, methyl-nitro-	1884, 2137, 3746, 3747, 4249		
335.	7469-77-4	1-Naphthalenol, 2-methyl-	1884, 3746, 3747, 4249, 5811b		
336.	135-19-3	2-Naphthalenol {2-naphthol; β-naphthol}	414, 568b, 765, 786–789, 789a, 869, 1025, 1365, 1378, 1626, 1649, 1879, 1884, 2079, 2195, 2939, 3059, 3263, 3302, 3474, 3616, 3746, 3747, 3753, 3797, 3999, 4005–4007, 4249, 4319, 5811b, 21A19	568b, 4249, 21A19	1378, 3395
337.	73850-19-8	2-Naphthalenol, dimethyl-	1884, 3746, 3747, 5811b		
338.	54703-51-4	2-Naphthalenol, 1,8-dimethyl-	3746, 3747, 4249		
339.	59534-36-0	2-Naphthalenol, methyl-	1884, 3745–3747, 3753, 5811b		
340.	1076-26-2	2-Naphthalenol, 1-methyl-	1378, 3746, 3747, 4249		1378
341.	71369-76-1	2-Naphthalenol, tetrahydro-	765, 2939, 4249		
342.	1125-78-6	2-Naphthalenol, 5,6,7,8-tetrahydro-	414, 2939, 3302		
343.		2-Naphthalenol, 5,6,7,8-tetramethyl-	765		
344.	73850-18-7	2-Naphthalenol, trimethyl-	1884, 3746, 3747, 4249, 5811b		
345.	30889-50-0	2-Naphthalenol, 3,5,8-trimethyl-	2765, 2766, 3746, 3747		
346.	108-95-2	Phenol 	37, 38, 50, 83, 100, 126a, 126b, 155, 157, 167, 172, 173a, 174a, 174b, 174c, 174e, 213, 237, 239, 248, 269, 270, 274–277, 293, 295, 337, 351, 359, 376, 392, 396, 397, 402, 414, 520, 521, 532, 539, 568b, 603, 615, 616, 636, 640, 663, 664, 688, 722, 723, 765, 789, 789a, 804, 828, 830a, 851, 859, 884, 891a, 912, 922c, 1051, 1063–1074, 1091, 1099, 1115, 1129, 1132, 1138, 1140, 1153, 1158, 1213,	100, 120, 404, 568b, 937, 984, 1085, 1590a, 1825, 1876, 1877a, 1980, 2014, 2338, 2339a, 2379a, 2386, 2389, 2544, 2607, 2862, 2917a, 2939, 3090, 3194, 3350, 3430, 3547, 3549, 3973, 3974a, 4064, 4202, 4249, 5079, 5093, 5811b	50, 1330, 1332, 1354, 1360, 1375a, 1377, 1378, 2387, 2506, 2507, 3395, 3401, 3402, 3405

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References		
		Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Phenol (cont.)	1215, 1232, 1236, 1283, 1284, 1292, 1303, 1329, 1330, 1332, 1333, 1336, 1339, 1348–1350, 1354, 1360, 1361,1364, 1365, 1369, 1371, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1423, 1426, 1427, 1437, 1442, 1445, 1449, 1450, 1492, 1494, 1502, 1589, 1647, 1648, 1649, 1673, 1674, 1699, 1709, 1741, 1744, 1751, 1760, 1764, 1766, 1789, 1791, 1797, 1803, 1807a, 1827, 1842, 1857, 1879, 1881, 1882 1884, 1906, 1928, 1966, 1981, 1995, 1999,2042–2045, 2062, 2079, 2082–2086, 2088, 2089, 2114, 2125, 2133, 2142, 2170, 2190, 2191, 2195, 2230, 2245, 2253, 2254, 2261, 2262a, 2270, 2274, 2295, 2306, 2307, 2311, 2312, 2313a, 2327c, 2351, 2374, 2376–2378, 2379a, 2387, 2397, 2399, 2400d, 2408, 2476, 2480, 2493, 2506, 2507, 2508, 2526, 2543, 2545, 2570, 2577, 2578, 2582, 2583, 2598, 2601a, 2605, 2607, 2628–2631, 2636, 2653, 2681, 2683, 2691–2695, 2719, 2731, 2735, 2737, 2739, 2740, 2747, 2761, 2762, 2775, 2777, 2799a, 2800,		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References		
		Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Phenol (cont.)	2820, 2857, 2858, 2876, 2899, 2927, 2939, 2983, 3007, 3043, 3059, 3065, 3087, 3088, 3090, 3093, 3095, 3105, 3111, 3121a, 3131, 3132, 3165, 3166, 3171–3175, 3187, 3190, 3228, 3251, 3255, 3257, 3263–3265, 3277, 3286, 3291, 3300, 3302, 3305, 3306, 3308, 3314, 3370, 3373, 3394, 3397, 3410, 3447, 3451–3453, 3454, 3457, 3462, 3468, 3470, 3476, 3482, 3486, 3488, 3493, 3497, 3500, 3551, 3553, 3555, 3557, 3559, 3572, 3576, 3577, 3616, 3625, 3650, 3671, 3712, 3716–3720, 3746, 3747, 3764, 3765, 3767, 3795, 3797, 3800, 3826, 3844, 3884, 3892, 3912a,3939, 3952, 3984, 3990a, 3992, 4005–4007, 4009, 4036, 4064, 4065, 4067, 4113, 4118, 4121, 4122, 4159, 4228, 4232, 4248, 4249, 4259, 4268, 4269a, 4290, 4301, 4304, 4311, 4314, 4317, 4319, 4322, 4328–4330, 4338, 4349, 4350, 4407, 4418, 4636, 4796, 4965, 5011, 5031, 5034, 5079, 5093, 5140, 5207, 5500, 5512, 5531, 5532, 5546, 5555, 5564, 5576, 5588, 5643a, 5811b, 5835, 5836, 5869a		

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
347.		Phenol, C_2-alkyl-	663, 2508, 2543, 2777		
348.		Phenol, C_3-alkyl-	663, 1364, 1371, 2543, 2761, 2762, 2765, 2766, 2773, 2775, 3410, 3559, 4248		
349.		Phenol, C_4-alkyl-	652, 663, 1364, 1365, 1371, 2543, 2761, 2765, 2766, 2773, 2775, 3410, 3746, 3747, 4248		
350.		Phenol, C_5-alkyl-	3746, 3747		
351.		Phenol, C_2-alkyl-ethenyl- {2 isomers}	3746, 3747		
352.		Phenol, C_4-alkyl-ethenyl-	3746, 3747		
353.		Phenol, C_5-alkyl-ethenyl-	3746, 3747, 4249		
354.		Phenol, alkyl-dimethoxy-	1586, 2767, 3557		
355.		Phenol, diethyl-	2570		
356.	25155-26-4	Phenol, dimethoxy-	3753, 5034		
357.		Phenol, dimethoxy-4-ethenyl-	2767		
358.	1300-71-6	Phenol, dimethyl- {xylenol}	125, 804, 828, 859, 1063–1066, 1068–1074, 1235, 1292, 1371, 1626, 1647, 1648, 1649, 1884, 1995, 2005, 2142, 2293, 2298, 2307, 2310, 2311, 2506, 2507, 2543, 2545, 2570, 2731, 2735, 2767, 2773, 2775, 2871, 3255, 3263, 3308, 3410, 3447, 3451, 3553, 3616, 3741, 3795, 4248, 4249, 4312, 4313, 4414, 5835	2338, 3188, 3350	2506, 2507, 3401
359.	73850-14-3	Phenol, dimethyl-ethenyl-	1884, 3746, 3747, 4249, 5811, 5811a, 5811b		
360.	73850-04-1	Phenol, dimethyl-4-ethenyl-	1884, 3746, 3747, 4249, 5811b		
361.	50984-45-7	Phenol, dimethyl-ethenyl-ethyl-	3746, 3747, 4249, 5811b		
362.		Phenol, dimethyl-ethenyl-2-methoxy-	3746, 3747, 4249		
363.	85528-07-0	Phenol, dimethylethyl-	5811, 5811a, 5811b		
364.	27178-34-3	Phenol, (1,1-dimethylethyl)-	1884, 3712, 4249		
365.	1329-97-1	Phenol, dimethyl-methoxy-	1884, 3712, 4249		
366.		Phenol, dimethyl-2-methoxy-	1884, 3746, 3747, 4249		
367.		Phenol, dimethyl-4-methoxy-	1884, 3746, 3747		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
368.		Phenol, dimethyl-2-nitro-	2137, 3491, 4249		
369.	31257-96-2	Phenol, ethenyl-	1426, 1427, 3741, 4249		
370.	50851-69-9	Phenol, ethenyl-ethyl-	1884, 3746, 3747, 4249, 5811b		
371.		Phenol, ethenyl-ethylmethyl-	1884, 3746, 3747, 4249		
372.		Phenol, ethenyl-2-methoxy-trimethyl-	3746, 3747, 4249		
373.	73850-05-2	Phenol, ethenyl-methyl-	1378, 1884, 3746, 3747, 5811b		1378
374.	73850-13-2	Phenol, ethenyl-trimethyl-	1884, 3746, 3747, 4249, 5811b		
375.	25429-37-2	Phenol, ethyl-	152, 157, 828, 1063–1066, 1068–1074, 1365, 1647, 1648, 2142, 2195, 2387, 2506, 2507, 2570, 2628, 2629, 2636, 2767, 3255, 3263, 3308, 3616, 3903, 4248, 4249, 4312, 5034, 5811b		2387, 2506, 2507, 3395, 3401, 3402
376.	80652-16-0	Phenol, ethyl-methoxy-	1884, 4249		
377.		Phenol, ethyl-2-methoxy-	1884, 3746, 3747		
378.	30230-52-5	Phenol, ethylmethyl-	652, 661, 1375a, 1377, 1378, 2195, 2570, 2871, 3308, 3746, 3747, 4249, 5811b		1375a, 1377, 1378
379.		Phenol, ethyl-methyl-nitro-	2137, 3491		
380.		Phenol, ethyl-nitro-	2137, 3491		
381.	26638-03-9	Phenol, methoxy-	152, 157, 2767, 4249		
382.	60825-46-9	Phenol-$^{14}C_6$, 2-methoxy-	2769, 2777, 4249		
383.	32391-38-1	Phenol, methoxy-methyl-	1884, 3712	5811b	
384.		Phenol, 2-methoxy-propyl-	4249		
385.	1319-77-3	Phenol, methyl- {cresol}	100, 105, 337, 376, 765, 828, 859, 1283, 1371, 1413, 1647, 1648, 1649, 2006, 2142, 2274, 2506, 2507, 2731, 2735, 3087, 3251, 3277, 3394, 3451, 3468, 3470, 3555, 3717, 3718, 3797, 4009, 4248, 4249, 4290, 4313, 4319, 4414, 4418, 5079, 5811b	100, 1980, 2389, 2544, 3350, 3430, 3555, 3973, 5811b	2506, 2507

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TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
386.	12167-20-3	Phenol, methyl-nitro-	2137, 3491, 4249		
387.		Phenol, methylpropylenyl-	4248, 4249		
388.	62744-64-3	Phenol, methylpropyl-	3746, 3747		
389.		Phenol, propenyl-	1364, 3746, 3747		
390.		Phenol, propyl-	1375, 1375b, 2761, 2762, 2766, 4249		
391.	66586-93-4	Phenol, tetramethyl-	312, 2767, 2777, 3557, 4249, 5811b		
392.	26998-80-1 73850-02-9	Phenol, trimethyl-	157, 1364, 1427, 1587, 2570, 2731, 2735, 2777, 3228, 3741, 4249, 5811, 5811a, 5811b	2338	
393.	3180-09-4	Phenol, 2-butyl-	414, 2554, 3712, 4249		
394.	95-57-8	Phenol, 2-chloro-	568b, 1928, 1994, 1995, 3712, 4249, 5811b		
395.	3743-22-4	Phenol, 2-(dimethylamino)-	3674, 3712, 4249		
396.	88-18-6	Phenol, 2-(1,1-dimethylethyl)-	2554, 3746, 3747, 4249, 5811b		
397.	25013-16-5	Phenol, 2-(1,1-dimethylethyl)-4-methoxy-	568b, 4249		
398.	695-84-1	Phenol, 2-ethenyl-	1063–1066, 1068–1074, 1378, 1426, 1427, 1879, 1884, 3712, 3746, 3747, 4249, 5811b		1378
399.	120550-69-8	Phenol, 2-ethenyl-6-methoxy-	90a, 3712, 5811b		
400.	135295-09-9	Phenol, 2-ethenyl-6-methyl-	91a, 1378, 3712, 5811b		1378
401.	94-86-0	Phenol, 2-ethoxy-5-propenyl- {5-propenylguaethol}		172a, 174b, 1053, 3266, 3370	
402.	90-00-6	Phenol, 2-ethyl-	50, 414, 568b, 851, 1063–1066, 1068–1075, 1153, 1360, 1364, 1371, 1375a, 1378, 1426, 1427, 1766, 1879, 1882, 2543, 2545, 2598, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 3095, 3255, 3302, 3410, 3452, 3712, 3716, 3717, 3719, 3746, 3747, 3797, 4249, 4317, 4319, 4796, 5011, 5811b	568b, 952, 1876, 1877a, 2917a, 4249, 5811b	50, 1360, 1375a, 1378, 3395, 3402
403.	13391-32-7	Phenol, 2-ethyl-4-methoxy-	1884, 2769, 3712, 5811, 5811b	5811, 5811b	
404.	90534-46-6	Phenol, 2-ethyl-6-methoxy-	90a, 3712, 5811b		
405.	6161-62-2	Phenol, 2-ethyl-3-methyl-	91a, 5811b		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
406.	3855-26-3	Phenol, 2-ethyl-4-methyl-	1063–1066, 1068–1074, 1378, 1586, 1884, 2767, 2769, 3557, 3712, 4249, 5811b		1378
407.	1687-61-2	Phenol, 2-ethyl-5-methyl-	91a, 1356, 1586, 2767, 3557, 3712, 4249, 5034, 5811b		
408.	1687-64-5	Phenol, 2-ethyl-6-methyl-	568b, 1356, 1371, 1378, 1586, 1884, 2545, 2767, 2769, 2775, 3410, 3553, 3557, 3559, 3712, 5811b		1378
409.	71607-97-1	Phenol, 2-ethyl-3-nitro-	2137, 3797, 4249		
410.		Phenol, 2-ethyl-4-nitro-	3712		
411.	90-05-1	Phenol, 2-methoxy- {guaiacol}	50, 376, 568b, 615, 723, 765, 789, 789a, 804, 830a, 851, 859, 966, 1063–1066, 1068–1074, 1089a, 1099, 1140, 1232, 1235, 1236, 1292, 1360, 1364, 1371, 1375, 1375a, 1375b, 1427, 1586, 1626, 1882, 1884, 1887a, 1906, 1928, 1963, 1995, 2042–2045, 2079, 2142, 2195, 2270, 2298, 2302, 2307, 2311, 2327c, 2379a, 2387, 2524a, 2545, 2577, 2598, 2601a, 2761, 2762, 2765–2767, 2777, 2858, 2939, 3059, 3090, 3255, 3266, 3302, 3308, 3394, 3410, 3453, 3457, 3462, 3555, 3557, 3559, 3719, 3746, 3747, 3764, 3767, 3797, 3876, 3952, 4248, 4249, 4313, 4317, 4319, 4414, 4796, 4999, 5011, 5034, 5079, 5811b	120, 172a, 174a, 174b, 404, 568b, 937, 952, 1053, 1063–1066, 1068–1074, 1102, 1590a, 1825, 1876, 1877a, 1980, 2338, 2379a, 2611, 2862, 2917a, 2939, 3059, 3090, 3194, 3266, 3350, 3430, 3543, 3547, 3555, 3560, 3561, 3797, 3973, 3974a, 4202, 4249, 5079, 5811b	50, 1360, 1375a, 2387, 3395
412.	60825-46-9	Phenol-$^{14}C_6$, 2-methoxy- {guaiacol-$^{14}C_6$}	2769, 2777, 4249		

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
413.		Phenol, 2-methoxy-methyl-	1884, 3746, 3747		
414.	18102-31-3	Phenol, 2-methoxy-3-methyl-	90a, 3712, 5811b		
415.	53587-16-9	Phenol, 2-methoxy-4-(1-methylethyl)-	90a, 3712, 4249, 5811b	2386, 4249	
416.	97-54-1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}	127, 568b, 1063–1066, 1068–1074,1375, 1375b, 1426, 1427, 1649, 2270, 2327c, 2543, 2545, 2761, 2762, 2767, 2773, 2777, 3251, 3280, 3300, 3302, 3462, 3557, 3712, 3797, 4005–4007, 4248, 4249, 5811b	120, 568b, 1063–1066, 1068–1074, 1091, 1221, 1626, 1649, 2079, 2270, 2283, 2917a, 2939, 3059, 3430, 3797, 3974a, 4249, 5079, 5180, 5811b	
417.	5932-68-3	Phenol, 2-methoxy-4-(1-propenyl)-, (*E*)- {*trans*-isoeugenol}	101, 3712, 3746, 3747, 5811b	1877a, 3430, 5811b	
418.	5912-86-7	Phenol, 2-methoxy-4-(1-propenyl)-, (*Z*)- {*cis*-isoeugenol}	101, 3712, 3746, 3747, 4249, 5811b	1877a, 3430, 5811b	
419.	97-53-0	Phenol, 2-methoxy-4-(2-propenyl)- {eugenol}	101, 127, 497, 568b, 1063–1066, 1068–1074, 1360, 1375, 1375a, 1375b, 1427, 1586, 1884, 2270, 2487, 2543, 2545, 2570, 2628, 2629, 2636, 2765–2767, 2773, 2939, 3251, 3280, 3300, 3302, 3308, 3453, 3557, 3712, 3746, 3747, 3797, 4005–4007, 4028, 4037, 4113, 4248, 4249, 5537, 5811b	120, 568b, 1102, 1221, 1626, 1825, 1854, 1876, 1877a, 2014, 2079, 2270, 2283, 2338, 2339, 2611, 2862, 2917a, 3059, 3194, 3430, 3797, 3973, 3974a, 4249, 5079, 5180, 5363, 5811b	1360, 1375a
420.	93-15-2	Phenol, 2-methoxy-methyl-4-(2-propenyl)- {eugenol, methyl-}	568b, 1741, 1743, 1744, 3265, 3300, 5512, 5537, 5811b	5515, 5811b	
421.	93-51-6	Phenol, 2-methoxy-4-methyl- {4-methylguaiacol}	568b, 1063–1066, 1068–1074, 1360, 1364, 1371, 1375, 1375a, 1375b, 1586, 2327c, 2543, 2767, 2773, 2775, 3266, 3410, 3553, 3557, 3712, 4249, 4796, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877a, 2014, 3266, 3370, 3430, 4249, 5811b	1360, 1375a
422.	2785-87-7	Phenol, 2-methoxy-4-propyl-	90a, 2570, 3712, 5811b	1876, 1877a, 4249, 5811b	
423.	19784-98-6	Phenol, 2-methoxy-5-(1-propenyl)-, (*E*)-	90a, 3712, 5811b		
424.	1195-09-1	Phenol, 2-methoxy-5-methyl-	90a, 3712	1877a	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
425.	58539-27-8	Phenol, 2-methoxy-5-propyl-	90a, 3712, 5811b		
426.	29275-83-0	Phenol, 2-methoxy-6-(1-propenyl)-, (*E*)-	3712		
427.	29275-82-9	Phenol, 2-methoxy-6-(1-propenyl)-, (*Z*)-	90a, 3712, 5811b		
428.	2896-67-5	Phenol, 2-methoxy-6-methyl-	90a, 3712, 5811b		
429.	32073-24-8	Phenol, 2-methoxy-propyl-	1884, 3746, 3747		
430.	93526-86-4	Phenol, 2-methoxy-trimethyl-	101, 1884, 3746, 3747, 4249, 5811b	5811b	
431.	95-48-7	Phenol, 2-methyl- {*o*-cresol}	50, 155, 172, 174a, 174b, 174c, 174e, 239, 274, 276, 277, 402, 414, 521, 532, 539, 568b, 603, 615, 616, 688, 722, 723, 765, 786, 787, 789, 789a, 830a, 851, 966, 1063–1066, 1068–1075, 1099, 1132, 1158, 1215, 1329, 1330, 1332, 1333, 1339, 1360, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1427, 1437, 1445, 1450, 1586, 1626, 1647, 1648, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1906, 1928, 1981, 1995, 2043, 2044, 2079, 2191, 2210, 2245, 2270, 2307, 2313a, 2387, 2526, 2543, 2545, 2557a, 2570, 2577, 2598, 2601a, 2628, 2629, 2636, 2681, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2820, 2857, 2876, 2939, 3007, 3059, 3088, 3090, 3095, 3105, 3131, 3171–3175, 3190, 3251, 3255, 3263, 3264, 3277, 3300,	568b, 937, 1825, 1876, 1877a, 2338, 2389, 2544, 3547, 4249, 5093, 5811b	50, 1330, 1332, 1360, 1375a, 1377, 1378, 2210, 2387, 3395, 3401, 3402

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Phenol, 2-methyl- {*o*-cresol} (cont.)	3302, 3370, 3394, 3397, 3410, 3447, 3452, 3453, 3476, 3486, 3488, 3493, 3553, 3557, 3559, 3616, 3671, 3712, 3716–3719, 3741, 3746, 3747, 3764, 3797, 3800, 3826, 3844, 3876, 3952, 3984, 3992, 4005–4007, 4228, 4249, 4259, 4268, 4313, 4317, 4319, 4350, 4354, 4407, 4414, 4796, 5011, 5034, 5079, 5093, 5500, 5532, 5564, 5576, 5588, 5643a, 5811b, 5836, 5869a		
432.	70-30-4	Phenol, 2,2′-methylenebis[3,4,6-trichloro-	4249		
433.	88-69-7	Phenol, 2-(1-methylethyl)- {2-isopropylphenol}	568b, 1378, 1884, 2543, 2773, 3559, 3712, 3746, 3747, 4248, 4249, 5811b	568b, 1053, 3266, 4249	1378
434.	1740-97-2	Phenol, 2-methyl-4-(1-methylethyl)-	2195, 3712		
435.	499-75-2	Phenol, 2-methyl-5-(1-methylethyl)- {carvacrol}	2195, 3266, 3308, 3555, 3712, 4249	172a, 174b, 1053, 3266, 5811b	
436.		Phenol, 2-methyl-(2-methylpropyl)-	4249		
437.	99-53-6	Phenol, 2-methyl-4-nitro-	2137, 3491, 3712, 4249, 5811b		
438.	3520-52-3	Phenol, 2-methyl-6-propyl-	1375, 1375b, 1884, 2767, 2769, 3557, 3746, 3747		
439.	73850-08-5	Phenol, (2-methylpropyl)-	5811, 5811a, 5811b		
440.	89-72-5	Phenol, 2-(1-methylpropyl)-	91, 1884, 3712, 3746, 3747, 4249, 5811b	5811b	
441.	4167-75-3	Phenol, 2-(2-methylpropyl)-	2554, 3712, 4249		
442.	88-75-5	Phenol, 2-nitro-	414, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
443.	2417-10-9	Phenol, 2-phenoxy-	1884, 3712, 3744		
444.	26761-75-1	Phenol, 2-(propen-1-yl)-	414, 1884, 3712, 3746, 3747, 5811, 5811a, 5811b		
445.	6380-21-8	Phenol, 2-(1-propenyl)-	91a, 5811b		
446.	1745-81-9	Phenol, 2-(2-propenyl)-	414, 568b, 1884, 3712, 3746, 3747, 4249, 4570a, 5811b		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
447.	644-35-9	Phenol, 2-propyl-	568b, 1360, 1371, 1375, 1375a, 1375b, 1378, 1884, 2769, 3410, 3712, 4249	568b, 1877a, 2386, 4249, 5811b	1360, 1375a, 1378
448.	591-27-5	Phenol, 3-amino-	1371, 2543, 2773, 2775, 3410, 3712, 4249		
449.	108-43-0	Phenol, 3-chloro-	278, 3712, 4249		
450.	585-34-2	Phenol, 3-(1,1-dimethylethyl)-	101, 1884, 3712, 3746, 3747, 4249, 5811b		
451.	618-45-1	Phenol, 3-(1-methylethyl)-	101, 1884, 3712, 3746, 3747, 4249, 5811b	4249, 4563	
452.	620-18-8	Phenol, 3-ethenyl-	1099, 1879, 1884, 3712, 3746, 3747, 4249, 5811b		
453.	73850-03-0	Phenol, 3-ethenyl-methyl-	1884, 3746, 3747, 5811, 5811a, 5811b		
454.	66164-30-5	Phenol, 3-ethenyl-4-methyl-	3712, 3746, 3747, 4249		
455.	73850-06-3	Phenol, 3 ethenyl-2,?,?-trimethyl-	5811, 5811a, 5811b		
456.	621-34-1	Phenol, 3-ethoxy-		2917a	
457.	620-17-7	Phenol, 3-ethyl-	155, 851, 1063–1066, 1068–1074, 1364, 1365, 1371, 1378, 1426, 1427, 1626, 1766, 1789, 1791, 1803, 1879, 1906, 1995, 2327c, 2543, 2628, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2800, 2876, 3059, 3095, 3302, 3308, 3410, 3712, 3716, 3717, 3719, 3746, 3747, 3764, 3765, 3797, 3800, 3903, 4249, 4317, 4319, 4350, 4407, 5811b	952, 1876, 1877a, 4249, 5811b	1378, 3395
458.	29760-89-2	Phenol, 3-ethyl-2-methoxy-	5811, 5811a, 5811b		
459.	1123-73-5	Phenol, 3-ethyl-2-methyl-	91a, 5811b		
460.	6161-67-7	Phenol, 3-ethyl-4-methyl-	91a, 1375a, 1377, 1378, 3712, 4249, 5811b		1375a, 1377, 1378

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
461.	698-71-5	Phenol, 3-ethyl-5-methyl-	1365, 1586, 1884, 2601a, 2761, 2762, 2765–2767, 2769, 3557, 3712, 4249, 5811b	1248, 2389, 2544, 4249, 5811b	
462.	150-19-6	Phenol, 3-methoxy-	1626, 1879, 1882, 1884, 2598, 3308, 3712, 3764, 3765, 3797, 4414, 4796, 5011, 5811b	952, 1876, 1877a, 4249, 5811b	3395
463.	108-39-4	Phenol, 3-methyl- {*m*-cresol}	50, 155, 172, 174a, 174b, 174c, 174e, 239, 274, 276, 277, 293, 402, 414, 521, 532, 539, 568b, 603, 615, 616, 688, 723, 765, 786, 787, 789, 789a, 830a, 851, 966, 1051, 1063–1066, 1068–1075, 1099, 1132, 1158, 1329, 1330, 1332, 1333, 1339, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1427, 1437, 1445, 1450, 1586, 1626, 1647, 1648, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1906, 1928, 1981, 1995, 2043, 2079, 2191, 2203, 2245, 2270, 2307, 2313a, 2327c, 2387, 2493, 2526, 2543, 2545, 2557a, 2570, 2577, 2598, 2628, 2681, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2857, 2858, 2876, 2939, 3007, 3059, 3088, 3090, 3095, 3131, 3165, 3166, 3171–3175, 3190, 3255, 3263, 3264, 3300, 3302, 3370, 3394, 3397,	120, 568b, 1825, 1876, 1877a, 2283, 2338, 2389, 2544, 2862, 2939, 3059, 3194, 3547, 3797, 3973, 3974a, 4249, 5079, 5093, 5811b	50, 1330, 1332, 1360, 1375a, 1377, 1378, 2387, 3395, 3401, 3402, 3405

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Phenol, 3-methyl- {*m*-cresol} (cont.)	3410, 3447, 3452, 3453, 3476, 3486, 3488, 3493, 3557, 3559, 3616, 3671, 3712, 3716–3719, 3741, 3746, 3747, 3764, 3765, 3800, 3826, 3844, 3876, 3952, 3984, 3990a, 3992, 4005–4007, 4228, 4249, 4268, 4313, 4317, 4319, 4350, 4351, 4407, 4414, 4796, 5011, 5014, 5034, 5079, 5093, 5500, 5532, 5564, 5576, 5588, 5643a, 5811b, 5836, 5869a		
464.	4920-77-8	Phenol, 3-methyl-2-nitro-	2137, 3491, 3712, 4010, 4011, 4249, 5811b		
465.	2581-34-2	Phenol, 3-methyl-4-nitro-	2137, 3491, 3712, 4010, 4011, 4249, 5811b		
466.	554-84-7	Phenol, 3-nitro-	2137, 3491, 3712, 4010, 4011, 4249, 5811b		
467.	713-68-8	Phenol, 3-phenoxy-	568b, 1587, 1884, 3108, 3712, 3745, 4249		
468.	88-32-4	Phenol, 3-(1,1-dimethyethyl)-4-methoxy-	4570a		
469.	79755-53-6	Phenol, 3-(1-propenyl)-	91a, 5811b		
470.	621-27-2	Phenol, 3-propyl-	101, 1884, 3712, 3746, 3747, 4249, 5811b		
471.	98-54-4	Phenol, 4-(1,1-dimethylethyl)-	101, 1884, 3190, 3712, 3746, 3747, 3992, 4249, 5811b	2338	
472.	99-89-8	Phenol, 4-(1-methylethyl)-	101, 1884, 2543, 2773, 3712, 3746, 3747, 4249, 5811b	2917a	
473.	99-71-8	Phenol, 4-(1-methylpropyl)-	101, 1884, 3712, 3746, 3747, 4249, 5811b	5811b	
474.	51-67-2	Phenol, 4-(2-aminoethyl)- {tyramine}	3491, 3674, 3712, 4249	1351, 2337, 3491, 3797, 3974a, 3978, 4249	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
475.	501-92-8	Phenol, 4-(2-propenyl)-	1063–1066, 1068–1074, 1364, 1586, 1884, 2767, 2769, 3557, 3712, 4249, 5811b	5811b	
476.	3690-05-9	Phenol, 4-(3-hydroxy-1-propenyl)- {coumaryl alcohol}		1102, 2338	
477.	537-33-7	Phenol, 4-(3-hydroxy-1-propenyl)-2,6-dimethoxy- {sinapyl alcohol}		1102, 2338,3973, 4249, 4438a, 5811b	
478.	458-35-5	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy- {coniferyl alcohol}	596, 1879, 1881, 1883, 1884, 3712, 3828, 4249, 5811b	1102, 2338, 3973	
479.	32811-40-8	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*E*)-		1879, 4249	
480.	69056-21-9	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*Z*)-		1879, 4249, 5811b	
481.	59832-96-1	Phenol, 4-butyl-2-methoxy-	90a, 3712, 5811b		
482.	2628-17-3	Phenol, 4-ethenyl-	1063–1066, 1068–1074, 1089a, 1099, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1879, 1881–1884, 1887a, 2387, 2493, 2524a, 2545, 2570, 2761, 2762, 2765–2767, 2777, 2857, 3255, 3394, 3397, 3557, 3712, 3746, 3747, 4159, 4249, 4796, 5811b	404, 1063–1066, 1068–1074, 1587a, 1590a, 2338, 2389, 2544, 3430, 3547, 3549, 5811b	1360, 1375a, 2387, 3395
483.		Phenol, 4-ethenyl-2-ethyl-	3712, 3747, 4249		
484.	7786-61-0	Phenol, 4-ethenyl-2-methoxy- {4-vinylguaiacol}	101, 1063–1066, 1068–1075, 1089a, 1364, 1586, 1879, 1881, 1883, 1884, 1887a, 2524a, 2545, 2570, 2767, 3255, 3266, 3397, 3410, 3557, 3712, 3746, 3747, 4159, 4249, 5811b	172a, 174b, 937, 1053, 1587a, 1590a, 1876, 1877a, 1878, 2338, 2389, 2544, 2917a, 3266, 3430, 3547, 3549, 4249, 5811b	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
485.	45803-83-6	Phenol, 4-ethenyl-2-methyl-	3712, 3746, 3747, 4249		
486.	123-07-9	Phenol, 4-ethyl- {*p*-ethylphenol}	50, 568b, 723, 851, 1075, 1360, 1364, 1371, 1375, 1375a, 1375b, 1426, 1427, 1586, 1626, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1981, 1995, 2543, 2545, 2598, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2876, 3088, 3095, 3266, 3302, 3308, 3397, 3410, 3493, 3555, 3557, 3559, 3712, 3716–3719, 3746, 3747, 3764, 3765, 3797, 3800, 4249, 4313, 4317, 4319, 4350, 4796, 5011, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877a, 2389, 2544, 2917a, 3266, 3430, 3547, 3555, 4249, 5811b	50, 1360, 1375a, 3395
487.	2785-89-9	Phenol, 4-ethyl-2-methoxy- {4-ethyguaiacol}	568b, 1063–1066, 1068–1074, 1364, 1371, 1375, 1375b, 1586, 1587, 1884, 2327c, 2543, 2765–2767, 2769, 3266, 3410, 3557, 3559, 3712, 3746, 3747, 4249, 5034, 5811b	568b, 1876, 1877a, 2014, 2338, 3266, 3430, 4249, 5811b	
488.	120550-71-2	Phenol, 4-ethyl-2-methoxy-5-methyl-	90a, 3712, 5811b		
489.	120550-70-1	Phenol, 4-ethyl-2-methoxy-6-methyl-	90a, 3712, 5811b		
490.	2219-73-0	Phenol, 4-ethyl-2-methyl-	1375, 1375b, 1586, 1884, 2767, 2769, 3557, 3712, 4249, 5811b		
491.	1123-94-0	Phenol, 4-ethyl-3-methyl-	91a, 1378, 3712, 4249, 5811b		1378
492.	71607-98-2	Phenol, 4-ethyl-3-nitro-	2137, 3712, 4249		
493.	150-76-5	Phenol, 4-methoxy-	414, 1586, 1626, 2387, 2570, 2598, 2767, 3255, 3257, 3265, 3555, 3712, 3764, 3797, 4319, 4414, 4796, 5011, 5811b	1876, 1877a, 2389, 2544, 3555, 5811b	2387, 3395

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
494.	106-44-5	Phenol, 4-methyl- {*p*-cresol}	37, 38, 50, 155, 156, 157, 172, 174a, 174b, 174c, 174e, 239, 274, 276, 277, 293, 402, 414, 521, 532, 539, 568b, 603, 615, 616, 688, 723, 765, 786, 787, 789, 789a, 830a, 851, 966, 1051, 1063–1066, 1068–1075, 1099, 1158, 1231, 1232, 1329, 1330, 1332, 1333, 1339, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1386, 1388–1390, 1427, 1437, 1445, 1450, 1586, 1626, 1647, 1648, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1906, 1928, 1981, 1995, 2043, 2079, 2133, 2191, 2210, 2245, 2270, 2311, 2313a, 2327c, 2387, 2493, 2526, 2543, 2545, 2557a, 2570, 2577, 2598, 2601a, 2628, 2681, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2820, 2857, 2876, 2939, 3007, 3059, 3088, 3095, 3131, 3165, 3166, 3171–3175, 3190, 3251, 3255, 3263, 3264, 3277, 3286, 3300, 3302, 3305, 3370, 3394, 3397, 3410, 3447, 3452,	404, 568b, 1085, 1825, 1876, 1877a, 2014, 2338, 2389, 2544, 2611, 2917a, 3430, 3547, 4249, 5093	50, 1330, 1332, 1360, 1375a, 2210, 2387, 3395, 3401, 3402, 3405

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Phenol, 4-methyl- {*p*-cresol} (cont.)	3453, 3476, 3486, 3488, 3493, 3553, 3557, 3559, 3616, 3671, 3712, 3716–3718, 3741, 3746, 3747, 3764, 3765, 3797, 3800, 3826, 3844, 3876, 3952, 3984, 3990a, 3992, 4005–4007, 4159, 4228, 4249, 4268, 4313, 4317, 4319, 4350, 4354, 4407, 4414, 4796, 5011, 5014, 5034, 5079, 5093, 5500, 5532, 5564, 5576, 5588, 5643a, 5811b, 5836, 5869a		
495.	4427-56-9	Phenol, 4-methyl-2-(1-methylethyl)-	414, 2761, 3712, 4249		
496.	119-33-5	Phenol, 4-methyl-2-nitro-	2137, 3712, 4010, 4011, 4249, 5811b		
497.	2042-14-0	Phenol, 4-methyl-3-nitro-	2137, 3712, 4249		
498.	4074-46-8	Phenol, 4-methyl-2-propyl-	1375a, 1377, 1378, 4249		1375a, 1377, 1378
499.	100-02-7	Phenol, 4-nitro-	414, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
500.	831-82-3	Phenol, 4-phenoxy-	4249		
501.	1988-89-2	Phenol, 4-(1-phenylethyl)-		2917a	
502.	101-53-1 7563-63-5	Phenol, 4-phenylmethyl-	2210, 3712, 4249		
503.	85960-81-2	Phenol, 4-(1-propen-1-yl)-, (*Z*)-	91a		
504.	539-12-8	Phenol, 4-(1-propen-1-yl)-	5811, 5811b		
505.	645-56-7	Phenol, 4-propyl-	1884, 3712, 3746, 3747, 4249, 5811b	1877a	
506.	2785-88-8	Phenol, 5-ethyl-2-methoxy-	90a, 3712, 5811b		
507.	1687-65-6	Phenol, 5-ethyl-2-methyl-	568b, 4249		
508.	71278-12-1	Phenol, 5-ethyl-2-methyl-4-nitro- {phenol, 3-ethyl-6-methyl-4-nitro-}	2137, 3712, 4249		
509.	89-83-8	Phenol, 5-methyl-2-(1-methylethyl)- {thymol}	568b, 1884, 2577, 3266, 3308, 3555, 3559, 3797, 4249, 5811b	172a, 174b, 568b, 1053, 1156, 1254, 1256, 2611, 3266, 4090, 4249, 5811b	
510.	5150-42-5	Phenol, 2,3-dimethoxy-	568b, 2570, 3712, 4249	568b, 1877a, 4249	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
511.	20578-97-6	Phenol, 2,3-dimethoxy-4-ethyl-	3712	1876, 1877a	
512.	526-75-0	Phenol, 2,3-dimethyl- {2,3-xylenol}	50, 568b, 851, 1075, 1360, 1364, 1365, 1371, 1375a, 1378, 1426, 1427, 1586, 1879, 1884, 1995, 2005, 2387, 2543, 2545, 2598, 2761, 2762, 2765–2767, 2773, 2775, 3088, 3302, 3395, 3410, 3557, 3712, 3716–3719, 3746, 3747, 3797, 4249, 4319, 4414, 4796, 5011, 5811b	568b, 952, 1876, 1877a, 4249, 5811b	50, 1360, 1375a, 1378, 2387, 3395
513.	18441-55-9	Phenol, 2,3-dimethyl-6-ethyl-	1378, 2767, 3557, 3712, 4249		1378
514.	34883-01-7	Phenol, 2,3-dimethyl-5-methoxy-	3712	2237	
515.	6665-95-8	Phenol, 2,3-dimethyl-6-nitro- {phenol, 5,6-dimethyl-2-nitro-}	2137, 3491, 3712, 4010, 4011, 4249		
516.	105-67-9	Phenol, 2,4-dimethyl- {2,4-xylenol}	50, 155, 293, 414, 568b, 722, 851, 966, 1132, 1360, 1371, 1375, 1375a, 1375b, 1377, 1378, 1426, 1427, 1586, 1626, 766, 1789, 1791, 1803, 1882, 1884, 1995, 2005, 2387, 2543, 2545, 2598, 2628, 2761, 2762, 2765–2767, 2773, 2775, 2800, 2876, 2939, 3095, 3302, 3308, 3410, 3453, 3488, 3493, 3557, 3559, 3712, 3716–3718, 3746, 3747, 3764, 3797, 3876, 3903, 4005–4007, 4249, 4313, 4317, 4319, 4350, 4354, 4407, 4414, 4796, 5011, 5811b	568b, 1132, 1825, 1876, 1877a, 4249, 5811b	50, 1360, 1375a, 1377, 1378, 2387, 3395, 3402
517.		Phenol, 2,4-dimethyl-6-ethyl-	2765–2767, 2769, 3557, 3712, 4249		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
518.	95-87-4	Phenol, 2,5-dimethyl- {2,5-xylenol}	50, 293, 414, 568b, 1075, 1132, 1360, 1364, 1365, 1371, 1375a, 1426, 1427, 1586, 1626, 1803, 1879, 1884, 1906, 1995, 2005, 2046, 2168, 2543, 2545, 2570, 2598, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2876, 2939, 3059, 3088, 3095, 3302, 3308, 3410, 3452, 3453, 3557, 3712, 3716–3719, 3746, 3747, 3764, 3767, 3797, 4249, 4319, 4414, 4796, 5011, 5811b	568b, 1132, 1876, 1877a, 4249, 5811b	50, 1360, 1375a, 3395
519.		Phenol, 2,5-dimethyl-6-nitro-	2137, 3712		
520.	1006-59-3	Phenol, 2,6-diethyl-	1884, 2769, 3557, 3712, 4249		
521.	4130-42-1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-	1371, 3712, 4249	404	
522.	128-37-0	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	568b, 1063–1066, 1068–1074, 1364, 1365, 1825, 1884, 2327c, 2767, 3410, 3553, 3557, 3712, 4159, 4249, 4570a	568b, 1825, 2386, 2917a, 3186, 3188, 3549, 3550, 4249	
523.	91-10-1	Phenol, 2,6-dimethoxy- {syringol}	568b, 952, 1063–1066, 1068–1074, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1879, 1884, 2043, 2045, 2327c, 2387, 2543, 2545, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 3266, 3302, 3394, 3410, 3553, 3557, 3712, 3797, 4249, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877a, 2339, 2386, 2917a, 3266, 3430, 4249, 5811b	1360, 1375a, 2387, 3395
524.		Phenol, 2,6-dimethoxy-ethenyl-	3557, 4249		
525.	28343-22-8	Phenol, 2,6-dimethoxy-4-ethenyl-	1364, 1884, 2767, 2769, 3255, 3712, 5811b	2338, 3430, 5811b	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
526.	14059-92-8	Phenol, 2,6-dimethoxy-4-ethyl-	1879, 1884, 2543, 2773, 3712	3430, 5811b	
527.	6638-05-7	Phenol, 2,6-dimethoxy-4-methyl-	1586, 1884, 2543, 2570, 2769, 2767, 2773, 3557, 3712	1877a, 2386, 3430, 4249, 5811b	
528.	20675-95-0	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*E*)-	3712, 3557, 4249	2339,3430	
529.	26624-13-5	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*Z*)-	3712	3430, 5811b	
530.	6627-88-9	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	1586, 1884, 2601a, 2767, 2769, 3557, 3712, 5811b	2338, 2339, 3430, 5811b	
531.	576-26-1	Phenol, 2,6-dimethyl- {2,6-xylenol}	50, 414, 568b, 851, 1099, 1360, 1365, 1371, 1375a, 1378, 1426, 1427, 1586, 1626, 1879, 1882, 1884, 1995, 2005, 2046, 2387, 2447, 2598, 2765–2767, 2773, 2777, 3255, 3302, 3308, 3394, 3410, 3452, 3557, 3712, 3716–3719, 3741, 3746, 3747, 3764, 3767, 3797, 4249, 4319, 4407, 4414, 4796, 5011, 5811b	568b, 962, 1876, 1877a, 2014, 4249, 5811b	50, 1360, 1375a, 1378, 2387, 3395
532.	71526-64-2	Phenol, 2,6-dimethyl-4-ethenyl-	1884, 2769, 3557, 3712, 4249		
533.	10570-69-1	Phenol, 2,6-dimethyl-4-ethyl-	1884, 2767, 2769, 3557, 3712, 4249		
534.		Phenol, 2,6-dimethyl-4-(2-propenyl)-		2338	
535.	2033-89-8	Phenol, 3,4-dimethoxy-	568b, 3952, 4249		
536.	95-65-8	Phenol, 3,4-dimethyl- {3,4-xylenol}	50, 155, 414, 568b, 830a, 1360, 1375a, 1378, 1426, 1427, 1586, 1626, 1789, 1879, 1881, 1883, 1884, 1928, 1995, 2005, 2387, 2447, 2598, 2628, 2761, 2762, 2765–2767, 2876, 3224, 3255, 3266, 3302, 3308, 3452, 3453, 3488, 3557, 3712, 3716–3719, 3746, 3747, 3764, 3797, 4249, 4317, 4319, 4407, 4414, 4796, 5011, 5811b	568b, 952, 1053, 1876, 1877a, 3266, 4249, 5811b	50, 1360, 1375a, 1378, 2387, 3395
537.	500-99-2	Phenol, 3,5-dimethoxy-	568b, 3712, 4249	568b, 1877a, 4249	

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

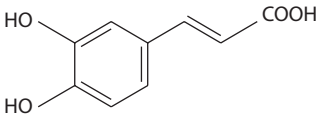
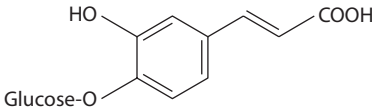
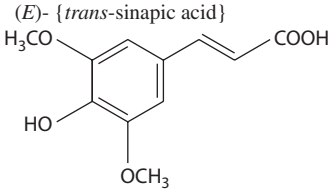
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
538.	108-68-9	Phenol, 3,5-dimethyl- {3,5-xylenol}	50, 155, 414, 568b, 615–617, 722, 723, 851, 1378, 1426, 1427, 1626, 1879, 1884, 1995, 2005, 2387, 2598, 2871, 2876, 2939, 3059, 3302, 3308, 3453, 3464, 3488, 3498, 3712, 3716–3719, 3746, 3747, 3797, 3800, 4249, 4319, 4407, 4414, 4796, 5011, 5811b	568b, 952, 1876, 1877a, 2917a, 4249, 5811b	50, 1378, 2387, 3395
539.	2785-85-5	Phenol, 3,5-dimethyl-2-methoxy-	90a, 1884, 3712, 5811b		
540.	71608-10-1	Phenol, 3,6-dimethyl-2-nitro- {phenol, 2,5-dimethyl-6-nitro-}	2137, 3712, 4249		
541.	72312-07-3	Phenol, 4,5-dimethoxy-2-methyl-		2917a	
542.	7771-25-7	Phenol, 4,5-dimethyl-2-methoxy-	90a, 3712, 5811b		
543.	2219-79-6	Phenol, 4,6-dimethyl-2-ethyl-	4249		
544.	2896-66-4	Phenol, 4,6-dimethyl-2-methoxy-	90a, 3712, 3746, 3747, 4249, 5811b		
545.	123844-48-4	Phenol, 5,6-dimethyl-2-methoxy-	90a		
546.	3238-38-8	Phenol, 2,3,4,6-tetramethyl-	1378, 2447, 3712, 4249, 5811b		1378
547.	527-35-5	Phenol, 2,3,5,6-tetramethyl- {durenol}	1378, 3302, 3557, 3712, 4249	404	1378
548.	526-85-2	Phenol, 2,3,4-trimethyl-	91a, 1378, 1586, 2543, 2767, 2773, 3557, 3712, 4147, 4249, 5811b	1877a, 2014, 4249	1378
549.	697-82-5	Phenol, 2,3,5-trimethyl- {isopseudocumenol}	50, 414, 568b, 851, 1364, 1378, 1427, 1586, 1626, 1789, 1995, 2387, 2543, 2767, 2773, 3302, 3308, 3557, 3712, 3716, 3717, 3746, 3747, 3797, 3903, 4249, 4313, 4317, 4319, 5811b	568b, 1877a, 2014, 4249, 5811b	1378, 2387
550.	2416-94-6	Phenol, 2,3,6-trimethyl-	568b, 1378, 1586, 1884, 2447, 2767, 3557, 3712, 3746, 3747, 4249, 5811b	568b, 1877a, 2014, 4249, 5811b	1378
551.	496-78-6	Phenol, 2,4,5-trimethyl- {pseudocumenol}	851, 1378, 3302, 3712, 3746, 3747, 4249, 5811b	1877a, 4249, 5811b	1378
552.	118-79-6	Phenol, 2,4,6-tribromo-		2650a, 4249	

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

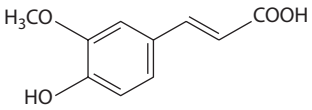
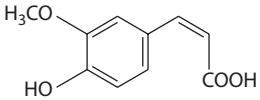
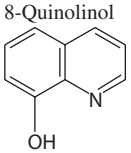
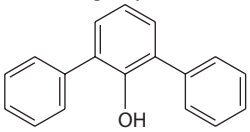
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
553.	527-60-6	Phenol, 2,4,6-trimethyl- {mesitol}	50, 396, 397, 568b, 1378, 1426, 1427, 1586, 1626, 1884, 1995, 2447, 2767, 2939, 3557, 3712, 3746, 3747, 3764, 3797, 4249, 4319, 5811b	568b, 952, 1825, 2389, 2544, 4249, 5811b	1378
554.	527-54-8	Phenol, 3,4,5-trimethyl-	568b, 1884, 2447, 2543, 2773, 3557, 3712, 3746, 3747, 4249, 5811b	568b, 1877a, 4249, 5811b	3395
555.	732-26-3	Phenol, 2,4,6-tris(1,1-dimethylethyl)-	1371	3547, 4249	
556.	51064-37-0	Phenylalanine, ar,ar-dihydroxy-		4249	
557.	24946-64-3	Plastochromenol {solanachromene isomer}		840	
558.	2034-60-8	1,2-Propanedione, 1-(4-hydroxy-3-methoxyphenyl)-	4249	5811b	
559.		Propanoic acid, 3-hydroxyphenyl-	1626, 3797		
560.		1-Propanone, 1-(dimethylhydroxyphenyl)-	3226, 3557, 4249		
561.		1-Propanone, 1-(3,5-dimethyl-4-hydroxyphenyl)-	2767, 4249		
562.	610-99-1	1-Propanone, 1-(2-hydroxyphenyl)-	1375, 1375b, 2767, 2769, 4249		
563.		1-Propanone, 1-(3-hydroxyphenyl)-	1586, 4249		
564.	13100-05-5	2-Propanone, 1-(2-hydroxyphenyl)-	1586, 1884, 2767, 3553, 3712, 3890, 4249		
565.		2-Propanone, 1-(3-hydroxyphenyl)-	1884, 3553, 3712	3186, 3188, 4249	
566.	19037-58-2	2-Propanone, 1-(3,5-dimethoxy-4-hydroxyphenyl)-	3553, 3712	5811b	
567.	2503-46-0 110053-51-5	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	568b, 1364, 1586, 1884, 2570, 2767, 3553, 3557, 3712, 4249, 5811b	568b, 3430, 4249, 5811b	
568.	770-39-8	2-Propanone, 1-(4-hydroxyphenyl)-	568b, 1364, 3553, 4249, 5811b		
569.	79407-66-2	2-Propenal, 3-(2,4-dihydroxyphenyl)-		3748, 3749, 3751, 4249	
570.	1202-41-1	2-Propenamide, 3-(3,4-dihydroxyphenyl)-		4249	
571.	59001-33-1	2-Propenamide, 3-(3,4-dihydroxyphenyl)-*N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]- {dicaffeoylspermidine}		4249, 4567	
572.	59576-98-6	2-Propenamide, 3-(4-hydroxyphenyl)-		3973, 5811b	
573.	29554-26-5	2-Propenamide, *N*-(4-aminobutyl)-3-(3,4-dihydroxyphenyl)-		4249, 4567, 5811b	
574.	501-13-3	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxy-3-methoxyphenyl)-		4249, 5811b	
575.	34136-53-3	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxyphenyl)-		4249	
576.	42369-86-8	2-Propenamide, *N,N′*-1,4-butanediylbis[3-(4-hydroxy-3-methoxyphenyl)-		4249, 5811b	
577.	31082-90-3	2-Propenoic acid, 3-(2,3-dihydroxyphenyl)-	3712, 3741, 3743, 4249, 4897, 5811b		

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
578.	331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid} 	1626, 1743, 1744, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3300, 3308, 3712, 3714, 3797, 4036, 4113, 4163, 4249, 4376, 5079, 5389, 5512, 5811b, 4A01	72, 120, 722, 835, 890, 1102, 1626, 1981, 2154, 2216, 2270, 2514, 2939, 2954, 3029, 3103, 3161, 3462, 3476, 3655b, 3660, 3700, 3748, 3749, 3751, 3973, 3974a, 4249, 4999, 5079, 5126, 5385, 5389, 5591, 5652, 5672. 5673, 5705, 5713, 5722, 5809, 5810, 5811b, 5830, 5831, 5900, 5908, 4A01	
579.	501-16-6	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*E*)- {*trans*-caffeic acid}	1626, 3302, 3308, 3712, 3741, 3743, 4163, 4376, 4377, 5811b	1626, 3748, 3749, 3751, 3797	
580.	4361-87-9	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*Z*)- {*cis*-caffeic acid}	1626, 2939, 3302, 3308, 3712, 3741, 3743, 4163, 4376, 4377, 5811b	1309, 1626, 2939, 3748, 3749, 3751, 3797	
581.	58994-15-3	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, monoamide with *N*-(3-aminopropyl)-1,4-butanediamine		4249, 4567	
582.	17093-82-2	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]- {1-*O*-caffeoylglucose} 		3797, 3974a, 4402	
583.	7362-37-0	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*E*)- {*trans*-sinapic acid} 	1626	1102, 3748, 3749, 3751	
584.	7361-90-2	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*Z*)- {*cis*-sinapic acid}	1626, 1884, 3302, 3712, 3797, 4377	1102, 3748, 3749, 3751	
585.	537-73-5	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-	3712, 4113, 4249		
586.	25522-33-2	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-, (*E*)-	3712, 5811b		
587.	1782-55-4	2-Propenoic acid, 3-(4,5-dihydroxy-3-methoxyphenyl)- {5-hydroxyferulic acid}		1102	
588.	1135-24-6	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)- {cinnamic acid, 3-hydroxy-4-methoxy-; ferulic acid}	3712, 5811b	5811b	
589.	530-59-6	2-Propenoic acid, 3-(4-hydroxy-3,5-dimethoxyphenyl)-	5811, 5811b		

(*continued*)

TABLE 9.22 (continued)
Phenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
590.	537-98-4	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid} 	1626, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3555, 3749, 3797, 4249, 4377, 5811b	404, 1102, 1626, 1884, 2216, 2389, 2544, 2939, 2954, 3103, 3161, 3555, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 4377	
591.	1014-83-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid} 	1626, 1842, 2216, 2939, 3255, 3257, 3302, 3712, 3741, 3743, 3749, 4249, 4377	1102, 1626, 2216, 2389, 2544, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3797, 3973, 3974a	
592.	2309-07-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester {ferulic acid, methyl ester}	3712, 4249, 4553a	5811b	
593.	25429-38-3	2-Propenoic acid, 3-(hydroxyphenyl)-	3712, 4249, 4553a		
594.	583-17-5 614-60-8	2-Propenoic acid, 3-(2-hydroxyphenyl)- {*o*-coumaric acid}	3265, 3741, 3743, 4113, 4249, 5811b	3109, 4249, 5811b	
595.	588-30-7	2-Propenoic acid, 3-(3-hydroxyphenyl)-		3748, 3749, 3751	
596.	14755-02-3	2-Propenoic acid, 3-(3-hydroxyphenyl)-, (*E*)-		3748, 3749, 3751, 4249	
597.	7400-08-0	2-Propenoic acid, 3-(4-hydroxyphenyl)- {coumaric acid}	101, 1626, 1842, 2543, 2939, 3302, 3308, 3712, 4113, 4163, 4377, 5811b	120, 908, 1102, 1626, 2386, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3973, 3974a, 4163, 4249, 4377, 4677	
598.	501-98-4	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*E*)- {*trans*-coumaric acid}	1626, 1842, 2775, 3302, 3741, 3743, 3939, 4163, 4377, 5811b	1626, 2270, 3748, 3749, 3751, 4163, 4377	
599.	4501-31-9	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*Z*)- {*cis*-coumaric acid}	1626, 1842, 2775, 3302, 3410, 3712, 3741, 3743, 4163, 4377, 5811b	1626, 3748, 3749, 3751, 4163, 4377	
600.	2983-65-5	2-Propen-1-one, 1-(4-hydroxy-3-methoxyphenyl)-	4249	5811b	
601.		Pyrenol	5486		4249, 4823
602.	3778-29-8	2-Quinolinecarboxylic acid, 4,6-dihydroxy- {6-hydroxykynurenic acid}		3491, 4249	
603.	492-27-3	2-Quinolinecarboxylic acid, 4-hydroxy-	5811, 5811a, 5811b		
604.	148-24-3	8-Quinolinol 	568b, 3280, 3286, 3302, 3491, 4160, 5811b	444, 568b, 1877a, 4249, 5811b, 5892	
605.	13207-66-4	8-Quinolinol, 5-amino-		2917a	
606.	5541-68-4	8-Quinolinol, 7-methyl-	1360, 1375a, 2761, 2762, 2765, 2766, 4249		1360, 1375a
607.	2432-11-3	1,1′,3′-Terphenyl-2′-ol 	2601a		

9.2 QUINONES

Even in the mid-1950s when knowledge of the composition of tobacco smoke was extremely limited and only a few phenols were known to be present in tobacco smoke, it was suggested that several of the phenols might be converted to the corresponding quinone during the smoking process.

This suggestion, coupled with the mouse-skin-painting bioassay results reported by Takizawa (3865a) that several simple quinones such as 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone), 1,2-naphthalenedione (1,2-naphthoquinone), and 1,4-naphthalenedione (1,4-naphthoquinone) were tumorigenic to mouse skin, raised serious questions about the desirability of adding phenols to the tobacco blend to enhance the odor and flavor of its smoke. Despite the many studies in which benzene was used as the solvent for testing of the tumorigenicity of PAHs, benzene seldom induced tumors in the skin-painted solvent-control group of laboratory animals [Hartwell (1543, 1544), Shubik and Hartwell (3664, 3665), Thompson et al. (3908)]. Similarly, naphthalene was found to be nontumorigenic in skin-painting studies.

The mouse-skin-painting bioassay results with 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) were subsequently confirmed by Tiedemann (3916a). Neither of the higher molecular weight tricyclic quinones 9,10-anthracenedione (9,10-anthraquinone) (3865a) nor 9,10-phenanthrenedione (9,10-phenanthrenequinone) (3865a) was reported to be tumorigenic to mouse skin.

In the early days of the studies on the specific tumorigenicity of various classes of compounds to mouse skin, investigators were intrigued by the activities exhibited by aromatic hydrocarbons, their dihydric phenols, and the quinones corresponding to the dihydric phenols. The results of mouse-skin-painting bioassays with various aromatic hydrocarbons ranging in complexity from monocyclic to hexacyclic, their dihydric phenols, and the corresponding quinones are summarized in Table 9.23.

From the studies on the chemical relationship between aromatic hydrocarbons and their quinones, the theory of the oxidation–reduction potential of quinones was proposed. A prime proponent of this theory was Fieser (1180b) who reported the reduction potentials of the following quinones:

- Several anthracenediones other than 9,10-anthracenedione [Conant and Fieser (790b); Fieser (1180a-1)]
- 9,10-Phenanthrenedione (9,10-phenanthraquinone) [Fieser (1180a-2)]
- 2,5-Cyclohexadiene-1,4-dione (*p*-benzoquinone) [Fieser (1180a-3)]
- Several naphthalenediones other than the 1,2- and 1,4-naphthalenediones[Fieser (1180a-4)]
- 7,12-Benz[*a*]anthracenedione (7,12-benz[*a*]anthraquinone), 7,14-dibenz[*a,h*]anthracenedione (7,14-benz[*a,h*]anthraquinone), 5,6-chrysenedione (5,6-chrysenequinone), 6,12-chrysenedione (6,12-chrysenequinone) [Fieser and Dietz (1180a-5)]
- 3,5-Cyclohexadiene-1,2-dione (*o*-benzoquinone) and 1,2-naphthalenedione (1,2-naphthoquinone [Fieser and Peters (1180a-6)]
- 9,10-Anthracenedione (9,10-anthraquinone) [Fieser and Peters (1180a-7)]
- 1,4-Naphthalenedione (1,4-naphthoquinone) [Fieser and Fieser (1180a-8)]

After the first demonstrations by Kennaway and Hieger (2078) of the tumorigenicity to mouse skin of DB[*a,h*]A, a PAH synthesized by Fieser and Dietz (1184), and of B[*a*]P by Barry et al. (194), the coal tar component isolated from coal tar and subsequently synthesized by Cook et al. (796a, 797), the tumorigenicity of a great number of PAHs and their derivatives was studied.

TABLE 9.23
Comparison of the Tumorigenicities of Aromatic Hydrocarbons, Their Diols (Phenols), and Their Diones (Quinones)

Hydrocarbon		Diol		Dione	
Benzene	–	1,4-Benzenediol (hydroquinone)	–	2,5-Cyclohexadiene-1,4-dione (*p*-benzoquinone)	+
		1,2-Benzenediol (catechol)	–	3,5-Cyclohexadiene-1,2-dione (*o*-benzoquinone)	?
Naphthalene	–	1,2-Naphthalenediol	–	1,2-Naphthalenedione (1,2-naphthoquinone)	+
		1,4-Naphthalenediol	–	1,4-Naphthalenedione (1,4-naphthoquinone)	+
Anthracene	–	9,10-Anthracenediol	–	9,10-Anthracenedione (9,10-anthraquinone)	–
Phenanthrene	–	9,10-Phenanthrenediol	–	9,10-Phenanthrenedione (9,10-phenanthraquinone)	–
Chrysene	±	5,6-Chrysenediol	–	5,6-Chrysenedione (5,6-chrysenequinone)	–
		6,12-Chrysenediol	–	6,12-Chrysenedione (6,12-chrysenequinone)	–
Benz[*a*]anthracene	±	7,12-Benz[*a*]anthracenediol	–	7,12-Benz[*a*]anthracenedione (7,12-benz[*a*]anthraquinone)	–
Dibenz[*a,h*]anthracene	+	7,14-Dibenz[*a,h*]anthracenediol	–	7,14-Dibenz[*a,h*]anthracenedione (7,14-Dibenz[*a,h*]anthraquinone)	–
Benzo[*a*]pyrene	+			Benzo[*a*]pyroquinone	–
Dibenzo[*b,def*]chrysene	+			7,14-Dibenzo[*b,def*]chrysenedione	–

–, negative response in mouse-skin-painting bioassay; +, positive response in mouse-skin-painting bioassay; ±, equivocal response in mouse-skin-painting bioassay.

Soon observed was the pronounced contrast between the gradation in specific tumorigenicities in the mouse-skin-painting bioassay from the nontumorigenicity of the mono- and bicyclic aromatic hydrocarbons benzene and naphthalene, respectively, to the potent tumorigenicities of the pentacyclic aromatic hydrocarbons DB[*a,h*]A and B[*a*]P *vs.* the tumorigenicities of the quinones 2,5-cyclohexadien-1,4-dione (*p*-benzoquinone), 1,2-naphthalenedione (1,2-naphthoquinone), and 1,4-naphthalenedione (1,4-naphthoquinone) and the nontumorigenicities of dibenzanthraquinone and benzopyroquinone. Neither the tricyclic aromatic hydrocarbons anthracene and phenanthrene nor their corresponding quinones have elicited tumors in the mouse-skin-painting bioassay. The tumorigenicities of the tetracyclic hydrocarbons benz[*a*]anthracene and chrysene have been classified as extremely weak or equivocal. None of their quinones has shown tumorigenicity in the mouse-skin-painting bioassay (see Table 9.23). Initially, it was found that the higher the tumorigenic potency of the quinones, particularly the benzoquinones and the naphthoquinones, the higher was the reduction potential of the quinone. In essence, the oxidation–reduction potential theory was eventually used in an attempt to relate the oxidation–reduction potential of the hydrocarbon–quinone system to the specific tumorigenicity observed in the mouse-skin-painting bioassays for PAHs and their quinones.

Although none of the diols (phenols) listed in Table 9.23 was found to be tumorigenic, in subsequent research dealing with the metabolism of tumorigenic PAHs, it was found that some of the dihydrodiols and dihydrodiol epoxides were tumorigenic to mouse skin [see review by Dipple et al. (983)]. However, it is obvious from examination of the structures of the dihydrodiols and dihydrodiol epoxides that none of these metabolites is a phenol.

As the laboratory data and understanding of chemical carcinogenesis increased dramatically pre- and post-World War II, exceptions to the theory of oxidation–reduction potential resulted in its being supplanted by other more meaningful theories, e.g., the relationship between electronic configuration, the activity of the so-called K region, and the inactivity of the so-called L region in aromatic compounds, particularly PAHs, and their tumorigenicity [see reviews by Coulson (829), Pullman and Pullman (3003)]. The interest in the theory of the electronic configuration–tumorigenesis relationship of PAHs was such that the 1953 review by Coulson was selected as the introductory chapter in Volume 1 of the newly instituted publication *Advances in Cancer Research.*

It is interesting to note that even in the early 1950s, the idea of the involvement of a hydroxylated PAH metabolite in tumorigenesis was already being discussed. For example, Pullman and Pullman (3003) wrote:

> It is nevertheless generally admitted that [dihydro]diols are probably intermediates in the metabolism of aromatic hydrocarbons.

Although their speculation as to the precise nature of its involvement was somewhat in error, the Pullmans (3003) did propose that a dihydroepoxide might also be involved in the metabolism of PAHs, the metabolite–cellular component interaction, and the tumorigenicity attributed to some of the PAHs.

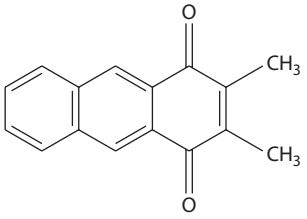
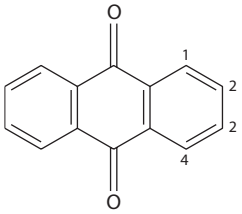
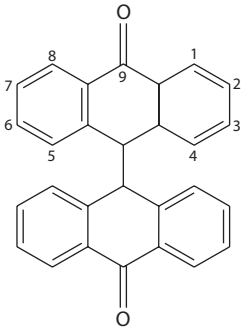
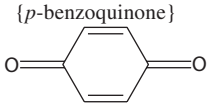
The oxidation–reduction potential of the aromatic hydrocarbon–quinone system was revisited some years later and its possible involvement in cigarette smoke. Schmeltz et al. (3510) reported that cigarette smoke condensate (CSC) possessed reducing properties sufficient to reduce 2,5-cyclohexadiene-1,4-dione (1,4-benzoquinone; *p*-benzoquinone) to 1,4-benzenediol (hydroquinone). This CSC-induced reduction apparently did not occur with 9,10-anthracenedione (9,10-anthraquinone).

Compared to the number of polycyclic aromatic hydrocarbons (PAHs) and phenols identified in tobacco smoke, the number of identified quinones is low despite the fact that many of the phenols after their pyrogenesis during the smoking process could realistically yield quinones. Table 9.24 lists the 49 quinones identified to date in tobacco and tobacco smoke. Of the 50 listed, 38 were identified in tobacco smoke, 19 in tobacco, and 7 in both. In his 1954 review of tobacco smoke components identified to that date, Kosak (2170) listed no quinone.

In view of tobacco smoke composition findings after the mid-1950s, the suggestion in the late 1950s by Rodgman that phenols were inappropriate additives for cigarette smoke flavor enhancement might have been an example of excessive caution. His suggestion was based on two factors: The promoting effect of phenols reported in 1955, 1956, and 1959 by Boutwell and his colleagues (414) plus the possible conversion during the smoking process of substituted phenols to corresponding quinones, several of which had been reported to be tumorigenic by Takizawa (3865a) and Tiedemann (3916a). Obviously, the latter situation occurred infrequently. The great discrepancy between the great number of phenols *vs.* the small number of quinones identified in tobacco smoke suggests that the phenol–quinone conversion does not occur in many instances or, if it does occur, the conversion results in the generation of extremely low levels of the quinone. As noted elsewhere, it has been estimated from examination of the many peaks and shoulders in the detailed glass capillary gas chromatograms from tobacco smoke and/or its fractions that the number of tobacco smoke components exceeds the number of identified tobacco smoke components by factors ranging from 10 to 25 [e.g., see Wakeham (4103)]. It is possible that quinones contribute to some of the extremely minor chromatographic peaks representing components as yet unidentified.

Table 9.25 lists the chronology of some of the major events pertinent to the identification of quinones in tobacco smoke. It is obvious that the number of significant events for these quinones is substantially less than those cataloged for the PAHs, the aza-arenes, the phenols, and the *N*-nitrosamines. More than likely, the difference is a direct reflection of the concern expressed relative to the tumorigenicity in laboratory animals of the various classes of compounds.

TABLE 9.24
Quinones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.		1,4-Anthracenedione, 2,3-dimethyl- 		3973, 3974a	
2.	84-65-1	9,10-Anthracenedione {9,10-anthraquinone} 	790b, 1211, 1884, 2191, 2195, 2196, 2200, 2203, 2210, 2860, 3308, 3510, 3557, 3797, 4249, 5811b	2939, 3560, 3561, 3633, 3797, 3973, 3974a, 4249, 5811b	2210, 3402
3.	20724-30-5	9,10-Anthracenedione, 1,2-diethyl-	246, 247, 278		
4.	117-12-4	9,10-Anthracenedione, 1,5-dihydroxy-	5480		
5.	71265-31-1	9,10-Anthracenedione, dimethyl-	246, 247, 1884, 3510		
6.	6531-35-7	9,10-Anthracenedione, 2,3-dimethyl-	278, 5811b		
7.	27936-34-1	9,10-Anthracenedione, methyl-	246, 247		
8.	84-54-8	9,10-Anthracenedione, 2-methyl-	1884, 3510, 5811b	3973, 3974a	
9.		9,10-Anthracenedione, trimethyl-	246, 247		
10.	434-85-5	[9,9′-Bianthracene]-10,10′(9*H*,9′ *H*)-dione {bianthrone; dianthraquinone} 	278, 4249		
11.	78919-13-8	Cyclohexadienedione {quinone}	652		
12.	106-51-4	2,5-Cyclohexadiene-1,4-dione {*p*-benzoquinone} 	74, 190, 282, 329, 392, 396, 790b, 876, 877, 1063–1066, 1068–1074, 1238, 1427, 1751, 1884, 2210, 2710, 2939, 3300, 3302, 3510, 4249, 4995, 4996, 5811b, 5869a		2210
13.	106-34-3	2,5-Cyclohexadiene-1,4-dione, compound with 1,4-benzenediol (1:1)	1378, 2379, 2767, 4249		1378
14.		2,5-Cyclohexadiene-1,4-dione, 2,3-dihydro-	1884, 3553		3401
15.		2,5-Cyclohexadiene-1,4-dione, 2,3-dihydro-2,2,6-trimethyl-	1884, 2769, 3476	2339a, 3550	

(*continued*)

TABLE 9.24 (continued)
Quinones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

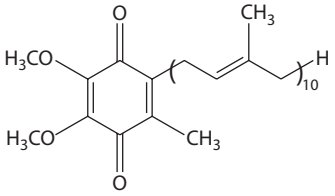
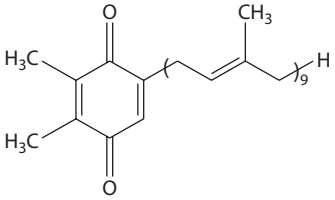
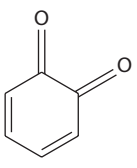
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
16.	303-98-0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-(3,7,11,15,19,23,27,31,35,39-decamethyl-2,6,10,14,18,22, 26,30,34,38-tetracontadecenyl)-6-methyl- {ubiquinone-10} 		1209, 1858	
17.	526-86-3	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethyl-	5811, 5811a		
18.	137-18-8	2,5-Cyclohexadiene-1,4-dione, 2,5-dimethyl-	1884, 2767, 2769		
19.		2,5-Cyclohexadiene-1,4-dione, 2,6-bis (1,1-dimethylethyl)-		2339a	
20.	527-61-7	2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl-	1360, 1370, 1375a, 2777, 4249		1360, 1375a
21.	4299-57-4	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethyl-5-(3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22, 26,30,34-hexatriacontanonaenyl)-, (all-*E*)- {plastoquinone-9} 		666, 840, 3875, 3916, 3971, 4249, 5811b	
22.	606-06-4	2,5-Cyclohexadiene-1,4-dione, 2-(3,7-dimethyl-2,6-octadienyl)-5,6-dimethoxy-3-methyl-, (*E*)-		1858, 4249	
23.	2474-72-8	2,5-Cyclohexadiene-1,4-dione, 2-hydroxy-	1586, 2767, 4249		
24.	3361-10-2	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15 15-tetramethylhexadecyl)-6-methyl-		1394, 4249, 4462	
25.	7559-04-8	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15 15-tetramethylhexadecyl)-3,5,6-trimethyl- [3R-(3R*,7R*,11R*)]-		4249, 4462	
26.		2,5-Cyclohexadiene-1,4-dione, 2-methoxy-	1586		
27.	553-97-9	2,5-Cyclohexadiene-1,4-dione, 2-methyl-	1884, 2194, 2195, 2767, 3302, 3308, 3510, 4249, 5811b		
28.	527-17-3	2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl-	568b, 1063–1066, 1068–1074,1360, 1375a, 1884, 2543, 2545, 2761, 2762, 2765–2767, 2769, 2773, 2777, 3557, 4249, 5811b		1360, 1375a
29.	935-92-2	2,5-Cyclohexadiene-1,4-dione, 2,3,5-trimethyl-	1063–1066, 1068–1074,1364, 1371, 1884, 2543, 2773, 2775, 3410, 3510, 4249		
30.	583-63-1	3,5-Cyclohexadiene-1,2-dione {*o*-benzoquinone} 	74, 3302, 4249	73b, 4156, 4249	

TABLE 9.24 (continued)
Quinones Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

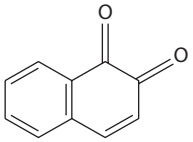
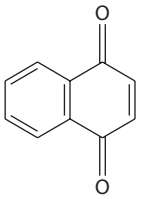
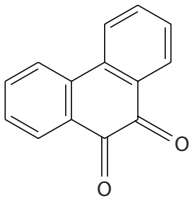
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	524-42-5	1,2-Naphthalenedione (1,2-naphthoquinone) 	278, 790b, 3300		
32.	130-15-4	1,4-Naphthalenedione (1,4-naphthoquinone) 	666, 790b, 1884, 2710, 3300–3302, 3510, 3744		
33.	117-80-6	1,4-Naphthalenedione, 2,3-dichloro-	3797	2095, 4249, 4666a	
34.	73850-17-6	1,4-Naphthalenedione, dimethyl-	662, 1884, 3744, 3746, 3747, 5811b		
35.	2197-57-1	1,4-Naphthalenedione, 2,3-dimethyl-	101, 662 1884, 3510, 3744, 3746, 3747, 5811b		
36.	482-70-2	1,4-Naphthalenedione, 2,7-dimethyl-	3744, 3746, 3747		
37.	68860-42-4	1,4-Naphthalenedione, 2,3-dimethyl-6-(4,8,12-trimethyltridecyl)-, (R*,R*)-	1178, 1884, 4249	1178, 4249	
38.	481-39-0	1,4-Naphthalenedione, 5-hydroxy- {juglone}		3973	
39.		1,4-Naphthalenedione, methyl-	662		
40.	58-27-5	1,4-Naphthalenedione, 2-methyl-	1884, 3510, 3744, 3746, 3747, 5811b		
41.	84-80-0	1,4-Naphthalenedione, 2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [R-[R*,R*-(*E*)]]- {Vitamin K1}		3348, 3349, 3797, 3974a	
42.	73850-15-4	1,4-Naphthalenedione, tetramethyl-	1884, 3557, 3744, 3746, 3747, 5811b		
43.	73850-16-5	1,4-Naphthalenedione, trimethyl-	662, 1884, 3604, 3744, 3746, 3747, 5811b		
44.	20490-42-0	1,4-Naphthalenedione, 2,3,6-trimethyl-	101, 666, 1360, 1371, 1375a, 1884, 2761, 2762, 2765–2767, 2777, 3410, 3510, 3557, 3744, 3746, 3747, 3797, 5811b	404, 2095, 3547, 5811b	1360, 1375a, 3404
45.	59832-90-5	1,4-Naphthalenedione, 2,6,7-trimethyl-	1884, 3744, 3746, 3747		
46.	84-11-7	9,10-Phenanthrenedione {phenanthrenequinone; phenanthraquinone} 	2191, 2200, 2210, 3302, 3308		2210
47.	3819-09-8	Plastoquinol		840	
48.	11005-16-6	Plastoquinone C		840, 1394, 3916	
49.	12778-15-3	Plastoquinone D		1394, 3882, 3916	
50.		Quinones	1744, 2195, 5512		

TABLE 9.25
Chronology of Identification of Quinones in Tobacco and/or Smoke

Year	Event
1924–1934	Fieser and his colleagues investigated the reduction of quinones and generated the theory of the oxidation–reduction potential of quinones. The reduction of the following quinones was studied: several anthracenediones other than 9,10-anthracenedione [Conant and Fieser (790b), Fieser (1180a)]; 9,10-phenanthrenedione (9,10-phenanthraquinone) (1180a); 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) [Fieser (1180a)]; several naphthalenediones other than the 1,2- and 1,4-naphthalenediones [Fieser (1180a)]; 3,5-cyclohexadiene-1,2-dione (*o*-benzoquinone) and 1,2-naphthalenedione (1,2-naphthoquinone) [Fieser and Peters (1180a)]; 9,10-anthracenedione (9,10-anthraquinone) [Fieser and Peters (1180a)]; 1,4-naphthalenedione (1,4-naphthoquinone) [Fieser and Fieser (1180a)]; 7,12-benz[*a*]anthracenedione (7,12-benz[*a*]anthraquinone), 7,14-dibenz[*a,h*]anthracenedione (7,14-benz[*a,h*] anthraquinone), 5,6-chrysenedione (5,6-chrysenequinone), 6,12-chrysenedione (6,12-chrysenequinone) [Fieser and Dietz (1180a)]. Later, the theory of the oxidation–reduction potential of quinones was advanced to explain the differences in tumorigenicity of the various quinones and their aromatic hydrocarbons sources
1940–1941	Takizawa (3865a) reported that several simple quinones [2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone), 1,2-naphthalenedione (1,2-naphthoquinone), 1,4-naphthalenedione (1,4-naphthoquinone)] were tumorigenic in mouse-skin-painting experiments
1942	Fieser (1180b) reviewed the theory of the oxidation–reduction potential of quinones. Because some nontumorigenic aromatic hydrocarbons (benzene, naphthalene) yielded tumorigenic quinones, some nontumorigenic aromatic hydrocarbons yielded nontumorigenic quinones, and some tumorigenic aromatic hydrocarbons (dibenz[*a,h*]anthracene) yielded nontumorigenic quinones, attempts were made to correlate the relationship between aromatic hydrocarbons, their quinones, the reduction potential of quinones, and the tumorigenicities (mouse skin) of the aromatic hydrocarbons *vs*. the tumorigenicities of their quinones
1953	Tiedemann (3916a) confirmed the finding of Takizawa on the tumorigenicity of 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) to mouse skin
1953–1955	The theory of oxidation–reduction potential of quinones was supplanted by other more meaningful theories, e.g., the relationship between electronic configuration, the activity of the so-called K region, and the inactivity of the so-called L region in aromatic compounds, particularly PAHs, and their tumorigenicity [see reviews by Coulson (829) and Pullman and Pullman (3003)]
1954	Kosak (2170) in his compilation of tobacco smoke components reported in the literature did not list a quinone
1957	Bonnet and Neukomm (396) suspected the presence of 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) in cigarette mainstream smoke because of the identification of 1,4-benzenediol (hydroquinone) when the smoke was collected under reducing conditions. Under similar reducing conditions, they were unable to identify 1,4-napthalenediol, concluding that 1,4-napthalenedione (1,4-naphthoquinone) was not present in the smoke
1959	Bentley and Berry (282) in their compilation of identified tobacco smoke components listed the report of 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) by Bonnet and Neukomm (396)
1959	In their review of tobacco and tobacco smoke composition, Johnstone and Plimmer (1971) listed no quinone in tobacco or tobacco smoke
1961	Onishi et al. (2860) reported the presence of 9,10-anthracenedione (9,10-anthraquinone) in tobacco smoke
1965	Kröller (2195) reported the presence of 9,10-anthracenedione (9,10-anthraquinone) and 9,10-phenanthrenedione (9,10-phenanthraquinone) in tobacco smoke
1965	To estimate the 1,4-benzenediol (hydroquinone) in tobacco smoke, Testa et al. (3891) used air oxidation to convert the 1,4-benzenediol (hydroquinone) to 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) which was subsequently derivatized and estimated. No effort was made to determine whether any 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) was already present in the smoke prior to the air oxidation
1968	In his review of tobacco and tobacco smoke composition, Stedman (3797) listed only two quinones, 9,10-anthracenedione (9,10-anthraquinone) in tobacco and 2,3,6-trimethyl-1,3-naphthalenedione (2,3,6-trimethyl-1,4-naphthoquinone) in tobacco smoke. He discussed the Bonnet and Neukomm (396) report. Because of the uncertainty of the Bonnet and Neukomm data and additional data from Testa et al. (3891), Stedman did not include 2,5-cyclohexadiene-1,4-dione (*p*-benzoquinone) as a tobacco smoke component. He also did not include the reports of the presence of 9,10-anthracenedione (9,10-anthraquinone) [Onishi et al. (2960), Kröller (2195)] or 9,10-phenanthrenedione (9,10-phenanthraquinone) (2195) in tobacco smoke
1968–1969	Bell et al. (246, 247) reported the presence of several alkylated 9,10-anthracenediones in tobacco smoke
1969–1978	RJRT R&D personnel identified numerous previously unidentified alkylated 2,5-cyclohexadiene-1,4-diones and 9,10-anthracenediones in tobacco smoke [Green et al. (1360, 1378), Schumacher et al. (3553), Heckman (1586), Newell et al. (2769)]
1976–1977	Schmeltz et al. (3510) identified several previously unidentified alkylated 2,5-cyclohexadiene-1,4-diones and 9,10-anthracenediones in tobacco smoke
1978–1980	Snook et al. (3747, 3748) identified a series of alkyl-, dialkyl-, trialkyl-, and tetraalkyl-1,4-naphthalenediones in tobacco smoke

10 Ethers

Assessment of the chronology of the number of ethers identified in tobacco and tobacco smoke provides another excellent example of the effect of the advancements in analytical technology on our ability to identify components in a complex mixture. In his 1954 review of the components identified to that date in tobacco smoke, Kosak (2170) lists only two ethers, 2-furancarboxaldehyde (furfural) and 1,6-anhydro-β-*D*-glucopyranose (levoglucosan). Johnstone and Plimmer (1971) did not list ethers as a specific class of components in tobacco and/or tobacco smoke but did mention the identification of several under different headings in their 1959 review, e.g., furan, 2-methylfuran, 2-furancarboxaldehyde (furfural) and two of its derivatives (3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol (α-tocopherol) and 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12,16,20,24,28,32-octamethyl-3,7,11,15,19,23,27,31-tritriacontaoctaenyl)-2*H*-1-benzopyran-6-ol (solanachromene)), the monosaccharides (glucose and fructose), the disaccharide (sucrose), the trisaccharides (raffinose and planteose), and the tetrasaccharide (stachyose). Overall, fewer than 30 ethers are listed by Johnstone and Plimmer (1971).

From 1959 to date, the number of ethers identified in tobacco and/or tobacco smoke has increased over 40-fold to 1243, 654 of which have been identified in tobacco smoke, 847 identified in tobacco, and 258 identified in both tobacco and tobacco smoke. In his 1968 review, Stedman (3797) tabulated the presence of five cyclic ethers in tobacco smoke, i.e., furan, methylfuran, 2,5-dimethylfuran, tetrahydrofuran, and tetrahydropyran. Currently, the number of identified ethers with a furan nucleus is almost 400, and the number with a pyran nucleus exceeds 275. The methoxy and ethoxy ethers number almost 300, phenoxy ethers number 22.

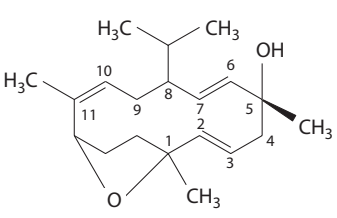
One type of ether that received considerable attention included the ethers derived from the cyclotetradecanols (see Figure 10.1). Because of their unusual structure, none of them were counted in the furan or pyran nucleus group. Over 25 of these ethers have been identified in tobacco and/or tobacco smoke (9, 12, 3351, 3352, 3360, 3361, 4089–4091).

As noted by Rodgman (3266), many components, including a number of ethers, used by the tobacco industry in its flavor formulations [see listing by Doull et al. (1053)] are known components of additive-free tobacco and/or its smoke. Thus, such additives are not strangers to tobacco and/or its smoke, but their addition increases the consumer acceptable flavor. Table 10.1 lists some of the tobacco and/or tobacco smoke ether components that have been or are used in flavor formulations.

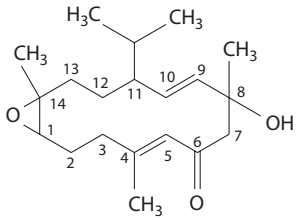
In Table 10.2 are listed the various ethers identified to date in tobacco, tobacco smoke, and tobacco substitute smoke. Of the 1243 ethers identified to date, 654 have been reported in tobacco smoke, 847 in tobacco, and 258 in both tobacco and tobacco smoke.

OVERALL SUMMARY OF OXYGEN-CONTAINING COMPONENTS OF TOBACCO AND/OR TOBACCO SMOKE: CHAPTERS 2 THROUGH 10

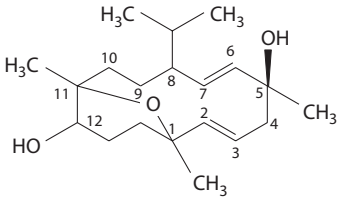
Table 10.3 summarizes the distribution in our catalogs in Chapters 2 through 10 of the *O*-containing components identified in tobacco and/or tobacco smoke. As we have noted in the introductions to each of the nine chapters, the numbers for the various classes of *O*-containing components have escalated tremendously since the last published review by Stedman (3797) in 1968 on tobacco and tobacco smoke components identified to that date.



1,5,11-Trimethyl-8-(1-methylethyl)-15-oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol,



8-Hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-15-oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one



1,5,11-Trimethyl-8-(1-methylethyl)-15-oxabicyclo[9.3.1]pentadeca-2,6-diene-5,12-diol,

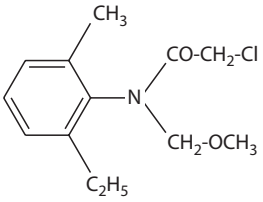
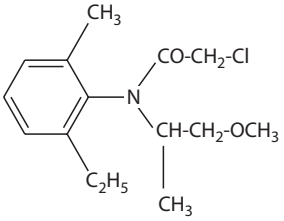
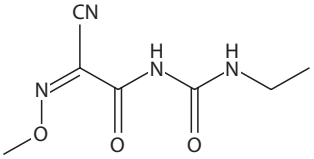
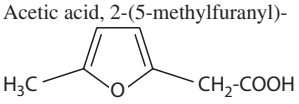
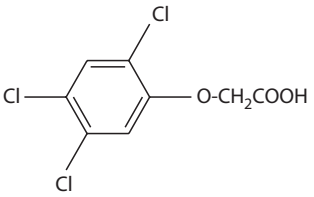
FIGURE 10.1 Cembranoid ethers identified in tobacco and/or tobacco smoke.

TABLE 10.1
Tobacco and/or Smoke Ethers Used in Flavor Formulations

			Identified in	
CAS No.	**Chemical Abstracts Nomenclature**	**As Listed by Doull et al. (1053)**	**Smoke**	**Tobacco**
120-14-9	Benzaldehyde, 3,4-dimethoxy-	Veratraldehyde	I	I
121-32-4	Benzaldehyde, 3-ethoxy-4-hydroxy-	Ethylvanillin	+	+
10031-82-0	Benzaldehyde, 4-ethoxy-	*p*-Ethoxybenzaldehyde	H	H
121-33-5	Benzaldehyde, 4-hydroxy-3-methoxy-	Vanillin	+	+
123-11-5	Benzaldehyde, 4-methoxy-	*p*-Methoxybenzaldehyde	+	+
151-10-0	Benzene, 1,3-dimethoxy-	*m*-Dimethoxybenzene	I	I
150-78-7	Benzene, 1,4-dimethoxy-	*p*-Dimethoxybenzene		
104-46-1	Benzene, 1-methoxy-4-(1-propenyl)-	Anethole	+	+
1076-56-8	Benzene, 3-methoxy-1-methyl-4-(1-methylethyl)-	4-Isopropyl-3-methoxy-1-methylbenzene	–	+
105-13-5	Benzenemethanol, 4-methoxy-	Anisyl alcohol	–	+
104-21-2	Benzenemethanol, 4-methoxy-, acetate	Anisyl acetate	+	+
104-93-8	Benzene, 1-methoxy-4-methyl-	*p*-Methylanisole	+	–
104-45-0	Benzene, 1-methoxy-4-propyl-	Dihydroanethole	H	–
623-15-4	3-Buten-2-one, 4-(2-furanyl)-	4-(2-Furyl)-3-buten-2-one	+	+
100-06-1	Ethanone, 1-(4-methoxyphenyl)-	Acetanisole	+	+
1193-79-9	Ethanone, 1-(2-furanyl 5-methyl)-	2-Acetyl-5-methylfuran	+	+
611-13-2	2-Furancarboxylic acid, methyl ester	Methyl 2-furoate	+	+
93-18-5	Naphthalene, 2-ethoxy-	β-Naphthyl ethyl ether	–	+
470-82-6	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl-	Eucalyptol	+	+
91-10-1	Phenol, 2,6-dimethoxy-	2,6-Dimethoxyphenol	+	+
7786-61-0	Phenol, 4-ethenyl-2-methoxy-	2-Methoxy-4-vinylphenol	+	+
123-07-9	Phenol, 4-ethyl-	*p*-Ethylphenol	+	+
90-05-1	Phenol, 2-methoxy-	Guaiacol	+	+
93-51-6	Phenol, 2-methoxy-4-methyl-	2-Methoxy-4-methylphenol	+	+
122-84-9	2-Propanone, 1-(4-methoxyphenyl)-	1-(*p*-Methoxyphenyl)-2-propanone	I	–

I, compound is an isomer of an identified component; H, compound is a homolog of an identified component.

TABLE 10.2
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	10312-83-1	Acetaldehyde, methoxy- $CH_3O\text{-}CH_2\text{-}CH{=}O$	1039		
2.	15972-60-8	Acetamide, 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)- {Alachlor®} 		2650a, 2913a, 3633, 4271a	
3.	51218-45-2	Acetamide, 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)- {Metolachlor®} 		2650b, 4271a	
4.	57966-95-7	Acetamide, 2-cyano-2-methoxyimino-*N*-(ethylcarbamoyl)- {Cymoxanil®} 		3633	
5.	5663-62-7	Acetamide, *N*-(2-furanylmethyl)-	568b, 1587, 4249, 5811b		
6.	94-75-7	Acetic acid, 2,4-dichlorophenoxy- {2,4-D}		3633, 5015, 5521, 5811b	
7.	162188-93-4	Acetic acid, (diethoxyphosphinyl)-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro[4.5]dec-7-yl ester, (±)-		4249	
8.	72360-04-4	Acetic acid, 2-(5-methylfuranyl)- 	91b, 5811b		
9.	123617-80-1	Acetic acid, 3-furanyl-	91b, 5811b		
10.	625-45-6	Acetic acid, methoxy- $H_3CO\text{-}CH_2\text{-}COOH$		429b, 1948, 4249	
11.	93-76-5	Acetic acid, 2,4,5-trichlorophenoxy- {2,4,5-T®} 		3633, 5015	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

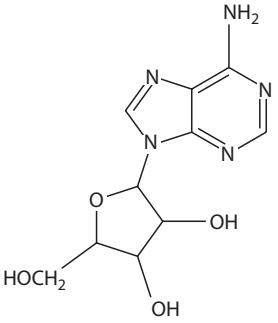
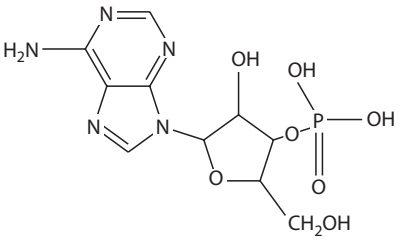
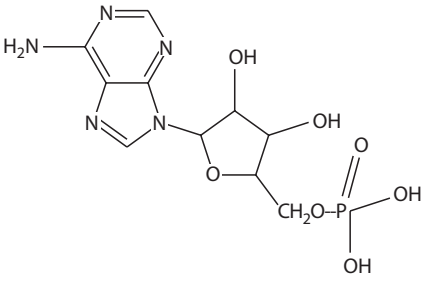
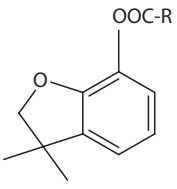
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
12.	58-61-7	Adenosine 		429b, 4249, 4828, 5540	
13.	28542-78-1	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-		2371a, 4249, 4523	
14.	6025-53-2	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*E*)-		683a, 2371a, 4066a, 4249	
15.	15896-46-5	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*Z*)-		2371a, 4249, 4582	
16.	26190-61-4	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-		2371a, 4249	
17.	53274-45-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*E*)-		2371a, 4249, 4778	
18.	52049-48-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*Z*)-		2371a, 4249, 4778	
19.	22663-55-4	Adenosine, *N*-(4-hydroxy-3-methylbutyl)-		960a, 2371a, 4249	
20.	7724-76-7	Adenosine, *N*-(3-methyl-2-butenyl)-		2371a, 4249, 4522	
21.	75081-82-2	Adenosine, *N*-[3-methyl-4-[(*O*-phosphono-β-*D*-glucopyranosyl)oxy]-2-butenyl]-, (*E*)-		429b, 4249, 4813	
22.	4294-16-0	Adenosine, *N*-(phenylmethyl)-		2371a	
23.	56-65-5	Adenosine 5′-(tetrahydrogen triphosphate)		429b	
24.	40922-97-2	Adenosine 5′-(tetrahydrogen triphosphate), *N*-(phenylmethyl)-		2371a	
25.	58-64-0	Adenosine 5′-(trihydrogen diphosphate)		429b	
26.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4708	
27.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249	
28.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
29.	55030-93-8	Adenosine 5′-(trihydrogen diphosphate), *N*-(3-methyl-2-butenyl)-		429b	
30.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′ → 5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′ → 5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
32.	22732-83-8	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester		4249, 4617	
33.	40811-89-0	Adenosine 5′-(trihydrogen diphosphate), *N*-(phenylmethyl)-		2371a, 4249	
34.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	
35.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
36.	84-21-9	3′-Adenylic acid 		429b, 4249, 4758	
37.	61-19-8	5′-Adenylic acid 		429b, 4249	
38.	20268-93-3	5′-Adenylic acid, *N*-(3-methyl-2-butenyl)-		4249, 4536	
39.	13484-66-7	5′-Adenylic acid, *N*-(phenylmethyl)-		4249	
40.	82560-54-1	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy) carbonyl)methylamino)thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}  R═-NH-S-N[CH(CH$_3$)$_2$]-(CH$_2$)$_2$-COOC$_2$H$_5$		3633	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

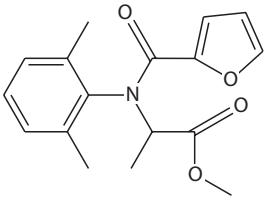
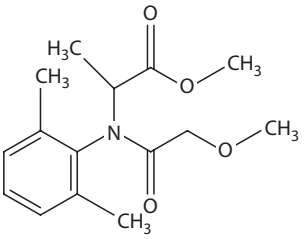
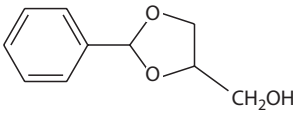
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
41.	57646-30-7	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(2-furanylcarbonyl)-, methyl ester {Furalaxyl®} 		3633	
42.	57837-19-1	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-, methyl ester {Ridomil®} 		2892a, 3633, 4271	
43.	154-17-6	*D*-Arabinohexose, 2-deoxy- {also known as *D*-Glucose, 2-deoxy-}		429b, 3075, 4249, 4599, 5811b	
44.	16449-30-2	*D*-Arabinohexose, 2-deoxy-4-*O*-β-*D*-glucopyranosyl-		4249, 4599	
45.		Arabitinol, 2,3-di-*O*-methyl- $HO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$		3669	
46.		Arabitinol, 2,5-di-*O*-methyl- $H_3CO\text{-}CH_2\text{-}(CHOH)_2\text{-}(CHOCH_3)\text{-}CH_3$		3669	
47.		Arabitinol, 3,5-di-*O*-methyl- $H_3CO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)\text{-}CHOH\text{-}CH_3$		3669	
48.		Arabitinol, 2,3,4-tri-*O*-methyl- $HO\text{-}CH_2\text{-}(CHOCH_3)_3\text{-}CH_3$		3669	
49.		Arabitinol, 2,3,5-tri-*O*-methyl- $H_3CO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$		3669	
50.	86-51-1	Benzaldehyde, 2,3-dimethoxy-	568b, 4249	568b, 4249	
51.	613-45-6	Benzaldehyde, 2,4-dimethoxy-		568b, 3219, 4249	
52.	93-02-7	Benzaldehyde, 2,5-dimethoxy-	5811	5811	
53.	4925-88-6	Benzaldehyde, 2,5-dimethoxy-4-methyl-	2601a		
54.	3392-97-0	Benzaldehyde, 2,6-dimethoxy-	2767, 3266, 3557, 4249	938, 1256, 3219, 3266, 4249	
55.	120-14-9	Benzaldehyde, 3,4-dimethoxy- {veratraldehyde}	568b, 1238, 4249	172a, 174b, 568b, 938, 1053, 1254, 1256, 3266, 3370, 3767a, 4249, 5811b	
56.	7311-34-4	Benzaldehyde, 3.5-dimethoxy-	568b, 4249	568b, 4249	
57.	134-96-3	Benzaldehyde, 3,5-dimethoxy-4-hydroxy- {syringaldehyde}	568b, 1238, 1884, 2042, 2043, 2046, 3302, 3308, 3712, 3797, 4163, 4249, 4379, 5811b	404, 568b, 3797, 3974a, 4249, 5811b	3395

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

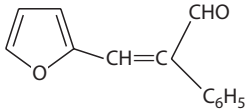
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
58.	708-76-9	Benzaldehyde, 4,6-dimethoxy-2-hydroxy-	568b, 4249	568b, 4249	
59.	121-32-4	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}	568b, 2731, 2735, 3266, 3712, 4050, 4249, 4566	568b, 633, 1053, 2281, 2282, 2478, 2699, 3266, 3643, 3894, 4050, 4249	
60.	10031-82-0	Benzaldehyde, 4-ethoxy-		172a, 174b, 1053, 3266	
61.	2539-53-9	Benzaldehyde, 4-ethoxy-3-hydroxy-		5811b	
62.	1319-88-6	Benzaldehyde glyceryl acetal 		172a, 174b, 1053, 3266	
63.	106799-60-4	Benzaldehyde, hydroxy-methoxy-		2339, 5811b	
64.	148-53-8	Benzaldehyde, 2-hydroxy-3-methoxy-	5034	3430, 5811b	
65.	121-33-5	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}	568b, 1105, 1238, 1352, 1358, 1360, 1361, 1364, 1375, 1375a, 1375b, 1586, 2042–2044, 2570, 2601a, 2640, 2762, 2765, 2767, 3224, 3266, 3302, 3308, 3553, 3557, 3712, 3745, 3797, 4050, 4249, 4379, 5034, 5811b	172a, 174b, 404, 568b, 633, 935, 1053, 1063–1066, 1068–1074, 1105, 1352, 1379, 1590a, 1825, 2281, 2338, 2339, 2339a, 2478, 2389, 2544, 2611, 2699, 2917a, 3159, 3215, 3219, 3266, 3370, 3550, 3643, 3767a, 3797, 3973, 3974a, 4050, 4249, 5811b	1360, 1375a, 3395
66.		Benzaldehyde, 4-hydroxy-3-methoxy-, labeled with ^{14}C {vanillin-^{14C}}	1105	1105	
67.		Benzaldehyde, methoxy-	3893, 4249, 5034		
68.	135-02-4	Benzaldehyde, 2-methoxy-	5811a		
69.	591-31-1	Benzaldehyde, 3-methoxy-	568b, 4249		
70.	123-11-5	Benzaldehyde, 4-methoxy- {*p*-anisaldehyde}	278, 568b, 1884, 3266, 4036, 4249, 5811b	45, 120, 172a, 174b, 568b, 1053, 1379, 2862, 2917a, 2939, 3059, 3266, 3370, 3797, 3905, 3973, 3974a, 4249, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
71.	90-04-0	Benzenamine, 2-methoxy- {*o*-anisidine}	2889, 3300, 3491, 3781, 4249, 4763, 5811b	1254	
72.	50868-72-9	Benzenamine, 2-methoxy-5-methyl-	568b, 4249	568b, 4249	
73.	536-90-3	Benzenamine, 3-methoxy- {*m*-anisidine}	568b, 2724, 2883, 2889, 3491, 3797, 4010, 4011, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	
74.	104-94-9	Benzenamine, 4-methoxy- {*p*-anisidine}	2889, 3491, 4010, 4011, 4249, 5811b	5811b	
75.		Benzene, chloromethoxy- {chloroanisole}		268	
76.	27598-81-8	Benzene, dimethoxy-	1427, 4249, 5811b		
77.	1125-88-8	Benzene, dimethoxy-methyl-	568b, 4249		
78.	91-16-7	Benzene, 1,2-dimethoxy- {veratrole}	568b, 1586, 1626, 2767, 2939, 3557, 4249, 5811b	568b, 1254, 2095, 3547, 4249	
79.		Benzene, 1,2-dimethoxy-4-ethenyl-	1586, 3557, 4249	2544, 4249	
80.	494-99-5	Benzene, 1,2-dimethoxy-4-methyl-	568b, 1586, 2767, 2778, 3557, 4249		
81.	93-16-3	Benzene, 1,2-dimethoxy-4-(1-propenyl)-	5811	5811	
82.	151-10-0	Benzene, 1,3-dimethoxy-		172a, 174b, 1053, 3266, 3370	
83.	150-78-7	Benzene, 1,4-dimethoxy-	297, 568b, 3266, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370, 3547, 4249	
84.	14753-08-3	Benzene, 1,4-dimethoxy-2-methyl-5-(1-methylethyl)-		568b, 4249, 4807, 5811b	
85.	3459-80-1	Benzene, [(1,1-dimethylethoxy)methyl]-		404	
86.	1004-66-6	Benzene, 1,3-dimethyl-2-methoxy-	5811a, 5811b		
87.	874-63-5	Benzene, 3,5-dimethyl-1-methoxy-	5811, 5811a, 5811b		
88.	83-66-9	Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro- {musk ambrette}		5811, 5811b	
89.	6380-23-0	Benzene, 4-ethenyl-1,2-dimethoxy-	568b, 2543, 2601a, 2767, 2773, 3557, 4249	568b, 2389, 2544, 4249, 5811b	
90.	637-69-4	Benzene, 1-ethenyl-4-methoxy-	568b, 4249, 4633		
91.	103-73-1	Benzene, ethoxy-	2775, 5811b		
92.	5076-72-2	Benzene, 1-ethoxy-4-methoxy	4570a		
93.	100-66-3	Benzene, methoxy- {anisole}	568b, 616, 1140, 1416, 1419, 1422, 1427, 1626, 2114, 2939, 3266, 3302, 4249, 5034	174b, 568b, 1379, 3266, 4249	
94.	21730-66-5	Benzene, methoxy-1-^{14}C- {anisole-1-^{14}C-}	2764, 4249	1379	
95.	26897-24-5	Benzene, methoxymethyl- {two isomers detected}	1427, 2731, 2735, 4249		
96.	538-86-3	Benzene, (methoxymethyl)- {benzyl methyl ether}		3539, 4249	
97.	578-58-5	Benzene, 1-methoxy-2-methyl- {*o*-methylanisole}	568b, 615, 796, 1626, 2939, 4249		
98.	100-84-5	Benzene, 1-methoxy-3-methyl- {*m*-methylanisole}	615, 796, 1626, 2939, 4249, 5811b		
99.	104-93-8	Benzene, 1-methoxy-4-methyl {*p*-methylanisole}	568b, 615, 795, 796, 1426, 1427, 1626, 2939, 3266, 4249, 5811b	172a, 174b, 404, 568b, 1053, 3266	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
100.	3794-96-5	Benzene, 2-methoxy-1-methyl-4-(1-methylethenyl)-		937, 1156, 4090, 4249	
101.	6379-73-3	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-		568b, 1156, 2093, 3555, 4090	
102.	1076-56-8	Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-		1053, 3266, 4249	
103.	40793-85-9	Benzene, 2-methoxy-1-methyl-4-(1-propenyl)-	568b, 4249		
104.	104-46-1	Benzene, 1-methoxy-4-(1-propenyl)- {anethole}	1884, 3193, 3266, 3302, 3555, 4249	1053, 1254, 1256, 2339a, 3266, 3547, 3555, 3905, 4249, 5811b	
105.	140-67-0	Benzene, 1-methoxy-4-(2-propenyl)- {estragole}	568b, 3302, 4249	568b, 1157, 4249	
106.	104-45-0	Benzene, 1-methoxy-4-propyl- {dihydroanethole}		1053, 3266	
107.	16277-67-1	Benzene, (3-methoxy-1-propenyl)-		4249	
108.	20469-61-8	Benzene, 1-methoxy-2,3,5-trimethyl-	5811, 5811a,		
109.	4028-66-4	Benzene, 2-methoxy-1,3,5-trimethyl-	5811, 5811a, 5811b		
110.	15457-05-3	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)- {Fluorodifen®}		3633	
111.	101-84-8	Benzene, 1,1′-oxybis- {diphenyl ether}	5811b	568b, 3543, 3560, 3561, 4249	
112.	103-50-4	Benzene, 1,1′-[oxybis(methylene)]bis- {dibenzyl ether}	568b, 2543, 2773, 2775, 4249	568b, 3561, 4249	
113.	55044-97-8	Benzene, 1,1′-[oxymethylene]bis(4-ethyl)-		2543, 4249	
114.	937-61-1	Benzene, propoxymethyl-	568b, 4249		
115.	938-22-7	Benzene, 1,2,3,5-tetrachloro-4-methoxy-		268, 4249	
116.	87-40-1	Benzene, 1,3,5-trichloro-2-methoxy-		268, 4249	
117.	634-36-6	Benzene, 1,2,3-trimethoxy-	38, 568b, 4249, 5811b	568b, 2339a, 2860, 2939, 3543, 3547, 3560, 3561, 3973, 3974a, 4249	
118.	135-77-3	Benzene, 1,2,4-trimethoxy-	282, 1971, 2939, 5811		
119.	621-23-8	Benzene, 1,3,5-trimethoxy-	282, 1971, 2939		
120.	487-11-6	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-		568b, 2860, 4249	
121.	2883-98-9	Benzene, 1,2,4-trimethoxy-5-(2-propenyl)-, (*Z*)- {α-Asarone®}		2917a	
122.	5273-86-9	Benzene, 1,2,4-trimethoxy-5-(2-propenyl)-, (*E*)- {β-Asarone®}		2917a, 5515	
123.	57568-60-2	Benzeneacetaldehyde, α-(2-furanylmethylene)- 		943, 1587, 3547, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

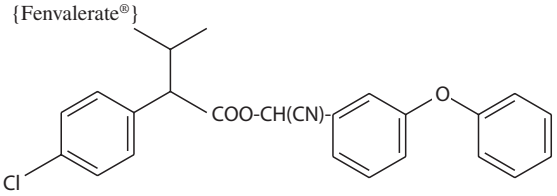
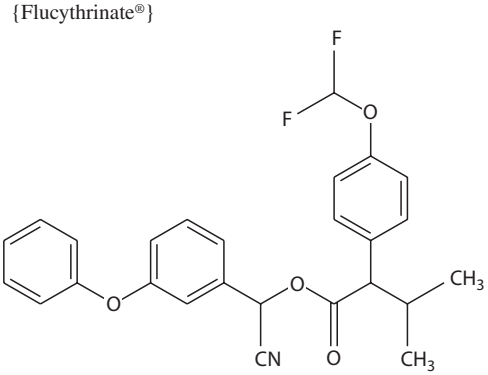
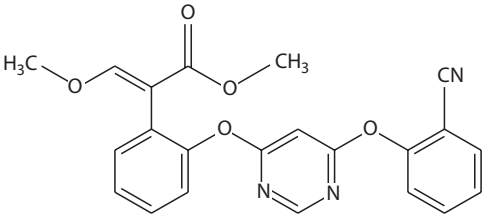
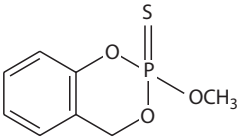
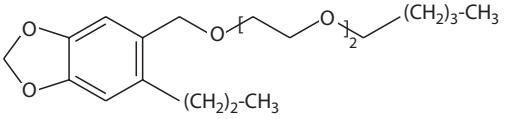
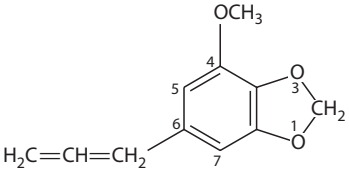
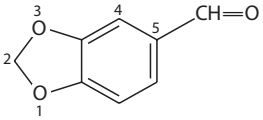
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
124.	65545-81-5	Benzeneacetaldehyde, α-(2-furanylmethylene)-, (*E*)-		5811	
125.	51630-58-1	Benzeneacetic acid, 4-chloro-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®} 	21A19	3585e, 21A19	
126.	70124-77-5	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Flucythrinate®} 		904	
127.	306-08-1	Benzeneacetic acid, 4-hydroxy-3-methoxy- {homovanillic acid}	3712, 3737, 3741, 3743, 4113, 4249, 5811b		
128.	131860-33-8	Benzeneacetic acid, methyl (α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)- {Azoxystrobin®} 		5568	
129.	934-00-9	1,2-Benzenediol, 3-methoxy-	2767, 3712, 4249	1877a	
130.	497-76-7	1,4-Benzenediol, β-*D*-glucopyranoside {arbutin}		5777, 5811	
131.	824-46-4	1,4-Benzenediol, 2-methoxy-	3712	3430, 5811b	
132.	2380-78-1	Benzeneethanol, 4-hydroxy-3-methoxy-	596, 3712, 4249, 4897	5811b	
133.	5349-60-0	Benzenemethanol, α-ethyl-4-methoxy-		568b, 4249	
134.	93-03-8	Benzenemethanol, 3,4-dimethoxy-		568b, 4249	
135.	498-00-0	Benzenemethanol, 4-hydroxy-3-methoxy-	568b, 4249, 5811a	5811a	
136.	105-13-5	Benzenemethanol, 4-methoxy- {anisyl alcohol}		172a, 174b, 568b, 1053, 3266, 3370, 3893, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
137.	104-21-2	Benzenemethanol, 4-methoxy-, acetate{anisyl acetate}	568b, 3553, 4249	172a, 174b, 568b, 1053, 3266, 3370, 3893, 4249	
138.	122-91-8	Benzenemethanol, 4-methoxy-, formate		172a, 174b, 1053, 3266, 3370	
139.	102-17-0	Benzenemethanol, 4-methoxy-, phenylacetate		172a, 174b, 1053, 3266, 3370	
140.	7549-33-9	Benzenemethanol, 4-methoxy-, propanoate		174b, 3266	
141.	1331-81-3	Benzenemethanol, ar-methoxy-		1217	
142.	80638-48-8	Benzenepropanal, 4-hydroxy-3-methoxy-	3712	5811b	
143.	24696-05-7	Benzenepropanoic acid, 2-(β-*D*-glucopyranosyloxy)-		4249, 4915	
144.		Benzenepropanoic acid, dihydroxy-methoxy-	3737, 3741, 3743		
145.	1135-23-5	Benzenepropanoic acid, 4-hydroxy-3-methoxy- {hydroferulic acid}	596, 3712, 3737, 3741, 3743, 4249		
146.	96937-36-9	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methoxy-	4249, 4897, 5811b		
147.	3811-49-2	4*H*-1,3,2-Benzodioxaphosphorin-2-sulfide, 2-methoxy- {Salithion®} 		3381, 3633, 4271a	
148.	51-03-6	1,3-Benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl- {piperonyl butoxide} 		3633, 4271a	
149.	607-91-0	1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)- {myristicin} 	568b, 2553, 3219, 3308, 3502, 4249, 5811b	568b, 2386, 3905, 4249, 5515, 5811b	
150.	94-59-7	1,3-Benzodioxole, 5-(2-propenyl)- {safrole}	568b, 2385a, 4249	568b, 3905, 4249	
151.	120-57-0	1,3-Benzodioxole-5-carboxaldehyde {piperonal; heliotropin} 	1238, 2478, 3266, 3894, 4249	172a, 174b, 1053, 1254, 1256, 1590a, 1662, 2478, 3266, 3370, 3643, 3894, 4249, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

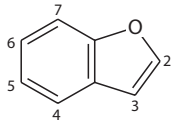
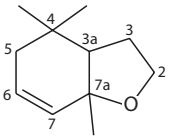
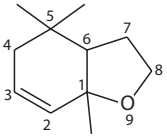
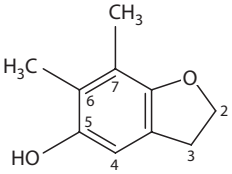
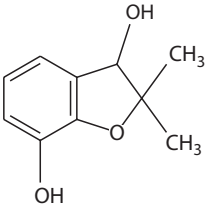
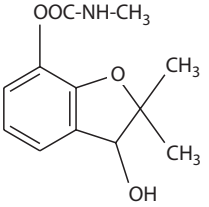
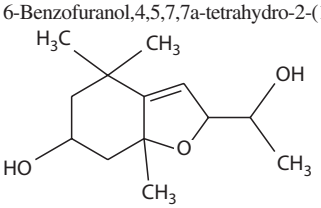
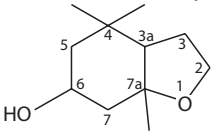
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
152.	271-89-6	Benzofuran {benzo[*b*]furan; coumarone} 	174e, 299, 568b, 1313, 1427, 1444, 1649, 1740, 1741, 1743, 1744, 1842, 2570, 2731, 2735, 2742, 2799a, 3193, 3255, 3265, 3300, 3410, 3714, 4249, 5034, 5512	5811b	3401
153.	25586-39-4	Benzofuran, dimethyl- {three isomers detected}	104, 2731, 2735, 2742, 3619, 3620, 3758, 3759, 4249, 5811b		
154.	58924-34-8	Benzofuran, ethyl-	3509a, 3757, 4249, 5811b		
155.	71265-37-7	Benzofuran, ethyldimethyl-	3757, 4249, 5811b		
156.	25586-38-3	Benzofuran, methyl- {three isomers detected}	104, 1649, 2570, 2731, 2732, 2735, 2742, 2761, 2762, 2765, 2766, 2799a, 3619, 3620, 3757, 3758, 3759, 4248, 4249, 5034, 5811b		
157.	13054-97-2	Benzofuran, octahydro-	2506, 4249		
158.	71265-38-8	Benzofuran, pentamethyl-	3757, 4249, 5811b		
159.	36618-49-2	Benzofuran, tetramethyl-	104, 2570, 2731, 2735, 4249, 5811b		
160.	36541-17-0	Benzofuran, trimethyl-	104, 2731, 2735, 3619, 3620, 3758, 3759, 4249, 5811b		
161.	496-16-2	Benzofuran, 2,3-dihydro- {coumaran}	568b, 1427, 2327c, 2601a, 2731, 2735, 3255, 3555, 4249, 4407, 5811b	568b, 2917a, 4249	
162.	71265-36-6	Benzofuran, 2,3-dihydromethyl-	2731, 2735, 4249		
163.	1746-11-6	Benzofuran, 2,3-dihydro-2-methyl-	5811b	404, 568b, 4249	3402a, 4249
164.	3782-00-1 28715-26-6	Benzofuran, 2,3-dimethyl-	568b, 2570, 2767, 3402a, 4249, 4407		
165.	3131-63-3	Benzofuran, 2-ethyl-	568b, 4249		
166.		Benzofuran, 2,3,3a,4,5,7a-hexahydro-4,4,7a-trimethyl-  Also known as 9-oxabicyclo[4.3.0]non-2-ene, 1,5,5-trimethyl- 			2339a
167.	4265-25-2	Benzofuran, 2-methyl-	299, 568b, 1586, 2767, 2777, 3255, 3557, 4249		3401
168.	36726-24-0	Benzofuran, 3-ethyl-	2570		

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
169.	21535-97-7	Benzofuran, 3-methyl-	568b, 4249		
170.	17059-52-8	Benzofuran, 5-methyl-	4407		
171.	494-90-6	Benzofuran, 4,5,6,7-tetrahydro-3,6-dimethyl-	568b, 3302, 4249		
172.		Benzofuran, 4-hydroxy-5,6-dimethyl-	2761, 2762, 2777		
173.	60026-12-2	Benzofuran, 5-hydroxy-6,7-dimethyl- 	8, 312, 568b, 1360, 1375a, 2543, 2761, 2769, 2773, 4249	404, 568b, 1156, 2386, 2389, 2544, 3549, 3550, 4090, 4249, 5811b	1360, 1375a
174.	35355-35-2	Benzofuran, 5-methoxy-6,7-dimethyl-		9a, 568b, 1156, 2389, 2544, 4090, 4249, 5811b	
175.	4265-16-1	2-Benzofurancarboxaldehyde	568b, 4249		
176.	17781-15-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl- 		5811, 5811b	
177.	16655-82-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate) {3-Hydroxycarbofuran®} 	1553, 21A19	1280, 1553, 3481, 5811b, 21A19	
178.	73051-72-6	2-Benzofuranmethanol, 2,4,5,6,7,7a-hexahydro-6-hydroxy-α,4,4,7a-tetramethyl-		234, 4249	
179.		2-Benzofuranmethanol, 2,4,5,7a-tetrahydro-4,4,7a- trimethyl-		3547, 4249	
180.		6-Benzofuranol,4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl- 		234, 1156, 3991, 4090	
181.	39815-67-3	6-Benzofuranol, octahydro-4,4,7a-trimethyl- 		943, 1149, 1149a, 1254, 1256, 3205, 3210, 3218, 3219, 3550, 4249, 4780, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

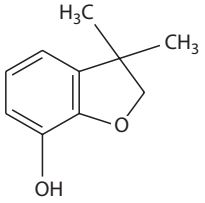
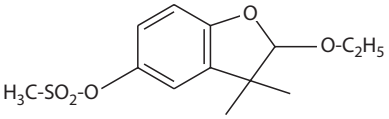
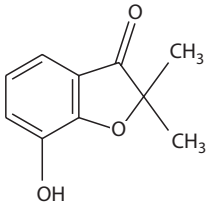
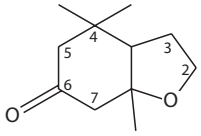
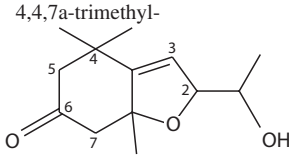
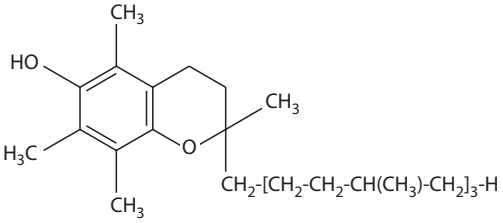
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
182.	1563-38-8	7-Benzofuranol, 2,3-dihydro-2,2-dimethyl- 		5811, 5811b	
183.	26225-79-6	7-Benzofuranol, 2,3-dihydro-3,3-dimethyl-2-ethoxy-, methanesulfonate {Ethofumesate®} 		3633, 4271a	
184.	17781-16-7	3(2*H*)-Benzofuranone, 7-hydroxy-2,2-dimethyl- 		5811, 5811b	
185.	117769-21-8	5(4*H*)-Benzofuranone, 2,7a-dihydro-2-(1-hydroxyethyl)-4,4-dimethyl-		4249, 5811b	
186.	39815-70-8	6(2*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl- 		037, 943, 1149, 1149a, 1156, 1254, 1256, 3206, 3210, 3218, 3219, 3550, 4090, 4249, 5811b	
187.	70875-03-5	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl- 		234, 1156, 1254, 1256 3206, 3210, 3218, 3549, 3991, 4090, 4249, 5811b	
188.	39815-73-1	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-		2544, 3219, 3549, 4249, 5811b	
189.	87323-67-9	Benzoic acid, hydroxymethoxy-	3737, 3741, 3743, 4249, 4897, 5811b		
190.	10366-91-3	Benzoic acid, 2-(β-*D*-glucopyranosyloxy)-		4249, 5811b	
191.	579-75-9	Benzoic acid, 2-methoxy- {*o*-anisic acid}		2389, 2544, 4249	
192.	3934-81-4	Benzoic acid, 2,3-dihydroxy-4-methoxy-	3712, 4113, 4249		
193.	645-08-9	Benzoic acid, 3-hydroxy-4-methoxy- {isovanillic acid}	2042, 3308, 3394, 3712, 3793, 3797, 5811b		
194.	87513-63-1	Benzoic acid, 3-hydroxy-6-methoxy-, methyl ester		2917a	
195.	586-38-9	Benzoic acid, 3-methoxy-	91b, 5811b		

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
196.	93-07-2	Benzoic acid, 3,4-dimethoxy-		1971, 4249	
197.	1918-00-9	Benzoic acid, 3,6-dichloro-2-methoxy- {Dicamba®}		3633, 3973, 4249, 4857, 5015, 5521, 5811b	
198.	32142-31-7	Benzoic acid, 4-(β-*D*-glucopyranosyloxy)-3-methoxy-		429b, 4249, 4915	
199.	530-57-4	Benzoic acid, 4-hydroxy-3,5-dimethoxy- {syringic acid}	1626, 1884, 2939, 3302, 3308, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 4378, 5811b	3797, 3973, 3974a	
200.	121-34-6	Benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid}	568b, 1235, 1427, 1626, 1884, 1886, 2042–2044, 2046, 2939, 3219, 3302, 3308, 3553, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	120, 568b, 908, 952, 1248, 1620, 2270, 2939, 2954, 3103, 3219, 3329, 3532, 3560, 3561, 3748, 3749, 3751, 3797, 3973, 3974a, 4092, 4249, 4677, 5811b	
201.	617-05-0	Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester		2917a	
202.	3943-74-6	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester	3712	5811b	
203.	121-98-2	Benzoic acid, 4-methoxy-, methyl ester {methyl anisate}		172a, 174b, 1053, 3266	
204.	239-30-5	Benzo[*b*]naphtho[2,1-*d*]furan	3757, 4249, 5811b		
205.	243-42-5	Benzo[*b*]naphtho[2,3-*d*]furan	726, 4249, 5811b		
206.	99881-86-4	2*H*-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-		5811, 5811b	
207.	19484-74-3	2*H*-1-Benzopyran-3-carboxylic acid, 7,8-dihydroxy-2-oxo-		4249, 4752	
208.	124052-01-3	2*H*-1-Benzopyran-3,4-dione, 2-(3,4-dihydroxyphenyl)-2,5,7-trihydroxy-		4249	
209.	1406-66-2	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)- {tocopherol}		5811	
210.	59-02-9	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- {α-tocopherol} 	1360, 1373, 1375a, 1842, 1884, 2601a, 2939, 3059, 3170, 3251, 3255, 3257, 3265, 3266, 3271, 3286, 3295, 3300, 3302, 3655a, 3684, 3685, 3797, 3875, 4159c, 4249	120, 174b, 486, 557, 667, 840, 1053, 1651, 2270, 2939, 3059, 3155, 3156, 3170, 3266, 3295, 3347, 3349, 3357, 3484, 3493, 3616, 3655a, 3707, 3755, 3797, 3811, 3875, 3971, 3973, 3974a, 4098a, 4236, 4249, 5079, 5811b	1360, 1375a
211.	148-03-8	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- {β-tocopherol}	2601a, 3484, 4249	3484, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

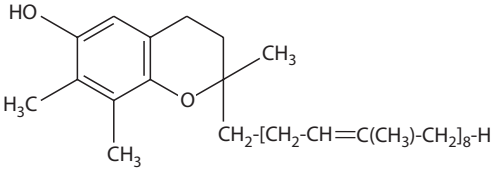
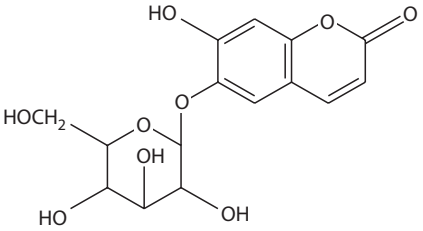
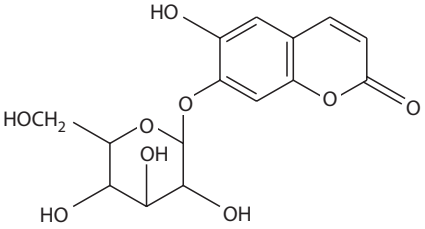
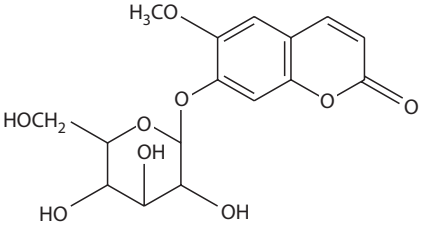
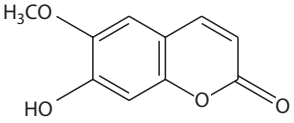
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
212.	7616-22-0	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-		1395a, 1971, 3611, 4249	
213.	56084-94-7	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12,16,20,24,28,32-octamethyl-3,7,11,15,19,23,27,31-tritriacontaoctaenyl)- [3*E*,7*E*,11*E*,15*E*,19*E*,23,*E*,27*E*] {solanochromene; solanachromene} 		120, 1971, 3059, 3346–3348, 3349, 3357, 3971, 3973, 3974a, 4249, 5811b	
214.	60091-00-1	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-		3797, 4249	
215.	531-75-9	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin} 	3257	1309, 2939, 2954, 3103, 3973, 3974a, 4249, 5711, 5811b	
216.	531-58-8	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin} 		1309, 1626, 3797, 4249, 5811b, 5838	
217.	531-44-2	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-methoxy- {scopolin} 		72, 120, 677b, 830a, 831, 834, 835, 840, 890, 966, 1102, 1309, 1626, 1863, 2338, 2395, 2557a, 2911c, 2954, 3194, 3629, 3631, 3646, 3738, 3797, 3973, 3974a, 3974b, 4156, 4249, 4269, 5649, 5650, 5809, 5811b, 5831	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
218.	92-61-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin} 	419, 568b, 1284, 1373, 1626, 1842, 1884, 1898, 2377, 2524a, 2767, 2939, 3059, 3096, 3168, 3302, 3308, 3553, 3602, 3797, 3891, 3995, 4005–4007, 4119, 4121, 4123, 4124, 4164, 4249, 4319, 4373–4375, 5512, 5811b	72, 120, 254, 404, 568b, 677b, 830a, 831, 834, 835, 840, 890, 966, 1063–1066, 1068–1074, 1112, 1626, 1863, 2014, 2270, 2313a, 2338, 2361, 2389, 2531, 2544, 2557a, 2810–2812, 2914, 2939, 2954, 3059, 3103, 3109, 3161, 3194, 3219, 3329, 3631, 3641, 3646, 3705, 3738, 3794, 3797, 3973, 3974a, 3974b, 3984, 4249, 4269, 4373–4375, 5079, 5081, 5127, 5235, 5591, 5616, 5650, 5652, 5704, 5705, 5745, 5766, 5788, 5808, 5811b, 5830, 5831, 5842, 5876, 5888, 5889	
219.	531-59-9	2*H*-1-Benzopyran-2-one, 7-methoxy-		4249	
220.		2*H*-1-Benzopyran-2-one, 8-methoxy-		4249, 4897	
221.	71050-53-8	2*H*-1-Benzopyran-2-one, 6-methoxy-7-(β-*D*-xylofuranosyloxy)- {scopoletin glucoside}		2939, 3797, 4249, 5650, 5808, 5809, 5830, 5842, 5888	
222.	18309-73-4	2*H*-1-Benzopyran-2-one, 6-methoxy-7-[(6-*O*-β-*D*-xylopyranosyl-β-*D*-glucopyranosyl)oxy]-		1863a, 2939, 4249, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

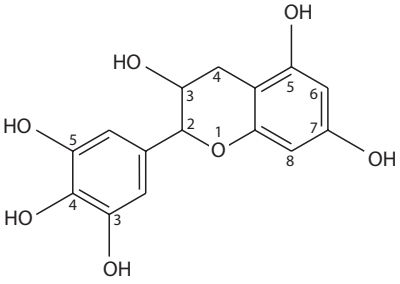
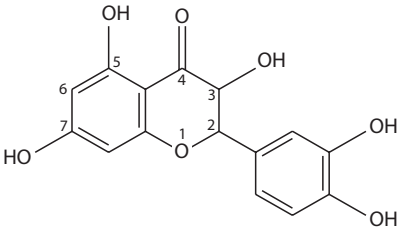
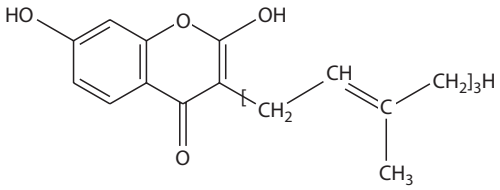
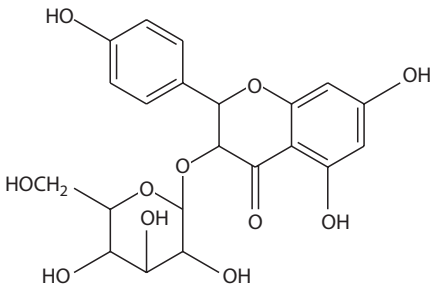
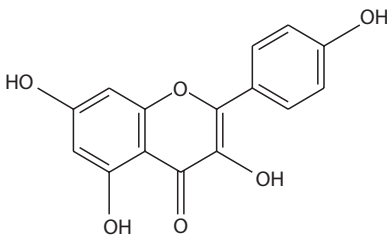
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
223.	970-73-0	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*E*)- 		429b	
224.	970-74-1	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*Z*)-		429b, 4249	
225.	124052-00-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,3,5,7-tetrahydroxy-		4249	
226.	21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		120, 1626, 1837a, 1971, 2023, 2270, 2939, 3059, 3194, 3555, 3667, 3794, 3797, 3973, 3974a, 4249, 5079, 5255, 5256, 5724, 5747, 5811b, 5888	
227.	117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin, 3,3a,4a,5,7-pentahydroxyflavone} 	3096, 3555, 5652, 5750, 5758, 5904	72, 120, 970, 1077b, 1837a, 2270, 2379, 2704a, 2939, 3059, 3462, 3555, 3685, 3794, 3797, 3974a, 4036, 4403, 4999, 5079, 5255, 5641, 5652, 5750, 5758, 5811b, 5904	
228.	7215-44-3 20188-84-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-O-β-*D*-glucopyranosyl- *D*-glucopyranosyl)oxy]-5,7-dihydroxy- {quercetin 3,3′-diglucoside}		4249, 5724, 5747, 5811, 5811b, 5888	
229.	1486-70-0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-methoxy-		3797, 3974a, 4249	
230.	2068-02-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5-hydroxy-3,7-dimethoxy-		3797, 3974a, 4249	
231.	491-50-9	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}		3797, 3974a, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
232.	124051-99-6	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-[[2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,6-dihydroxy-3-oxo-4-benzofuranyl]oxy]-2,3-dihydro-3,5-dihydroxy-		4249	
233.	480-41-1	4*H*-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)- {naringenin}		970, 3797, 3974a, 4249	
234.	643-57-2	4*H*-1-Benzopyran-4-one, 2,7-dihydroxy-3-(3,7,11-trimethyldodeca-2,6,10-trienyl)- {ammoresinol} 		3763, 5079	
235.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3,4-dihydroxyphenyl)- {3a,4a,5,7-tetrahydroxy-3-methylflavone}		4147, 5776, 5888	
236.		4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-3-methyl-2-(3-methyl-4-hydroxyphenyl)- {4a,5,7-trihydroxy-3,3a-dimethylflavone}		4147, 5888	
237.		4*H*-1-Benzopyran-4-one, 3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone}		5776	
238.	480-10-4	4*H*-1-Benzopyran-4-one, 3-(b-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glucoside; 3,4a,5,7-tetrahydroxyflavone glucoside} 		120, 641, 830a, 835, 838, 840, 966, 970, 1626, 1971, 2023, 2270, 2939, 3059, 3161, 3555, 3646, 3738, 3797, 3974a, 4072a, 4249, 5079, 5724, 5753, 5758	
239.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5,7-tetrahydroxyflavone, 3-glucoside}		1625, 4147, 5353, 5724, 5834, 5888	
240.	57523-93-0	4*H*-1-Benzopyran-4-one, octahydro-2,5,5,7a-tetramethyl-		5811, 5811b	
241.	529-44-2	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricetin}		5811, 5811b	
242.	520-18-3	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(4-hydroxyphenyl)- {kaempferol; 3,4a,5,7-tetrahydroxyflavone} 	3095a, 3555, 3794, 4249, 5652, 5758	1626, 1971, 2939, 3059, 3555, 3794, 4249, 5652, 5758, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

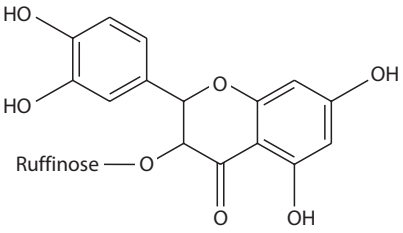
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
243.	55136-76-0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
244.	142235-82-3	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2090b	
245.	19895-95-5	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	
246.	522-12-3	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl) oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {quercetrin}	970	4036, 4249, 4573	
247.	17912-87-7	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl) oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricitrin}		5811, 5811b	
248.	55696-57-6	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-		4249	
249.	55804-74-5	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
250.	153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} 		69, 72, 120, 248, 385, 598, 828b, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1063–1066, 1068–1074, 1309, 1329, 1333, 1485, 1626, 1971, 2014, 2079, 2153a, 2270, 2313a, 2338, 2361, 2379, 2395, 2514, 2529, 2531, 2557a, 2704a, 2810–2812, 2939, 3059, 3096, 3161, 3367a, 3400, 3462, 3551, 3555, 3628, 3629, 3631, 3641, 3646, 3700, 3705, 3738, 3767, 3794, 3974a, 3974b, 3984, 3999, 4005–4007, 4036, 4156,	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} (cont.)		4157, 4249, 4403, 4999, 5079, 5110, 5156, 5157, 5189, 5204, 5217, 5304, 5305, 5310, 5576, 5591, 5596, 5641, 5652, 5661, 5681, 5697, 5698, 5724, 5747, 5750, 5780, 5788, 5808, 5809, 5811b, 5831, 5834, 5888, 5889	
251.	17650-84-9	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		1309, 4249, 5811b	
252.	30311-61-6	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy- {rutin-7-glucoside}		2023, 4147, 5777, 5811b, 5888	
253.	34336-18-0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249, 5811b	
254.	29859-91-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		4249	
255.	27554-19-4	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		1309, 4249	
256.	58934-57-9	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		4249	
257.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5, 7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-glucoside}		4147, 5888	
258.		4*H*-1-Benzopyran-4-one,7-(β-*D*-rhamnoglucopyranosyloxy)-3, 5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone, 7-rhamnoglucoside}		4147, 5888	
259.		4*H*-1-Benzopyran-4-one, 3-(β-*D*-rhamnoglucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-rhamnoglucoside}		3095a, 4372, 5888	
260.	828-82-0	4*H*-1-Benzopyran-4-one, 3-ethyl-	568b, 4249		
261.	520-34-3	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)- {diosmetin}		120, 4249, 4959	
262.	4382-17-6	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-methoxy-		3797, 4249	
263.		4*H*-1-Benzopyran-4-one, hydroxy-	1586, 2767, 4249		
264.	38445-24-8	4*H*-1-Benzopyran-4-one, 6-hydroxy-	1586, 2767		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

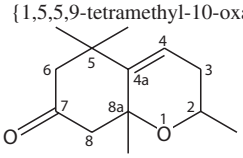
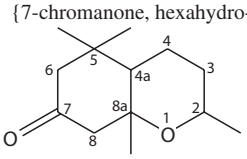
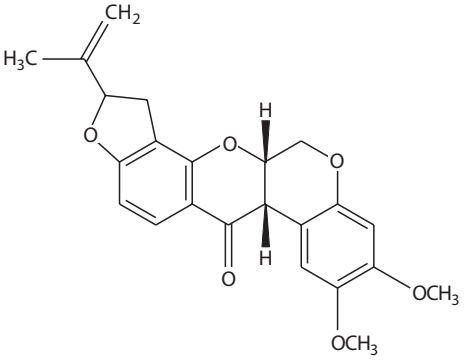
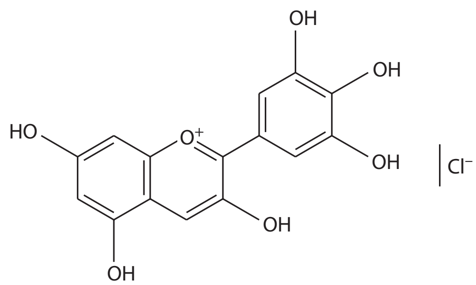
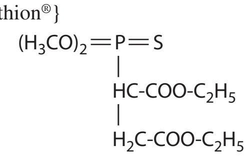
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
265.	10236-47-2	4*H*-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}		970, 1305b, 3797, 3974a, 4249	
266.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,5′,7-pentahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2023, 4249	
267.		4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,7-tetrahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		4249	
268.		5*H*-1-Benzopyran-7-one, 2,3,6,7,8,8a-hexahydro-2,5,5,8a-tetramethyl-		568b, 4249	
269.		7*H*-1-Benzopyran-7-one, 2,4a,5,6,8,8a-hexahydro-2,5,5,8a-tetramethyl-		404, 3547, 4249	
270.	20194-67-6	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-2,5,5,8a-tetramethyl-{1,5,5,9-tetramethyl-10-oxabicyclo[4.4.0]dec-6-en-3-one} 	297, 568b, 2767, 2769, 3557, 4249, 5811b	568b, 937, 943, 1063–1066, 1068–1074, 1149, 1156, 1254, 1256, 1590a, 2338, 2339b, 2386, 2389, 2544, 2611, 3218, 3543, 3545, 3546, 3550, 3560, 3561, 4048, 4090, 4098a, 4249, 5811b	
271.	52811-22-0	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-5,5,8a-trimethyl-	5811, 5811a, 5811b	5811, 5811a, 5811b	
272.	5835-18-7	7*H*-1-Benzopyran-7-one, octahydro-2,5,5,8a-tetramethyl-{7-chromanone, hexahydro-2,5,5,8a-tetramethyl-} 	568b, 1586, 2570, 2767, 2769	568b, 943, 1063–1066, 1068–1074, 1149, 1156, 1254, 1256, 1590a, 2282, 2338, 2339b, 2386, 2917a, 3205, 3218, 3223, 3545, 3550, 4090, 4098a, 5811b	
273.	83-79-4	Benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6a*H*)-one, 1,2,12,12a-tetrahydro- 8,9-dimethoxy-2-(1-methylethenyl)-, [2R-(2α,6aα,12aα)]- {Rotenone®} 		3633, 3634, 21A14, 21A49	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
274.	528-58-5	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride		4249, 4681	
275.	22688-80-8	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride		4249, 4681, 4710	
276.	528-53-0	1-Benzopyrylium, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-, chloride 		2855a, 4249, 4681	
277.	18719-76-1	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-, chloride		928b, 4249, 4710	
278.	33978-17-5	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride		4249, 4681	
279.	27548-56-7	3-Benzoxepin-7-methanol, 5a,6,7,8,9,9a-hexahydro-α,α,5,9a-tetramethyl-, (5aα,7α,9aα)-(-)-		4249, 5811b	
280.	102488-10-8	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-		5811, 5811b	
281.	53093-94-0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-,(*Z*)-(±)-		52, 4249	
282.	53093-95-1	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-,(*E*)-(±)-		52, 4249	
283.	53093-96-2	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethyl)-,(*Z*)-(±)-		52, 404	
284.	53093-97-3	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethyl)-,(*E*)-(±)-		52, 404	
285.		Butanal, 4-(2-hydroxyethoxy)- $HO\text{-}CH_2CH_2\text{-}O\text{-}(CH_2)_3\text{-}CH{=}O$	3553, 4249		
286.	121-75-5	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester {Malathion®} 	1618, 1619, 1884, 3634, 4249, 5811b, 21A19	1219b, 1219c, 1618, 1884, 2058a, 2650b, 3633, 3634, 3767a, 3973, 4249, 4271a, 21A19	
287.	1438-90-0	1,2-Butanedione, 1-(2-furanyl)-	568b, 4249		
288.		1-Butanol, 2-ethoxy-		2339a	
289.	91599-03-0	1-Butanol, 4-[(7-β-*D*-glucopyranosyl-7*H*-purin-6-yl)amino]-2-methyl-		4249	
290.	155728-85-1	2-Butanol, 1-(4-bromophenoxy)-3-[(phenylmethyl)amino]-, (R*,R*)-		4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

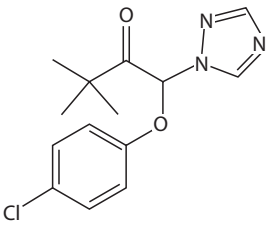
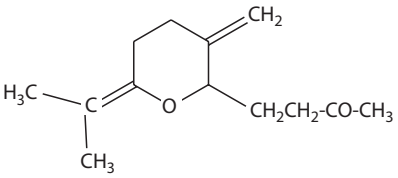
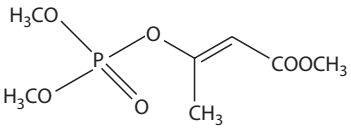
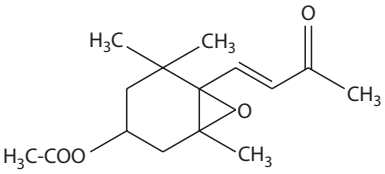
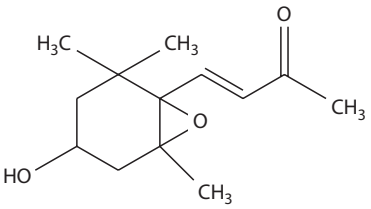
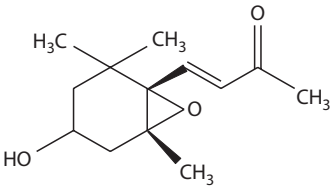
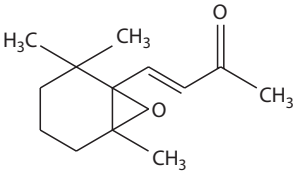
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
291.	43121-43-3	2-Butanone,1-(4-chlorophenoxy)-3, 3-dimethyl-1-(1,2,4-triazol-1-yl)- {Triadimefon®} 		3633	
292.	699-17-2	2-Butanone, 4-(2-furanyl)-	5811, 5811a, 5811b	5811b	
293.	104-20-1	2-Butanone, 4-(4-methoxyphenyl)-		172a, 174b, 1053, 3266	
294.	158815-72-6	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)-		4249, 5811b	
295.	158815-73-7	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)-		4249, 5811b	
296.	160115-51-5	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)- (+)-		4249	
297.	160115-52-6	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)- (-)-		4249	
298.		2-Butanone, 4-[5,6-dihydro -3-methyl-6-(1-methylethyl)-pyran-2-yl]-		3547, 4249	
299.	13679-56-6	2-Butanone, 4-(5-methyl-2-furanyl)-	2570, 4249	3547, 4249	
300.		2-Butanone, 4-(2-methyl-5-(1-methylethyl)-2-furanyl)-		3545	
301.		2-Butanone, 4-(2-methyl-6-(1-methylethyl)-2-tetrahydropyranyl)-		404, 3547, 4249	
302.		2-Butanone, 4-(4,5-dihydro-3-methylene-6-dimethylmethylene-2-pyranyl)- 		3545	
303.	7786-34-7	2-Butenoic acid, 3[(dimethoxyphosphinyl)oxy]-, methyl ester {Mevinphos®; Phosdrin®} 		1219, 2058a, 3379, 3379a, 3380, 3633, 4271a	
304.	72074-11-4	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*] furan-2-yl)-, [2S-[2α(*E*),3aα,5aβ,9aα,9bβ]]-		4249	
305.	87584-34-7	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*] furan-2-yl)-, [2R-[2α(*E*),3aβ,5aα,9aβ,9bα]]-		4249, 5811b	
306.	62512-25-8	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-		4249, 4715	
307.	160550-77-6	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		4249, 4715	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
308.	50281-40-8	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1R-[1α(*E*),4β,6α]]- 		1, 4249, 4573	
309.	50281-41-9	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1S-[1α(*E*),4α,6α]]-		1	
310.	36340-49-5	3-Buten-2-one, 4-(1,2-epoxy-2,6,6-trimethyl-cyclohexyl)-, (*E*)-		5811, 5811b	
311.	623-15-4	3-Buten-2-one, 4-(2-furanyl)-	568b, 1238, 1587, 3266, 4249, 5811b	568b, 1053, 3266, 3893, 4249	
312.	81540-27-4	3-Buten-2-one, 4-(2-furanyl)-3-methyl-	568b, 4249	568b, 4249	
313.	50281-42-0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1S-[1α(*E*),4α,6α]]- 		1, 1156, 3547, 4090, 4249, 4780, 5811b	
314.	61116-99-2	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1R-[1α(*E*),4β,6α]]- 		1, 1156, 2338, 4090, 4249, 4780	
315.	23120-57-2	3-Buten-2-one, 4-(5-methyl-2-furanyl)-	568b, 1587, 4249, 5811b		
316.	66434-99-9	3-Buten-2-one, 4-(5-methyl-2-furanyl)-, (*E*)-		3547, 4249	
317.	23267-57-4	3-Buten-2-one, 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- 		937, 2339b, 2386, 2544, 2917a, 4249, 5811b	
318.	14660-91-4	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S,9′-*cis*)- {neoxanthin}		943, 2338, 2339a, 3973, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

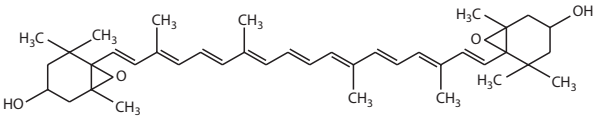
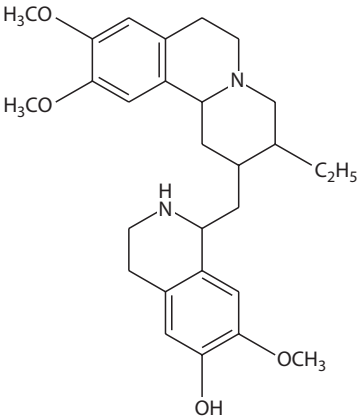
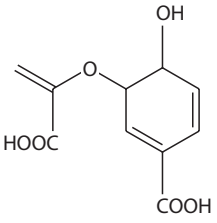
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
319.	30743-41-0	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′, 5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S)-		943, 2338, 2339a, 2939, 3973, 4249	
320.	126-29-4	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S)- {violaxanthin} 		543a, 585, 830a, 832, 835, 838, 943, 971, 972, 1156, 2338, 2339b, 2939, 3194, 3218, 3797, 3973, 3974a, 4090, 5811b	
321.	26927-07-1	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S,9-*cis*)-		429c	
322.	68831-78-7	β,β-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-,(3S,3′R,5R,6S,9-*cis*)-		429c, 5811b	
323.	17539-43-4	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-		429c	
324.	28368-08-3	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,6′R)-		429c	
325.	512-29-8	β,ε-Carotene-3,3′-diol, 5,8-epoxy-5,8-dihydro-, (3S,3′R,5R,6′R,8R)- {flavoxanthin}		2939, 3797, 3974a	
326.	528-50-7	Cellobiose		3075, 3468, 5811b	
327.	9004-34-6	Cellulose	5811b	120, 172, 248, 277, 337, 385, 385a, 420, 451, 535, 539, 601, 602, 629, 665, 722, 1053, 1063–1066, 1068–1074, 1077, 1228, 1289, 1329, 1330, 1333, 1352, 1878a, 1885, 1887, 1933a, 2014, 2042, 2044, 2046, 2070, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2454, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2913, 2919, 2939, 3029, 3059, 3087, 3192,	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Cellulose (cont.)		3264, 3266, 3305, 3371, 3372, 3393, 3395, 3401, 3402, 3404, 3405, 3409, 3430, 3449, 3450, 3462, 3468, 3551, 3665a, 3702, 3797, 3871, 3973, 3974a, 3975, 3976, 4104, 4151, 4249, 4261, 4262, 4418, 4999, 5079, 5189, 5344, 5811b, 5841	
328.		Cellulose, labeled with ^{14}C {cellulose-^{14}C}		2764, 4249	
329.	9000-11-7	Cellulose, carboxymethyl ether		172b, 2086a, 4249, 4465	
330.	9004-57-3	Cellulose, ethyl ether		429b, 4249	
331.	9004-67-5	Cellulose, methyl ether		429b, 4249	
332.	483-17-0	Cephalin		5079, 5375	
					
333.	617-12-9	1,5-Cyclohexadiene-1-carboxylic acid, 3-[(1-carboxyethenyl)oxy]-4-hydroxy-, (3R-*E*)- {chorismic acid}		429b, 4249, 4476	
					

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

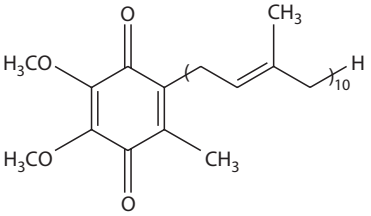
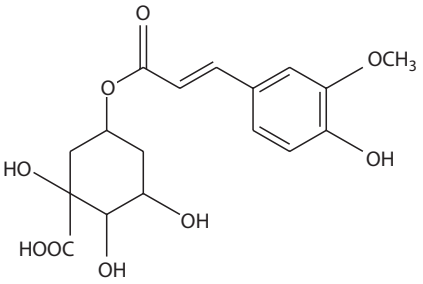
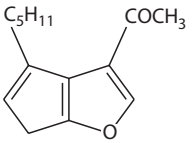
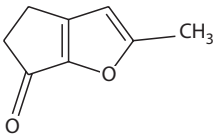
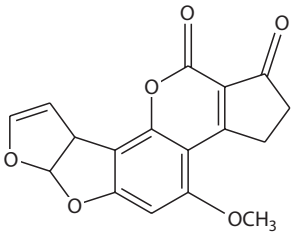
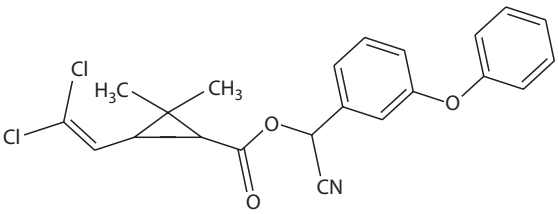
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
334.	303-98-0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-(3,7,11,15,19,23,27,31,35,39-decamethyl-2,6,10,14,18,22,26,30,34,38-tetracontadecenyl)-6-methyl- {ubiquinone-10} 		1209, 1858	
335.	606-06-4	2,5-Cyclohexadiene-1,4-dione, 2-(3,7-dimethyl-2,6-octadienyl)-5,6-dimethoxy-3-methyl-, (*E*)-		1858, 4249	
336.		2,5-Cyclohexadiene-1,4-dione, 2-methoxy-	1586		
337.	933-40-4	Cyclohexane, 1.1-dimethoxy-	568b, 4249		
338.	18349-16-1	Cyclohexane, 1.1-dimethoxy-3-methyl-	568b, 4249		
339.	18349-20-7	Cyclohexane, 1.1-dimethoxy-4-methyl-	568b, 4249		
340.	29887-60-3	Cyclohexane, 1,2-dimethoxy-, (*E*)-		2917a	
341.	1899-29-2 27044-07-1	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)- {3-*O*-feruloylquinic acid}  Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-		3797, 3973, 3974a, 4249, 4402, 4913, 5811b	
342.	62512-22-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-		4249, 4715, 5811b	
343.	77699-19-5	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-		4249, 4715	
344.	159813-37-3	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [4R-[4R*(1*E*,3S*)]]-		4249, 4715	
345.	54835-70-0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-4-hydroxy-3,5,5-trimethyl-, [R-[R*,S*-(*E*)]]-		321c, 1361, 4249, 4713	
346.	62512-23-6	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butyl]-3,5,5-trimethyl-		4249, 4715, 5811b	
347.	91048-13-4	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butylidene]-3,5,5-trimethyl-		4249, 4715	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
348.		Cyclopenta[*b*]furan, 3-acetyl-4-pentyl-	3553, 4249	404	
					
349.		Cyclopenta[*b*]furan-6-one, 4,5-dihydro-2-methyl-	3553, 4249	404	
					
350.	1162-65-8	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_1}	158a, 2024, 2484, 3721, 3970, 3986 [added aflatoxin B_1 not transferred intact to smoke]	158a, 2024, 2484, 3721, 3970, 3975 [not found in tobacco]	
					
351.	7220-81-7	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione,2,3,6a,8,9,9a-hexahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_2}		4039b, 4254, 4754	
352.	78210-65-8	2-Cyclopenten-1-one, 2-(2-furanyl)-	568b, 1587, 4249, 5811b		
353.	22323-97-3	2-Cyclopenten-1-one, 2-methoxy-	5811, 5811a, 5811b		3404, 4249
354.	14189-85-6	2-Cyclopenten-1-one, 2-methoxy-3-methyl-	1371, 2543, 2773, 2775, 3410, 4249		
355.		2-Cyclopenten-1-one, 3-(2-furanyl)-	2543, 2773, 2775, 4249		
356.	52315-07-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-,cyano(3-phenoxyphenyl)methyl ester {Cypermethrin®}	21A19	904, 1219b, 1219c, 3188a, 3585e, 3633, 4249, 4271a, 5568, 21A19	
					
357.	67375-30-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-,cyano(3-phenoxyphenyl)methyl ester {α-Cypermethrin}	21A19	3633, 21A19	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

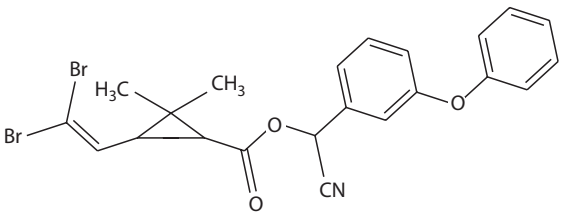
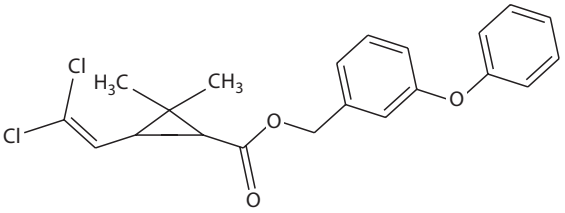
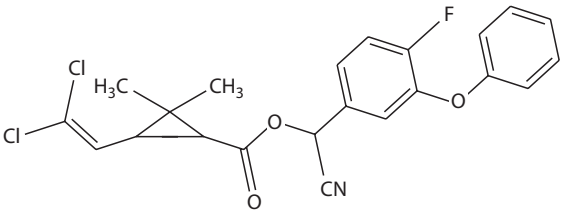
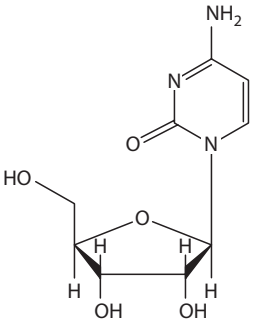
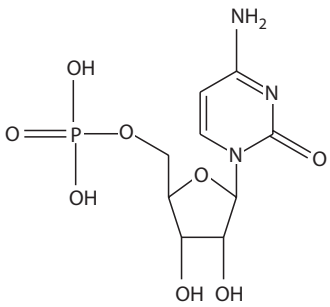
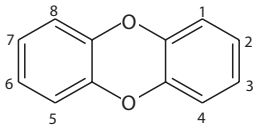
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
358.	52918-63-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl)methyl ester {Deltamethrin®} 	21A19	904, 1219b, 1219c, 3585e, 3633, 4271a, 21A19	
359.	52645-53-1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl)methyl ester {Permethrin®; Spartan®} 		904, 1219a, 1219b, 1219c, 2346, 2892a, 3188a, 3585e, 3633	
360.	68359-37-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester {Cyfluthrin®} 		904, 3633	
361.	65-46-3	Cytidine {2(1*H*)-pyrimidinone, 4-amino-1-β-*D*-ribofuranosyl-} 		429b, 4249, 4477, 4554a	
362.	65-47-4	Cytidine 5′-(tetrahydrogen triphosphate)		429b, 4249, 4474, 4505	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
363.	63-37-6	5′-Cytidylic acid 		429b, 4249, 4299, 4774	
364.	262-12-4	Dibenzo[*b,e*][1,4]dioxin 	1217, 2490, 2491, 3265, 3300, 3715		
365.		Dibenzo[*b,e*][1,4]dioxin, polychloro-	854, 4249		
366.	35822-46-9	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,8-heptachloro-	177, 1217, 2160, 2391, 2490, 2491, 3265, 3300, 4249	2160, 4249	
367.	58200-70-7	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,9-heptachloro-	177, 4249		
368.	39227-28-6	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,7,8-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
369.	57653-85-7	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,6,7,8-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
370.	19408-74-3	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8,9-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
371.	40321-76-4	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8-pentachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
372.	1746-01-6	Dibenzo[*b,e*][1,4]dioxin, 2,3,7,8-tetrachloro-	177, 1217, 2490, 2491, 3265, 3300, 3685, 4249, 5869a	933, 4249	
373.	37871-00-4	Dibenzo[*b,e*][1,4]dioxin, heptachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249, 5811b		
374.	34465-46-8	Dibenzo[*b,e*][1,4]dioxin, hexachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249, 5811b		
375.	3268-87-9	Dibenzo[*b,e*][1,4]dioxin, octachloro-	177, 1217, 2391, 2490, 2491, 2897, 3300, 4249, 5811b		
376.	36088-22-9	Dibenzo[*b,e*][1,4]dioxin, pentachloro-	1217, 2391, 2490, 2491, 3265, 3300		
377.	41903-57-5	Dibenzo[*b,e*][1,4]dioxin, tetrachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249, 5811b		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

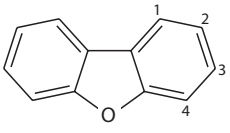
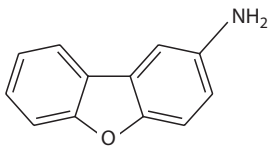
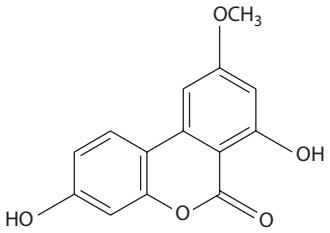
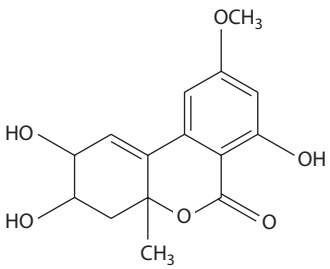
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
378.	132-64-9	Dibenzofuran {2,2′-biphenylene oxide} 	104, 568b, 1371, 1375a, 1377, 1649, 1712, 1748, 2510, 2543, 2570, 2596a, 2731, 2735, 2767, 2799a, 3410, 3500, 3514, 3557, 3619, 3620, 3741, 3758, 3759, 4248, 4249, 5811b	568b, 1248, 2094, 2339a, 3547, 4249, 5811b	1375a, 1377
379.	29062-95-1	Dibenzofuran, dimethyl-	3619, 3620, 3557, 3758, 3759, 4249, 5811, 5811a, 5811b		
380.	38998-75-3	Dibenzofuran, heptachloro-	1217, 3265, 3300, 4249		
381.	55684-94-1	Dibenzofuran, hexachloro-	1217, 3265, 3300, 4249		
382.	60826-62-2	Dibenzofuran, methyl-	2731, 2735, 2799a, 3514, 3557, 3619, 3620, 3758, 3759, 4249, 4594, 5811b		
383.	39001-02-0	Dibenzofuran, octachloro-	1217, 3265, 3300, 4249		
384.	30402-15-4	Dibenzofuran, pentachloro-	1217, 3265, 3300, 4249		
385.	30402-14-3	Dibenzofuran, tetrachloro-	1217, 3265, 3300, 4249		
386.		Dibenzofuran, polychloro- {dioxins}	177, 854, 1217, 2490, 2491, 3265, 3300, 3715, 4249		
387.	67562-39-4	Dibenzofuran, 1,2,3,4,6,7,8-heptachloro-	177, 1217, 2160, 2391, 2490, 2491, 3265, 3300, 4249	2160	
388.	55673-89-7	Dibenzofuran, 1,2,3,4,7,8,9-heptachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
389.	70648-26-9	Dibenzofuran, 1,2,3,4,7,8-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
390.	91538-84-0	Dibenzofuran, 1,2,3,4,7,9-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
391.	67517-48-0	Dibenzofuran, 1,2,3,4,8-pentachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300		
392.	57117-44-9	Dibenzofuran, 1,2,3,6,7,8-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
393.	72918-21-9	Dibenzofuran, 1,2,3,7,8,9-hexachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300		
394.	57117-41-6	Dibenzofuran, 1,2,3,7,8-pentachloro-	177, 1217, 2391, 2490, 2491, 3265, 3300, 4249		
395.	60851-34-5	Dibenzofuran, 2,3,4,6,7,8-hexachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249		

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
396.	57117-31-4	Dibenzofuran, 2,3,4,7,8-pentachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249		
397.	83704-32-9	Dibenzofuran, 2,3,4,8-tetrachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249		
398.	51207-31-9	Dibenzofuran, 2,3,7,8-tetrachloro-	1217, 2391, 2490, 2491, 3265, 3300, 4249		
399.	7320-50-5	Dibenzofuran, 1-methyl-	104, 568b, 1748, 2510, 2731, 2735, 3514, 4249, 5811b		
400.	7320-51-6	Dibenzofuran, 2-methyl-	104, 1748, 2510, 2731, 2735, 4249, 5811b		
401.	7320-52-7	Dibenzofuran, 3-methyl-	568b, 1748, 2510, 2731, 2735, 3514, 4249, 5811b		
402.	7320-53-8	Dibenzofuran, 4-methyl-	104, 1748, 2510, 2731, 2735, 3514, 4249, 5811b		
403.	3693-22-9	2-Dibenzofuranamine	1735, 4249		
					
404.	4106-66-5	3-Dibenzofuranamine	568b, 642, 4249		
405.	26894-49-5	6*H*-Dibenzo[*b,d*]pyran-6-one, 3,7(3,9 or 7,9)-dihydroxy-9(7 or 3)-methoxy-1-methyl-		4249, 4756	
					
406.	29752-43-0	6*H*-Dibenzo[*b,d*]pyran-6-one, 9-methoxy-4a-methyl-2,3,4,4a-tetrahydro-2,3,7-trihydroxy-(2α,3β,4aβ)-		4249, 4756	
					
407.	5894-59-7	Digalacturonic acid		5811, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

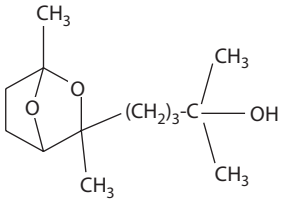
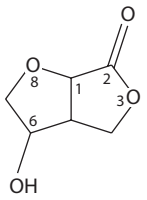
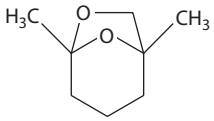
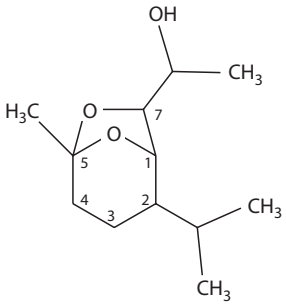
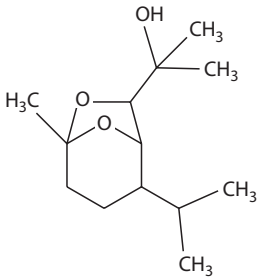
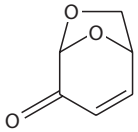
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
408.	60-57-1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aα,3β,6β,6aα,7β,7aα)- {Dieldrin®}	518, 644, 1000, 1006, 2697, 21A19	518, 644, 1029, 1000, 1006, 1219, 1219a, 1219b, 1333, 1740, 2650a, 2650b, 2697, 3188a, 3633, 3767a, 3770, 3797, 3915, 3973, 3977, 4271a, 5811b, 21A19	
409.	72-20-8	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aβ,3α,6α,6aβ,7β,7aα)- {Endrin®}	415, 419, 518, 644, 1000, 1006, 1457, 1884, 2697, 3634, 4249, 21A19	415, 419, 518, 644, 1000, 1006, 1028, 1029, 1219, 1219a, 1333, 1457, 1740, 1884, 2318, 2389, 2544, 2650b, 2697, 2939, 3188a, 3633, 3634, 3637, 3767a, 3770, 3915, 3973, 3977, 4249, 4271a, 5811b, 21A19	
410.	14816-18-3	3,5-Dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile, 4-ethoxy-7-phenyl-, 4-sulfide		1492a	
411.	117210-53-4	2,7-Dioxabicyclo[2.2.1]heptane, 1,3-dimethyl-3-(4-methyl-3-pentenyl)-, endo-		429b, 5811b	
412.	117305-90-5	2,7-Dioxabicyclo[2.2.1]heptane, 1,3-dimethyl-3-(4-methyl-3-pentenyl)-, exo-		4249, 5811b	
413.	117210-54-5	2,7-Dioxabicyclo[2.2.1]heptane-3-butanol, α,α,1,3-tetramethyl- 		5811, 5811b	
414.	121927-15-9	13,14-Dioxabicyclo[10.2.2]hexadec-6-ene-2,3,5-triol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2S*,3R*,5S*)]		4249	
415.	52886-15-4	2,9-Dioxabicyclo[3.3.1]nonan-4-ol,1,3,3-trimethyl-6-(1-methylethyl)- {two isomers reported}		3547, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
416.	110053-63-9	3,8-Dioxabicyclo[3.3.0]octan-2-one, 6-hydroxy-	5811, 5811a, 5811b		
					
417.	28401-39-0	6,8-Dioxabicyclo[3.2.1]octane, 1,5-dimethyl- {frontalin}		2339a	
					
418.	58001-00-6	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,5-dimethyl- [1α,2β,5α,7α(R*)]		1149, 1149a	
					
419.	58001-10-8	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-, (2-endo,7-exo)-(±)-		4249	
					
420.	52992-36-6	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-		4249, 5811b	
421.	37112-31-5	6,8-Dioxabicyclo[3.2.1]oct-2-en-4-one, (1S)- {levoglucosenone}	1350, 1354, 1375a, 1377, 2388, 2777, 5811b	3430, 5811b	1375a, 1377, 2387, 2388
					
422.		1,3-Dioxalane, 4-methyl-	568b, 4249		
423.		1,3-Dioxalane, 4-methyl- {isomer}	568b, 4249		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

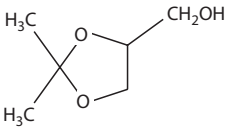
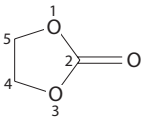
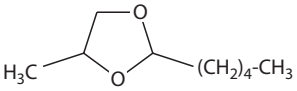
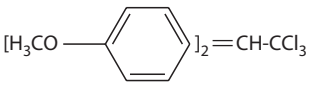
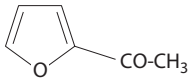
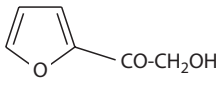
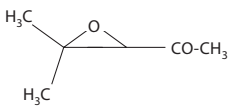
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
424.	5464-28-8	1,3-Dioxalane-4-methanol	568b, 4249		
425.	100-79-8	1,3-Dioxalane-4-methanol, 2,2-dimethyl- 	568b, 1375, 3553, 3557, 4249, 5811b		
426.	96-49-1	1,3-Dioxalan-2-one {ethylene glycol carbonate} 	568b, 1375, 1586, 1882, 2570, 2767, 3553, 3557, 4249, 5811b		3405
427.	931-40-8	1,3-Dioxalan-2-one, 4-(hydroxymethyl)- {glycerol carbonate}	568b, 1371, 1375, 3255, 3553, 3557, 4249, 5811b		
428.	108-32-7 9005-37-2	1,3-Dioxalan-2-one, 4-methyl- {1,2-propylene glycol carbonate}	568b, 3553, 4249, 5811b	2389, 2544, 4249, 5811b	
429.	505-22-6	1,3-Dioxane	568b, 4249		
430.	86687-05-0	1,3-Dioxane, 5-hydroxy-	568b, 4249		
431.	123-91-1	1,4-Dioxane	568b, 4249		
432.	16279-34-8	1,4-Dioxane, 2-methyl-	1357, 4249		
433.	26563-74-6	1,3-Dioxolane, 4-methyl-2-pentyl-, (*Z*)- 	5811		
434.	38419-69-1	6*H*-3,10b-Epoxy-1*H*-naphtho[2,1-*b*]pyran, decahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]-		4249	
435.	534-15-6	Ethane, 1,1-dimethoxy-	568b,4249		
436.	104-66-5	Ethane, 1,2-diphenoxy- C_6H_5-O-CH_2CH_2-OC_6H_5		2339a	
437.	540-67-0	Ethane, methoxy- C_2H_5-O-CH_3	2950, 4249		
438.	60-29-7	Ethane, 1,1′-oxybis- {ethyl ether}	1419, 1472, 4249, 4570a	984, 4249	
439.	72-43-5	Ethane, 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)- {Methoxychlor®} 		3188a, 3663, 3770, 4249, 4271a	
440.	534-82-7	1,2-Ethanediol, 1-(4-hydroxy-3-methoxyphenyl)-		4249	
441.	30934-97-5	Ethanol, 2,2-dimethoxy- $(H_3C\text{-}O)_2$═CH-CH_2-OH	3406, 4249, 5811b		
442.	111-46-6	Ethanol, 2,2′-oxybis- {diethylene glycol} $(HO\text{-}CH_2CH_2)_2$═O	43, 568b, 627, 1603, 2170, 2171, 2543, 2549, 2761, 2767, 2773, 2777, 2939, 3302, 3308, 3553, 4319, 5079, 5189, 5286, 5811b	568b, 627, 1241, 1296, 2188, 2195, 2246, 2788, 3264, 3605, 3689, 3797, 3974a, 4249, 5205, 5206, 5228, 5254, 5286, 5307, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
443.	78-51-3	Ethanol, 2-butoxy-, phosphate (3:1) $[H_3C\text{-}(CH_2)_3\text{-}O\text{-}(CH_2)_2]_3{\equiv}P{=}O$	3553, 5811b		
444.	112-27-6	Ethanol, 2,2′-(1,2-ethanediylbis(oxy))bis- {triethylene glycol} $HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$	174e, 331, 627, 974, 1371, 1603, 2761, 2762, 2939, 3302, 3797, 3835, 4249, 4319, 5811b	627, 1241, 1296, 2188, 2192, 2193, 2195, 2788, 2939, 3264, 3797, 3974a, 4249, 5811b, 5903	
445.	111-21-7	Ethanol, 2,2′-[1,2-ethanediylbis(oxy)]bis-, diacetate	2762, 4249, 5811b	3593	
446.	110-80-5	Ethanol, 2-ethoxy- $HO\text{-}CH_2CH_2\text{-}O\text{-}CH_2CH_3$	2761, 2762, 2765, 2766, 2777, 4249, 4570a	2917a	
447.	109-86-4	Ethanol, 2-methoxy- $HO\text{-}CH_2CH_2\text{-}O\text{-}CH_3$	3559	2385a, 3905, 4249	
448.	112-60-7	Ethanol, 2,2′-[oxybis(2,1-ethanediyloxy)]bis- {tetraethylene glycol} $HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$		3264	
449.	122-99-6	Ethanol, 2-phenoxy- $C_6H_5O\text{-}CH_2CH_2\text{-}OH$		1256, 2339a, 4249	
450.	1192-62-7	Ethanone, 1-(2-furanyl)- {2-acetylfuran} 	37, 38, 339, 568b, 1140, 1215, 1238, 1338, 1339, 1365, 1371, 1378, 1419, 1427, 1586, 1590, 1958, 1960, 2337, 2387, 2506, 2507, 2543, 2545, 2570, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 3255, 3397, 3410, 3530, 3555, 3797, 4249, 4407, 4570a, 5034, 5811b	404, 568b, 937, 953, 984, 1590, 1590a, 2337, 2339a, 2386, 2389, 2544, 2917a, 3188, 3547, 3555, 3561, 4249, 5811b	1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404
451.	19859-79-1	Ethanone, 1-(2-furanyl)-2-(acetyloxy)-	568b, 1375, 1375b, 1586, 2767, 3553, 3557, 5811b		
452.	17678-19-2	Ethanone, 1-(2-furanyl)-2-hydroxy- 	568b, 3553, 3557, 4249, 5811b	568b, 3797, 4249	3402, 3404, 3405, 4249
453.	703-98-0	Ethanone, 1-(2-hydroxy-3-methoxyphenyl)-	1375, 1375b, 3712, 4249		
454.	703-23-1	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-	2570, 3712		
455.		Ethanone, 1-[[3,4-dihydro-6-(1-methylethyl)-inden-4-yl]-pyran-2-yl]-		3547, 4249	
456.	4478-63-1	Ethanone, 1-(3,3-dimethyloxiranyl)- {mesityl oxide epoxide} 		404	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
457.	66611-15-2	Ethanone, 1-(3-benzofuranyl)-	568b, 1587, 4249, 5811b		
458.	14313-09-8	Ethanone, 1-(3-furanyl)-	2767, 2769, 4249		
459.	3420-59-5	Ethanone, 1-(3-hydroxy-2-furanyl)- {isomaltol}		2917a	
460.		Ethanone, 1-(3-hydroxy-2-methoxyphenyl)-	1360, 1375a		1360, 1375a
461.	6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-	1375, 1375b, 1586, 1884, 2767, 2769, 3557, 3712, 4249		
462.	586-37-8	Ethanone, 1-(3-methoxyphenyl)-	796, 1626, 2939, 4249		
463.	1676-63-7	Ethanone, 1-(4-ethoxyphenyl)-	2487		
464.	493-33-4	Ethanone, 1-(4-hydroxy-2-methoxyphenyl)-	1360, 2327c, 2761, 2762, 3712, 4249		
465.	2478-38-8	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	3712	404, 3430, 5811b	
466.	498-02-2	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)- {acetovanillone}	568b, 1360, 1364, 1375, 1375a, 1375b, 1586, 1884, 2327c, 2765–2767, 2769, 2773, 3557, 3712, 4249, 5811b	404, 568b, 938, 2917a, 3430, 3767a, 4249	1360, 1375a
467.	100-06-1	Ethanone, 1-(4-methoxyphenyl)- {acetanisole}	336, 616, 1626, 2939, 3224, 3266, 4249, 5811b	172a, 174b, 336, 1053, 2389, 2544, 3266, 3370, 4249	
468.	1193-79-9	Ethanone, 1-(5-methyl-2-furanyl)- {2-acetyl-5-methylfuran}	568b, 1427, 1586, 2337, 2570, 2731, 2735, 2767, 2775, 3553, 3555, 3557, 4249, 4570a, 5811b	404, 568b, 965, 1053, 1662, 2337, 2339a, 2386, 2389, 2544, 3188, 3205, 3219, 3266, 3543, 3547, 3555, 3560, 3561, 3905, 4249, 5811b	
469.		Ethanone, 1-(5-methyl-2-furanyl)-2-hydroxy-═Furan, 2-(1-oxo-2-hydroxyethyl)-5-methy-	568b, 4249		
470.	25154-45-4	Ethanone, 1-(furanyl)-	3404, 4249, 5811b		
471.	71278-10-9	Ethanone, 1-(methyl-2-furanyl)-	1427, 4249		
472.	74430-25-4	Ethanone, 1-(methylfuranyl)-	4249	5811b	
473.	25252-64-6	Ethanone, 1-(tetrahydro-2-furanyl)-	4249		
474.	121198-50-3	Ethanone, 1-(tetrahydrofuranyl)-	2387	5811b	2387
475.	13678-73-4	Ethanone, 1-[1-(2-furanylmethyl)-1*H*-pyrrol-2-yl]-		404, 568b, 3547, 3555, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
476.	51297-35-9	Ethanone, 1-[3-(1-ethyl-2-methylpropyl)oxiranyl]-		4249	
477.	120056-06-6	Ethanone, 1-[3-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)oxiranyl]-, [1S-[1α(2S*,3R*),2β,4a]]		4249, 5811b	
478.	55087-82-6	Ethanone, 1-[5-(hydroxymethyl)-2-furanyl]-	568b, 1586, 2767, 3553, 3557, 4249, 5811b		
479.	52812-41-6 102518-81-0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-		404, 940, 942, 3546, 3547, 3555, 3561, 4249, 5811, 5811b	
480.	57934-85-7 102518-82-1	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-, (exo,exo)-(±)-		4249, 4573, 5811, 5811b	
481.	29732-48-7	Flavylium, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride		4249, 4527, 4710	
482.		Flavylium, 3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-3′,4′,5,7-tetrahydroxy-, chloride		4249, 4527, 4644	
483.	72693-10-8	Formamide, *N*-(2-furanylmethyl)-	568b, 1587, 4249, 5811b		
484.	9037-90-5	*D*-Fructan		429b, 4249, 4806	
485.	10247-46-8	*D*-Fructofuranose		429b, 3333a, 4923	
486.	71385-82-5	β-*D*-Fructofuranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2155, 4249	
487.	79082-92-1	β-*D*-Fructofuranose, 2,6-bis(dihydrogen phosphate)		429b, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

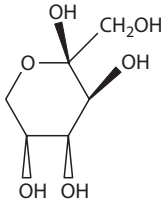
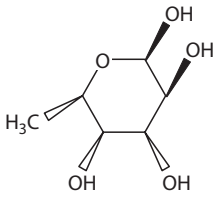
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
488.	57-48-7	*D*-Fructose {levulose} 	1089a, 1352, 1360, 1361, 1375a, 1887a, 1944, 2079, 2145, 2321, 2524a, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	71, 120, 321b, 480, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1141, 1142, 1289, 1352, 1361, 1435a, 1916, 1971, 2070, 2270, 2283, 2313a, 2337, 2338, 2381, 2532, 2818, 2911c, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3462, 3551, 3555, 3580, 3667, 3797, 3871, 3913, 3973, 3974a, 3974b, 4159, 4249, 4275, 4411, 5079, 5105, 5108, 5109, 5114, 5189, 5344, 5387, 5449, 5562, 5652, 5748, 5768, 5811b, 5819	1360, 1375a
489.	51767-72-7	*D*-Fructose, labeled with ^{13}C {*D*-Fructose-^{13}C}		976a, 4249, 4720	
490.		*D*-Fructose, labeled with ^{14}C {*D*-Fructose-^{14}C}		5644	
491.	29118-61-4	*D*-Fructose, 1-(2-carboxy-1-pyrrolidinyl)-1-deoxy-, (S)-		434, 1063–1066, 1068–1074, 1351, 2337, 2339b, 3555, 3639, 3923, 3973, 3974a, 4159, 4249, 5811b	
492.	488-69-7	*D*-Fructose, 1,6-bis(dihydrogen phosphate)		429b, 4249, 4720	
493.	70954-04-0	*D*-Fructose, 1-[(1-carboxy-2-hydroxypropyl)amino]-1-deoxy-,[R-(R*,S*)]-		434, 1351, 3555, 3973, 3974a	
494.	34393-27-6	*D*-Fructose, 1-[(3-amino-1-carboxy-3-oxopropyl)amino]-1-deoxy-,(S)-		1351, 2337, 4362	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
495.	10003-63-1	*D*-Fructose, 1-[(3-carboxypropyl)amino]-1-deoxy-		1351, 2337, 3639, 3923, 3973, 3974a, 5811b	
496.	70906-15-9	*D*-Fructose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		4159, 4249	
497.	643-13-0	*D*-Fructose, 6-(dihydrogen phosphate)		429b, 4249, 4670	
498.	36119-15-0	*D*-Fructose, mono(dihydrogen phosphate)		429b, 4249, 4960	
499.	2438-80-4	Fucose 		3075, 5811b	
500.	110-00-9	Furan 	112, 199, 199, 299, 480, 568b, 605, 639, 722, 1063–1074, 1140, 1284, 1348–1352, 1374, 1375a, 1377, 1378, 1412–1414, 1416, 1418, 1419, 1449, 1586, 1589, 1634, 1740, 1741, 1743, 1744, 1842, 1875, 2002, 2003, 2063, 2079, 2270, 2293, 2310, 2313a, 2337, 2508, 2520, 2543, 2570, 2634, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2939, 2940, 2942, 2946, 3059, 3105, 3132, 3193, 3251, 3260, 3265, 3300, 3302, 3308, 3557, 3583, 3584, 3714, 3797, 3901, 4052, 4056, 4162, 4249, 4257, 4290, 4319, 5034, 5508, 5512, 5770, 5811b	5811b	1228, 1375a, 1377, 1378, 2244, 3401, 4052, 4056
501.		Furan, C_3-alkyl- {3 isomers detected}		3188	
502.	64079-00-1	Furan, butyl-		1157, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

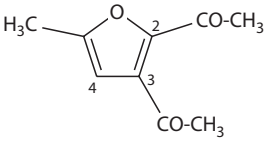
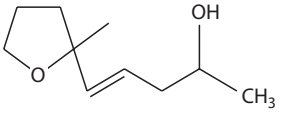
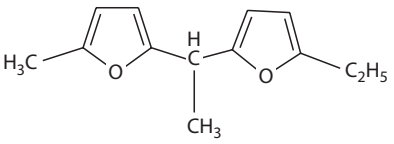
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
503.		Furan, 2,3-diacetyl-5-methyl- 		3543	
504.	28802-49-5	Furan, dimethyl-	105, 156, 1215, 1412–1414, 1416, 1418, 1637, 2634, 2857, 3308, 3692, 3901, 4005–4007, 4104, 4249, 4319, 5034, 5811b		
505.	31093-57-9	Furan, ethenyl-	5811, 5811b		
506.		Furan, ethenyl-methyl-	642, 4249		
507.	27252-25-1	Furan, ethyl-		1157, 4249	
508.	12758-54-2	Furan, hexenyl-methyl-	2735, 4249, 5811, 5811a		
509.	27137-41-3	Furan, methyl-	105, 167, 1140, 1215, 1284, 1352, 1412–1414, 1416, 1418, 1637, 1966, 2142, 2506, 2507, 2799a, 3255, 3308, 3897, 3901, 4249, 4360, 5034, 5811b		2506, 2507
510.	64079-01-2	Furan, pentyl-		1157, 1587, 4249	
511.	27252-26-2	Furan, propyl-		1157, 4249	
512.	109-99-9	Furan, tetrahydro-	568b, 1140, 1374, 1375a, 1377, 1378, 1412–1414, 1416, 1418, 2782, 2804, 3302, 3308, 3557, 3797, 3901, 4249, 4319, 5034, 5811b	568b, 3561, 4249	1375a, 1377, 1378
513.	41239-48-9	Furan, tetrahydro-2,5-diethyl-	568b, 4249		
514.		Furan, tetrahydro-2-methyl-2-(4-hydroxy-1-pentenyl)- 		1156, 2389, 2544, 4090	
515.	3208-40-0	Furan, tetrahydro-2-(3-phenylpropyl)-		1053, 3266	
516.	13678-51-8	Furan, 2-(2-furanylmethyl)-5-methyl-	568b, 2731, 2735, 4249, 5811b		
517.	10504-11-7	Furan, 2-(2-methyl-1-propenyl)-	568b, 1587, 4249, 5811b		
518.	4868-20-6	Furan, 2-(3-hexenyl)-5-methyl-, (*Z*)-	2731, 2735, 2767, 4249		

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

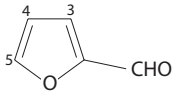
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
519.	1197-40-6	Furan, 2,2′-methylenebis-	2731, 2735, 3555, 5811b	4249, 4809	
520.	110484-93-0	Furan, 2,2′-methylenebis(5-ethyl)-	4249		
521.	13679-43-1	Furan, 2,2′-methylenebis(5-methyl)-	568b, 2735, 4249, 5811b		
522.	1191-99-7	Furan, 2,3-dihydro-	5811, 5811a		
523.	121213-25-0	Furan, 2,3-dihydro-2-methoxy-	4249	5811b	
524.	1708-25-4	Furan, 2,3-dihydro-2-methyl-	568b, 4249		
525.	34314-83-5	Furan, 2,3-dihydro-4-methyl-	3559	5811b	
526.	14920-89-9	Furan, 2,3-dimethyl-	157, 4249		
527.	3710-43-8	Furan, 2,4-dimethyl-	568b, 4249		
528.	1708-29-8	Furan, 2,5-dihydro-	1102a	5811b	
529.	13314-90-4	Furan, 2,5-dihydro-2,5-bis(methylene)-	2731, 2735		
530.	332-77-4	Furan, 2,5-dihydro-2,5-dimethoxy-	568b, 4249		
531.	13436-43-6	Furan, 2,5-dihydro-2-methoxy-	4249	5811b	
532.	1708-30-1	Furan, 2,5-dihydro-2-methyl-	3559		
533.	10504-06-0	Furan, 2,5-diethyl-		984	
534.	625-86-5	Furan, 2,5-dimethyl-	111, 112, 199, 156, 157, 299, 314, 480, 568b, 605, 1063–1066, 1068–1074, 1140, 1153, 1154, 1313, 1348–1350, 1354, 1365, 1374, 1375a, 1377, 1419, 1586, 1589, 1634, 1947, 1975, 2002, 2003, 2079, 2091, 2270, 2293, 2310, 2337, 2543, 2545, 2570, 2765, 2767, 2777, 2782, 2799a, 2804, 2822, 3302, 3308, 3508, 3530, 3557, 3797, 3897, 4052, 4056, 4162, 4249, 4257, 4360, 5480a, 5770, 5811b	568b, 984, 2917a, 3561, 3973, 5811b	1228, 1354, 1375a, 1377, 2244, 3401, 4052, 4056
535.	110484-94-1	Furan, 2-[1-(5-ethyl-2-furanyl)ethyl]-5-methyl- 	4249		
536.	4466-24-4	Furan, 2-butyl-	568b, 3553, 4249	568b, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
537.	1487-18-9	Furan, 2-ethenyl-	314, 568b, 1422, 2545, 2777, 4249, 5034, 5770, 5811b	568b, 984, 4249	3401
538.	10504-13-9	Furan, 2-ethenyl-5-methyl-═furan, 5-ethenyl-2-methyl-	314, 568b, 642, 2545, 4249, 5811, 5811b		
539.	13679-86-2	Furan, 2-ethenyltetrahydro-2-methyl-5-(1-methylethenyl)-		2386, 4249	
540.	3208-16-0	Furan, 2-ethyl-	299, 314, 568b, 1063–1066, 1068–1074, 1365, 1371, 1587, 2570, 2773, 2777, 3410, 4407, 5811b	568b, 1550, 2917a, 4249	
541.	1703-52-2	Furan, 2-ethyl-5-methyl-	299, 568b, 1063–1066, 1068–1074, 1365, 1587, 2545, 3410, 4249, 5770, 5811b		
542.	60858-07-3	Furan, 2-(3-hexenyl)-5-methyl-	5811, 5811b		
543.	534-22-5	Furan, 2-methyl-	111, 112, 239, 299, 314, 480, 568b, 605, 1063–1066, 1068–1074, 1140, 1153, 1154, 1348–1351, 1354, 1374, 1375, 1375a, 1375b, 1377, 1378, 1416, 1419, 1437, 1449, 1495, 1586, 1589, 1632, 1634, 1875, 1947, 2002, 2003, 2063, 2079, 2091, 2270, 2293, 2310, 2543, 2545, 2559, 2559a, 2570, 2765, 2767, 2773, 2775, 2777, 2782, 2804, 2822, 2857, 2939, 2942, 3059, 3132, 3254, 3302, 3308, 3482, 3530, 3557, 3797, 4052, 4056, 4104, 4162, 4249, 4257, 4290, 4319, 5770, 5811b	568b, 984, 1550, 2339a, 3561, 3973, 4249, 5811b	1228, 1354, 1375a, 1377, 1378, 2244, 3401, 4052, 4056
544.		Furan, 2-methyl-5 (1-methylethenyl)-		2339a	
545.	96-47-9	Furan, 2-methyltetrahydro-	568b, 2270, 2293, 2310, 3302, 4249		
546.	3777-69-3	Furan, 2-pentyl-		404, 1157, 1550, 2336, 2339a, 4249, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
547.	17113-33-6	Furan, 2-phenyl-	568b, 2570, 4249		
548.	55484-04-3	Furan, 2-(4-pyridyl)-	4407, 4249		
549.	42933-00-6 54869-11-3	Furan, 3-(4,8,12-trimethyltridecyl)- {phytofuran}	901, 4249	404, 901, 943, 1250, 1256, 1590a, 2386, 2917a, 3549, 3550, 4249, 5811b	
550.	930-27-8	Furan, 3-methyl-	299, 314, 348, 568b, 1063–1066, 1068–1074, 1365, 2545, 4249, 5770, 5811b	568b, 984, 1550, 4249, 5811b	3401
551.	13423-15-9	Furan, 3-methyltetrahydro-	568b, 4249	568b, 4249	
552.	13679-41-9	Furan, 3-phenyl-	568b, 4249	568b, 937, 2339a, 4249	
553.	10504-04-8	Furan, 2,3,5-trimethyl-	5770		
554.	2745-26-8	2-Furanacetic acid	568b,1063–1066, 1068–1074, 1375a, 1377, 3553, 4249		1375a, 1377
555.	4915-21-3	2-Furanacetic acid, ethyl ester	568b, 4249		
556.	617-90-3	2-Furancarbonitrile	568b, 2726, 2731, 2735, 2777, 4249		
557.	13714-86-8	2-Furancarbonitrile, 5-methyl-	2726, 2727, 2731, 2735, 2777, 3491, 4249, 5811b		
558.	39276-09-0	Furancarboxaldehyde	3865b, 4249, 4553		
559.	98-01-1	2-Furancarboxaldehyde {furfural; 2-furaldehyde} 	157, 172, 174a, 239, 270, 299, 314, 375, 376, 402, 564, 568b, 722, 775, 916, 924, 1039, 1099, 1140, 1215, 1238, 1239, 1338, 1339, 1348–1350, 1354, 1361, 1364, 1371, 1375, 1375a, 1375b, 1377, 1378, 1416, 1418, 1419, 1427, 1437, 1586, 1589, 1590, 1634, 1649, 1666, 1949, 1958, 1960, 1971, 2079, 2088, 2089, 2170, 2200, 2270, 2337, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2573–2375, 2591,	120, 404, 524, 568b, 965, 984, 1063–1066, 1068–1074, 1550, 1590, 1590a, 1949, 2079, 2337, 2339a, 2386, 2389, 2544, 2860a, 2917a, 2939, 3188, 3194, 3547, 3555, 3626, 3648, 3873, 3973, 3974a, 4202, 4249, 5073, 5079, 5132, 5234, 5303, 5811b	1228, 1354, 1375a, 1377, 1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		2-Furancarboxaldehyde {furfural; 2-furaldehyde} (cont.)	2604, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 2887, 2939, 3106, 3127, 3187, 3190, 3255, 3257, 3300, 3302, 3308, 3324, 3397, 3410, 3462, 3530, 3553, 3555, 3557, 3559, 3648, 3653, 3795, 3822, 3826, 3913, 3992, 4079, 4159, 4202, 4259, 4319, 4378, 4407, 5034, 5073, 5079, 5099, 5100, 5124, 5140, 5359, 5420, 5770, 5811b, 5835		
560.		2-Furancarboxaldehyde, hydroxy-	1375a, 1377		1375a, 1377
561.	25376-49-2	2-Furancarboxaldehyde, (hydroxymethyl)-		924, 2939, 4249	
562.	26895-04-5	2-Furancarboxaldehyde, methyl-	297, 2506, 2507, 2767, 4249, 5034, 5811b		2506 (0), 2507 (0), 3402, 3404
563.	33342-48-2	2-Furancarboxaldehyde, 3-methyl-	568b, 1357, 4249		
564.	32529-53-6	2-Furancarboxaldehyde, 5-acetyl-	568b, 1140, 2570, 4249	568b, 2389, 2544, 3547, 4249, 5811b	
565.	10551-58-3	2-Furancarboxaldehyde, 5-[(acetyloxy)methyl]-	5811b	404, 3557, 4249	
566.	23074-10-4	2- Furancarboxaldehyde, 5-ethyl-	5811, 5811a, 5811b		
567.	67-47-0	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	341, 568b, 722, 723, 924, 1063–1066, 1068–1074, 1350, 1354, 1360, 1364, 1365, 1371, 1375a, 1377, 1882, 1958, 1960, 2337, 2387, 2493, 2543, 2545, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 2939, 3302, 3308, 3397, 3410, 3462, 3530, 3553, 3557, 3559, 4159, 4163, 4249, 4378, 4379, 4407, 5034, 5811b	120, 568b, 965, 984, 2337, 2389, 2544, 2722, 2860a, 2930, 2917a, 2939, 3194, 3430, 3547, 3549, 3797, 3973, 3974a, 4249, 5811b	1354, 1375a, 1360, 1375a, 1377, 2387, 3393, 3401, 3402, 3404, 3405

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
568.	21300-07-2	2-Furancarboxaldehyde, 5-methoxy-		3823, 4249	
569.		2-Furancarboxaldehyde, 5-(methoxy-?-methyl)-		833, 4249	3402, 3404,
570.	1917-64-2	2-Furancarboxaldehyde, 5-(methoxymethyl)-	3404, 4249, 5811b		3402, 3404
571.	620-02-0	2-Furancarboxaldehyde, 5-methyl-	156, 157, 299, 568b, 722, 775, 1099, 1140, 1215, 1364, 1365, 1337, 1339, 1360, 1371, 1375, 1375a, 1375b, 1378, 1427, 1590, 1949, 1971, 2337, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2628, 2629, 2636, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 3302, 3397, 3410, 3530, 3553, 3555, 3557, 3648, 3795, 3797, 3826, 4104, 4159, 4249, 4407, 5073, 5811b	120, 404, 524, 568b, 965, 984, 1063–1066, 1068–1074, 1590, 1590a, 1949, 2337, 2386, 2389, 2544, 2860a, 2917a, 2939, 3188, 3430, 3543, 3547, 3555, 3560, 3561, 3648, 3797, 3974a, 4249, 5073, 5811b	1360, 1375a, 1378, 2387, 2506, 2507, 3401, 3402, 3404
572.		2-Furancarboxaldehyde, 5-(2-phenylethenyl)-	568b, 4249	568b, 4249	
573.	498-60-2	3-Furancarboxaldehyde	299, 568b, 1063–1066, 1068–1074, 2506, 2507, 2545, 2731, 2735, 3255, 3559, 4249, 5811b	404, 568b, 4249, 5811b	2244, 2506, 2507, 3401, 3402, 3404
574.	29988-76-9	Furancarboxamide	2767, 3557	2337a	
575.	609-38-1	2-Furancarboxamide	568b, 1586, 2787, 3553, 3557, 3559, 4249, 5811b	568b, 2336, 4249	
576.		2-Furancarboxamide, *N*-ethyl-	568b, 4249	568b, 4249	
577.	61190-74-7	2-Furancarboxamide, *N*-(2-furanylmethyl)-	568b, 4249	568b, 4249	
578.	26447-28-9	Furancarboxylic acid	689b, 5811b	3430, 5708	
579.	1334-76-5	Furancarboxylic acid, methyl ester {methyl furoate}	5811, 5811a, 5811b		
580.	88-14-2	2-Furancarboxylic acid {furoic acid}	568b, 1132, 1063–1066, 1068–1074, 1099, 1235, 1365, 1375, 1375a, 1375b, 1377, 1882, 2337, 2761, 2762, 2765–2767, 2777, 2939, 3053, 3059, 3060, 3061, 3255, 3302, 3308, 3394, 3410, 3496, 3553, 3557, 4159, 4249, 5811b	120, 568b, 965, 1999, 2014, 2337, 2338, 2337a, 2389, 2544, 2722, 2862a, 2863, 2939, 3053, 3060, 3973, 3974a, 4249, 5811b	1375a, 1377, 3393, 3402, 3404

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

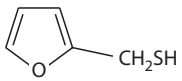
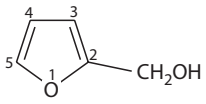
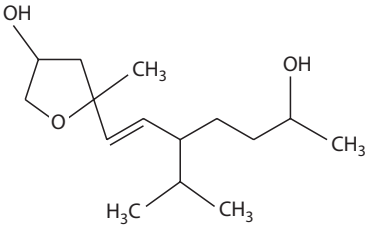
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
581.	61892-61-3	2-Furancarboxylic acid, 2-(acetyloxy)ethyl ester	568b, 1375a, 1377, 4249	568b, 1883, 4249	1375a, 1377
582.	614-99-3	2-Furancarboxylic acid, ethyl ester {ethyl 2-furoate}		1053, 3266	
583.	3736-81-0	2-Furancarboxylic acid, 4-[(2,2-dichloroacetyl)-methylamino]phenyl ester	5811, 5811a, 5811b		
584.	71278-16-5	2-Furancarboxylic acid, 3-hydroxy-	1375a, 1377	1883, 4249	1375a, 1377
585.	6338-41-6	2-Furancarboxylic acid, 5-(hydroxymethyl)-	1089a, 1886m, 1887a, 2524a, 3741, 3743, 4249, 5811b		3393
586.	1917-15-3	2-Furancarboxylic acid, 5-methyl-	568b, 1075, 1882, 3394, 3553, 4249, 5811b		3393
587.	611-13-2 1334-76-5	2-Furancarboxylic acid, methyl ester {methyl 2-furoate}	568b, 1884, 3266, 4249, 5811b	568b, 984, 1053, 3266, 4249, 5811b	
588.	3885-29-8	2-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester	568b, 3553, 4249, 5811b		
589.	488-93-7	3-Furancarboxylic acid	568b, 3553, 4249, 5811b		
590.	636-44-2	3-Furancarboxylic acid, 2,5-dimethyl-	91b, 5811b		
591.	6947-94-0	3-Furancarboxylic acid, 2-methyl-	91b, 5811b		
592.	4412-96-8	3-Furancarboxylic acid, 3-methyl-	3327a, 5811b		
593.	21984-93-0	3-Furancarboxylic acid, 5-methyl-	91b, 568b, 2767, 2777, 3553, 4249, 5811b		
594.	13129-23-2	3-Furancarboxylic acid, methyl ester		2917a	
595.	5204-91-1	3-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester	568b, 3553, 4249		
596.	823-82-5	2,5-Furandicarboxaldehyde	568b, 1364, 3553, 4249, 5811b	568b, 3547, 4249	3401
597.	61892-94-2	3,4-Furandiol, tetrahydro-3-methyl-	3553, 5811b		
598.	98-02-2	2-Furanmethanethiol 		1053, 3266, 4249	
599.	40795-25-3	Furanmethanol	1205a, 5034	5811b	
600.	98-00-0	2-Furanmethanol {furfuryl alcohol} 	172, 568b, 1099, 1140, 1215, 1338, 1339, 1350, 1352, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1378, 1427, 1461, 1586, 1882, 1963, 2088, 2270, 2337, 2387, 2493, 2506, 2507, 2543, 2545, 2570, 2607, 2628, 2629, 2636, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2857, 2939, 3059, 3255, 3302, 3308, 3397, 3410, 3553, 3555, 3557, 3559, 3648, 3795, 3797, 4104, 4159, 4249, 4319, 4407, 5811b	120, 404, 524, 543a, 568b, 937, 953, 984, 1063–1066, 1068–1074, 1590a, 1848, 2079, 2337, 2339a, 2386, 2389, 2544, 2607, 2649, 2861a, 2917a, 2939, 3059, 3547, 3549, 3550, 3555, 3648, 3797, 3905, 3973, 3974a, 4052, 4249, 5079, 5811b	1360, 1375a, 1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404, 3405

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
601.	623-17-6	2-Furanmethanol, acetate	568b, 2337, 2731, 2735, 3555, 4249, 5811b	404, 568b, 2337, 3547, 4092, 4249	
602.		2-Furanmethanol, 2,3-dihydro-5-methoxy-	2775		
603.	60047-17-8	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-		404, 937, 2389,2544, 3555, 4249	
604.	5989-33-3 60047-17-8	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*Z*)- {*cis*-linalool oxide}		172a, 174b, 404, 568b, 1053, 2336, 2338, 2339a, 2386, 2389, 2544, 2917a, 3266, 3555, 4249	
605.	23007-29-6	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*E*)- {*trans*-linalool oxide}		172a, 174b, 568b, 1053, 2339a, 2917a, 3266	
606.	13493-97-5	2-Furanmethanol, formate		568b, 2389, 2544, 3547, 3555, 4249, 5811b	
607.	55664-77-2	2-Furanmethanol, methyl-		4012, 4249	
608.	3857-25-8	2-Furanmethanol, 5-methyl-	1586, 1882, 2543, 2767, 2775, 3410, 3557, 5811b	404, 1590a, 2917a, 3547, 3549	
609.	54774-28-6	2-Furanmethanol, 5-methyltetrahydro-		2917a	
610.	61481-02-5	2-Furanmethanol, 5-(1-pyrrolidinylmethyl)-	4249		
611.	97-99-4	2-Furanmethanol, tetrahydro-	222–224, 568b, 2543, 2773, 4249	568b, 2389, 2544, 4249, 5811b	
612.	4412-91-3	3-Furanmethanol	4249	5811b	
613.	29848-46-2	3-Furanol, tetrahydro-5,5-dimethyl-	3553, 4249		
614.	66607-70-3	3-Furanol, tetrahydro-5-[6-hydroxy-3-(1-methylethyl)-1-heptenyl]-5-methyl-		1156, 3851, 4090	
					
615.		2(3*H*)-Furanone, dihydro-5-methyl-5-(5-methyl-2-furanyl)-		2934b	
616.	3511-31-7	3(2*H*)-Furanone	4249	5811b	
617.	22929-52-8	3(2*H*)-Furanone, dihydro-	4249	5811b	
618.	33909-95-4	3(2*H*)-Furanone, dihydro-2,5-dimethyl-, (*E*)-			2388, 4249

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

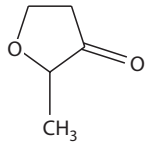
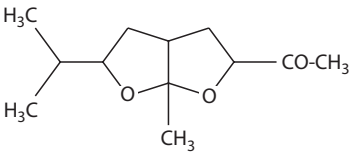
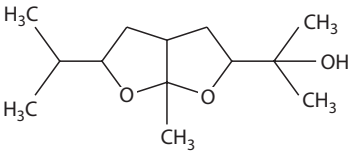
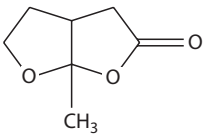
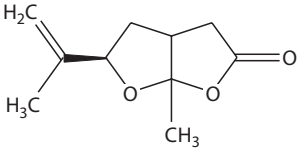
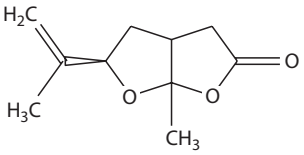
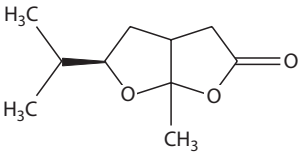
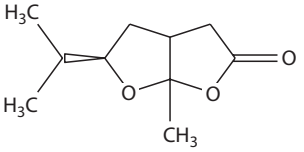
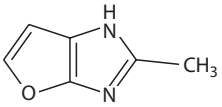
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
619.	33794-61-5	3(2*H*)-Furanone, dihydro-2,5-dimethyl-, (*Z*)-			2388, 4249
620.	3188-00-9	3(2*H*)-Furanone, dihydro-2-methyl- {2-methyltetrahydrofuran-3-one} 	1371, 2735, 3266, 3410, 4249, 5770, 5811b	172a, 174b, 984, 1053, 1590a, 2336, 2389, 2544, 2917a, 3188, 3266, 3370, 3547, 3555, 4249, 5811b	3404, 4249
621.	89364-27-2	3(2*H*)-Furanone, dihydro-4-methyl-	4249	5811b	
622.		3(2*H*)-Furanone, dihydro-5-methyl-5-propyl-		3547, 4249	
623.	14400-67-0	3(2*H*)-Furanone, 2,5-dimethyl-	1075, 2775, 4249		
624.	27538-09-6	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl-		174b, 3266	
625.	17678-20-5	3(2*H*)-Furanone, 4-hydroxy-2-(hydroxymethyl)-5-methyl-	1375, 1375b, 4249		
626.	3658-77-3	3(2*H*)-Furanone, 4-hydroxy-2,5-dimethyl- {furaneol}	568b, 1063–1066, 1068–1074, 1364, 1370, 1371, 1882, 2493, 2570, 2601a, 2767, 3266, 3397, 4249, 4407, 5811b	172a, 174b, 568b, 1053, 2917a, 3266, 3370, 4249, 5811b	
627.	484-20-8	7*H*-Furo[3,2-*g*][1]benzopyran-7-one, 4-methoxy-		898a	4249, 4513
628.		Furo[3,2-*b*]furan, tetrahydro-2-acetyl-3a-methyl-5-(1-methylethyl)- 		3543, 3545	
629.		Furo[3,2-*b*]furan-2(3*H*)-methanol, tetrahydro-α,α,3a-trimethyl-5-(1-methylethyl)- 		3543, 3545	
630.	60026-27-9	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl- 		2544, 3543, 4249, 5811b	
631.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethenyl)- 		3543	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
632.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethenyl)-		3543	
					
633.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethyl)-		3543, 3545	
					
634.		Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethyl)-		3543, 3545	
					
635.	61893-05-8	1*H*-Furo[2,3-*d*]imidazole, 2-methyl-	1351, 3553, 4249		
					
636.	72686-97-6	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, (2α,3aα,5aβ,8β,9aS*)-		4249, 4594	
637.	72747-21-8	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, [2R-(2α,3aβ,5aα,8α,9aR*)]-		4249, 4594	
638.	37209-50-0	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, acetate, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberin}	4249, 4642	4249, 4594, 4642, 5811b	
639.	56857-64-8	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberol}		4101, 4249, 4594, 4910, 5071, 5811b	
640.		Galactitol, 2,3-di-*O*-methyl- HOH_2C-[$CH(OCH_3)$]$_2$-$(CHOH)_2$-CH_2OH		3669	
641.		Galactitol, 2,4-di-*O*-methyl- HOH_2C-$CH(OCH_3)$-CHOH-$CH(OCH_3)$-CHOH-CH_2OH		3669	
642.		Galactitol, 2,6-di-*O*-methyl- HOH_2C-$CH(OCH_3)$-$(CHOH)_3$-CH_2OCH_3		3669	
643.		Galactitol, 2-*O*-methyl-		3669	
644.		Galactitol, 3-*O*-methyl-		3669	
645.		Galactitol, 2,3,4,6-tetra-*O*-methyl-		3669	
646.		Galactitol, 2,3,4-tri-*O*-methyl-		3669	
647.		Galactitol, 2,3,6-tri-*O*-methyl-		3669	
648.		Galactitol, 2,4,6-tri-*O*-methyl-		3669	
649.	9036-66-2	*D*-Galacto-*L*-arabinan	4249, 4751a	429b, 2939, 3797, 4249	
650.	33818-21-2	α-*D*-Galactofuranose, 1,6-anhydro-	2321, 4249, 5811b		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

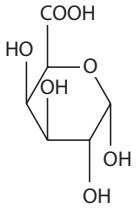
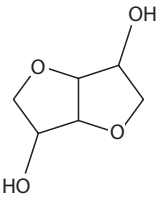
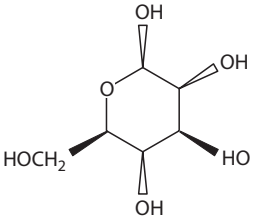
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
651.	107389-81-1	Galactoglucomannan		5811b	
652.	9040-29-3	*D*-Galacto-*D*-gluco-*D*-mannan		429b, 4249, 4583	
653.	644-76-8	β-*D*-Galactopyranose, 1,6-anhydro-	2321, 4249, 5811b		
654.	26656-33-7	*D*-Galactopyranuronic acid, homopolymer		4249	
655.	6118-79-2	2-*O*-α-*D*-Galactopyranuronosyl-*L*-mannose, 6-deoxy-		5811, 5811b	
656.	1948-54-5	Galactose, 2-amino-2-deoxy-		3797, 3974a, 4249	
657.	35381-83-0	Galactose, diether with 1,2,3-propanetriol (1:2)		908, 4249, 4640, 8A09	
658.	59-23-4	*D*-Galactose	3266, 4249, 5580	120, 158, 344a, 933, 1053, 1263, 2070, 2270, 2338, 2939, 3075, 3266, 3555, 3797, 3973, 3974a, 4249, 4411, 5079, 5114, 5768, 5785, 5811b	
659.	7535-00-4	*D*-Galactose, 2-amino-2-deoxy- {galactosamine}		3973, 4224, 4226, 4422, 5811b	
660.	1949-89-9	*D*-Galactose, 2-deoxy-		3075	
661.	97234-09-8	*D*-Galactoside, [(1-oxohexadecatrienyl)oxy][(1-oxooctadecatrienyl) oxy]propyl, (all-*Z*)-		4249	
662.	97234-10-1	*D*-Galactoside, [(1-oxohexadecyl)oxy][(1-oxooctadecatrienyl)oxy] propyl, (*Z*,*Z*,*Z*)-		4249	
663.	97276-55-6	*D*-Galactoside, [(1-oxooctadecadienyl)oxy] [(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249	
664.	97232-94-5	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl *O*-*D*-galactosyl-, (all-*Z*)-		4249, 4570	
665.	97170-15-5	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl, (all-*Z*)-		4249, 4570	
666.	97233-43-7	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl *O*-*D*-galactosyl-, (all-*Z*)-		4249, 4570	
667.	97170-14-4	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		4249, 4570	
668.	97275-71-3	*D*-Galactoside, 2,3-dihydroxypropyl, 2′(or 3′)-hexadecanoate 3′(or 2′)-octadecadienoate, (*Z*,*Z*)-		4249	
669.	100092-00-0	Galactoxyloglucan {amyloid}		5811, 5811b	
670.	14982-50-4	Galacturonic acid 	2321, 4249	120, 344a, 722, 2079, 2939, 3107, 3555, 3797, 3973, 3974a, 4249, 5079, 5114, 5189, 5306	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
671.	25990-10-7	Galacturonic acid, homopolymer		1051a, 1971, 4249, 5079, 5114	
672.	685-73-4	*D*-Galacturonic acid	2321, 4249	344a, 722, 2070, 2270, 2939, 3797, 4249, 5811b	
673.	34150-36-2	*D*-Galacturonic acid, anhydro-		4249, 4933	
674.	25249-06-3	*D*-Galacturonic acid, homopolymer		1051a, 1334e, 1971, 4249	
675.	554-91-6	Gentiobiose		120, 2079, 2270, 3075, 3667, 5079, 5288	
676.	652-67-5	*D*-Glucitol, 1,4:3,6-dianhydro- 	5811, 5811a, 5811b		
677.	7425-74-3	β-*D*-Glucofuranose, 1,6-anhydro-	1883, 2939, 4249, 5811b	429b, 5811b	2466, 3402, 3405, 4249
678.	4451-30-3	β-*D*-Glucofuranose, 1,5:3,6-dianhydro-	5811, 5811a, 5811b	5811, 5811a, 5811b	
679.	66537-22-2	Glucometasaccharinic acid, γ-lactone	2493, 5811b	4249	
680.	492-62-6	α-*D*-Glucopyranose 		2079, 3667, 4249	
681.	492-61-5	β-*D*-Glucopyranose	5811b	2079, 3667, 4249	
682.		α-*D*-Glucopyranose, 1-acetate 2,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
683.	28977-67-5	β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylvalerate) β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylpentanoate)	1352, 1373, 3251, 3278, 3286, 3302, 4249, 5811b	1352, 1373, 2338, 3185, 3215, 3473, 3535, 3542, 3560, 3561, 3607, 4249, 4575, 4990	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

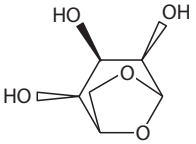
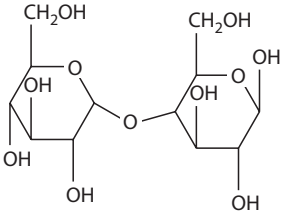
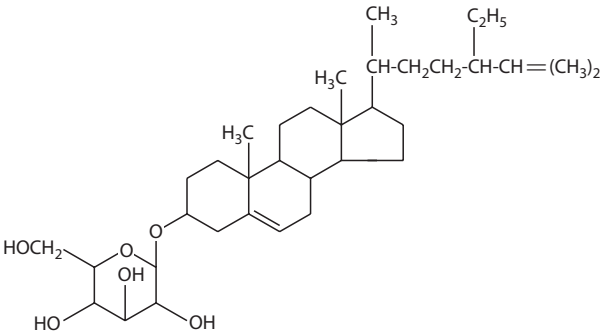
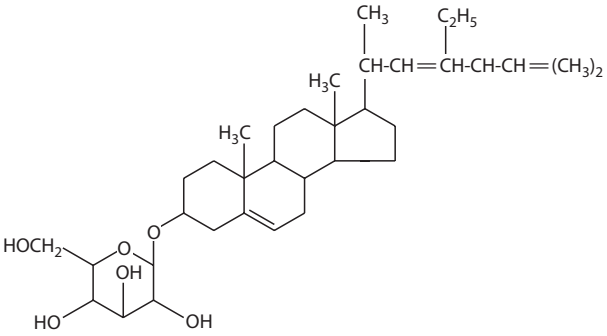
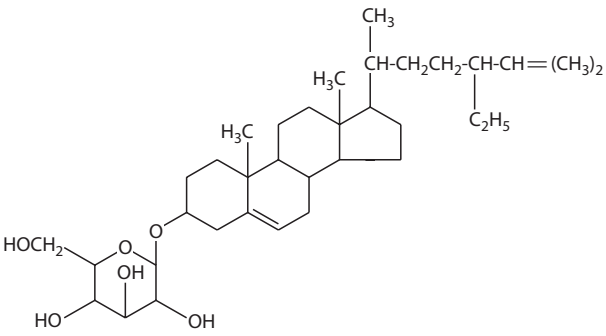
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
684.	60517-74-0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)		5811b	
685.	25545-13-5	*D*-Glucopyranose, 4-(4-hydroxybenzoate)		4249, 4915	
686.	23445-11-6	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)		4249, 4915	
687.	41682-52-4	β-*D*-Glucopyranose, 1-(3-phenyl-2-propenoate)		429b, 4249, 4915	
688.	59-56-3	α-*D*-Glucopyranose, 1-(dihydrogen phosphate)		120	
689.	498-07-7	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan} 	277, 568b, 1089a, 1351, 1354, 1364, 1371, 1375a, 1377, 1378, 1586, 1887a, 1971, 2170, 2270, 2493, 2524a, 2601a, 2607, 2761, 2762, 2765–2767, 2777, 2850, 2939, 3302, 3308, 3462, 3553, 3557, 3653, 3797, 3963, 4199, 4200, 4202, 4249, 5079, 5811b	568b, 2607, 3430, 3973, 4249, 5079, 5811b	1354, 1375a, 1377, 1378, 3402, 3405, 4249
690.	61891-55-2	β-*D*-Glucopyranose, 1,6-anhydro-, monoacetate	568b, 3553, 4249, 5811b		
691.	10139-18-1	α-*D*-Glucopyranose, 1,6-bis(dihydrogen phosphate)		429b	
692.	21056-52-0	β-*D*-Glucopyranose, 1-benzoate		4249, 4915	
693.	69-79-4 4482-75-1 9005-84-9	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin; α-maltose} 		120, 429b, 1063–1066, 1068–1074, 1835b, 2079, 2270, 2283, 3018, 3075, 3555, 3667, 3974a, 4249, 4411, 4841a, 5079, 5189, 5344, 5449, 5768, 5785, 5819	
694.		α-*D*-Glucopyranose, 1,2,3,4,5-penta((+)-3-methylbutanoate)		3556	
695.	133-99-3	β-*D*-Glucopyranose, 4-*O*- β-*D*-glucopyranosyl- {β-maltose}		429b, 2079, 3555, 3667, 3974a, 4249-	
696.	64461-84-3	β-*D*-Glucopyranose, 6-(3-phenyl-2-propenoate)		3367a, 4249, 4915	
697.		α-*D*-Glucopyranose, 1,3,4,6-tetrakis((+)-3-methylbutanoate)		3556	
698.		α-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
699.		β-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		3556	
700.	7724-09-6	β-*D*-Glucopyranoside, (2-hydroxyphenyl)methyl-		4249, 4790	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
701.	7073-61-2	β-*D*-Glucopyranoside, (3β)-cholest-5-en-3-yl- {cholesteryl glucoside}	648, 1434, 4249, 4534	390, 4249	
702.	32214-82-7	β-*D*-Glucopyranoside, (3β)-ergost-5-en-3-yl- {campesteryl glucoside}	648, 2018, 2019, 2079, 3308, 3667, 4249	2018, 2019, 4249, 5777	
703.		β-*D*-Glucopyranoside, 3-hexen-1-yl- {3-hexen-1-yl glucoside; leaf acid glucoside}		740	
704.	474-58-8 20431-48-5	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl- {β-sitosteryl glucoside} 	648, 2018, 2019, 2939, 3296, 3302, 3308, 4249	1079, 2018, 2019, 2270, 2939, 3296, 3302, 3346, 3349, 4249	
705.	19716-26-8	β-*D*-Glucopyranoside, (3β,22E)-stigmasta-5,22-dien-3-yl- {stigmasteryl glucoside} 	648, 908, 2018, 2019, 2939, 3296, 3302, 3308, 4249, 4534	908, 2018, 2019, 3302, 3346, 3349, 4249	
706.	51064-38-1	β-*D*-Glucopyranoside, (3β,24S)-stigmast-5-en-3-yl- {γ-sitosteryl glucoside} 	2018	120, 2087, 3346, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

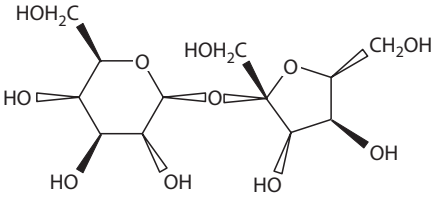
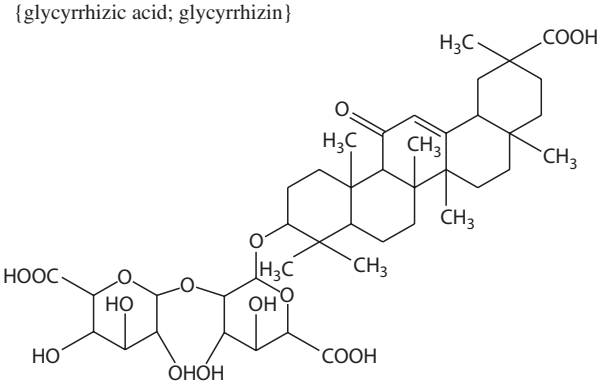
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
707.	57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose} 	1264, 1265, 1361, 4249, 5811b	71, 120, 172c, 248, 321b, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1264, 1265, 1289, 1361, 1933a, 1958, 1960, 1971, 2070, 2079, 2270, 2283, 2313a, 2337, 2532, 2818, 2911c, 2939, 2947c, 3059, 3075, 3266, 3370, 3398, 3409, 3449, 3461, 3462, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3973, 3974a, 3974b, 4249, 4411, 4990, 5079, 5108, 5109, 5126, 5189, 5449, 5562, 5679, 5692, 5748, 5768, 5811b, 5819, 5836, 5896	
708.	126-14-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate		1053, 3266	
709.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-		4990	
710.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-3′-acetyl-		4990	
711.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-4′-acetyl-		4990	
712.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-		4990	
713.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′-*O*-acetyl-		4990	
714.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-4′-*O*-acetyl-		4990	
715.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′,4′-*O*-diacetyl-		4990	
716.		α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-1′,3′,4′-*O*-triacetyl-		4990	
717.	470-55-3	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)-*O*-α-*D*-galactopyranosyl-(1→6)-{stachyose}		429b, 1971, 3797, 4249, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
718.	512-69-6	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)- {raffinose}		3075, 1971, 3797, 4249, 5768, 5811b	
719.	13101-54-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→4)- {erlose}		429b, 3667, 4249	
720.	25954-44-3	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-β-*D*-glucopyranosyl-(1→6)-		429b, 4249, 4460	
721.	98913-58-7	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 3-methylpentanoate		4249, 5811b	
722.	154063-13-5	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(2-methylbutanoate)		3606	
723.	97614-61-4	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(3-methylpentanoate)		3606, 5811b	
724.	106033-38-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(3-methylpentanoate), [2(S),3(S),4(S)]-		4249, 5811b	
725.	41055-68-9	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, labeled with ^{13}C		4249, 4720,	
726.	21291-36-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→6)-		429b, 3667, 4249	
727.	88848-61-7	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl 2-*O*-β-*D*-glucopyranosyl-, [1S-(1α,2β,3α,7β)]-		4249, 4716, 4717, 5811b	
728.	99499-89-5	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl *O*-6-deoxy-α-*L*-mannopyranosyl-(1→4)-*O*-β-*D*-glucopyranosyl-(1→4)-, [1S-(1α,2β,3α,7β)]-		4249, 5811b	
729.	138-52-3	β-*D*-Glucopyranoside, 2-(hydroxymethyl)phenyl-		4249, 4790	
730.	136448-99-2	β-*D*-Glucopyranoside, 2-[5-(acetyloxy)-1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl]-2-hydroxypropyl-, 2,3,4,6-tetraacetate, [2R-[2α(S*),5α,8β,8aα]]-		4249, 5811b	
731.	75039-16-6	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl-, mono(dihydrogen phosphate) (ester), (*E*)-		4249, 4813	
732.	62512-96-3	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)butyl-		4249	
733.	78081-83-1	β-*D*-Glucopyranoside, 3-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-1-methyl-2-propenyl-		4249, 4713	
734.	63648-83-9	α-*D*-Glucopyranoside, 3-*O*-acetyl-β-*D*-fructofuranosyl-		4249	
735.	470-57-5	α-*D*-Glucopyranoside, *O*-α-*D*-galactopyranosyl-(1→6)-β-*D*-fructofuranosyl {theanderose}		3667, 4249	
736.	1464-44-4	β-*D*-Glucopyranoside, phenyl-		689a, 2527, 4249	
737.	1405-86-3	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid; glycyrrhizin} 		174e, 242, 743, 1356, 1361, 1671, 2313a, 3390, 3555, 4623, 5019, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

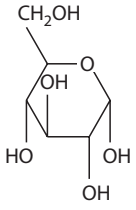
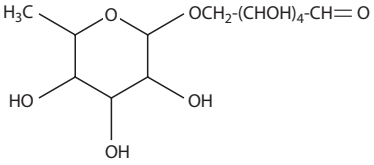
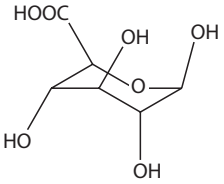
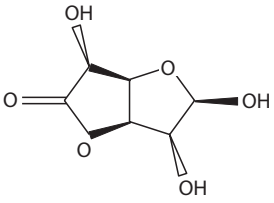
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
738.	53596-04-0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated; glycyrrhizin ammoniated}		172a, 174b, 1053, 3266	
739.	50-99-7 26655-34-5	α-*D*-Glucose 	1264, 1265, 1352, 1360, 1361, 1371, 1375a, 1883, 1944, 2145, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	72, 120, 172c, 174b, 248, 321b, 480, 727, 840, 924, 933, 1053, 1063–1066, 1068–1074, 1077b, 1128a, 1141, 1142, 1264, 1265, 1289, 1352, 1361, 1835b, 1835d, 1863, 1916, 1933a, 1971, 2070, 2079, 2270, 2283, 2313a, 2338, 2339b, 2381, 2394a, 2532, 2704a, 2850, 2911c, 2913, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3913, 3973, 3974a, 4103, 4159, 4249, 4275, 4411, 4999, 5079, 5108, 5109, 5126, 5189, 5255, 5344, 5449, 5562, 5655, 5656, 5698, 5748, 5768, 5774, 5811b, 5819, 5831	1360, 1375a
740.	110187-42-3	Glucose, labeled with ^{13}C {-Glucose-^{13}C}		4249, 4720	
741.	9050-36-6	α-*D*-Glucose, labeled with ^{14}C {α-*D*-Glucose-^{14}C}		1264, 1265, 5644, 25A30, 25A74	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
742.	3416-24-8	*D*-Glucose, 2-deoxy-, 2-amino- {glucosamine}		1032, 1063–1066, 1068–1074, 2445a, 3705, 3797, 3973, 3974a, 4224, 4226, 4249, 4422, 5540, 5811b	
743.	90-74-4	*D*-Glucose, 6-*O*-(6-deoxy-α-*L*-mannopyranosyl)- {rutinose} 		1971; 5777, 5811	
744.	1398-61-4	*D*-Glucose, β-(1,4)-2-acetamido-2-deoxy-		1102	
745.	28905-12-6	β-*D*-Glucose	1354, 1360, 1375a, 2761, 2762, 2765, 2766, 2777	3667, 4275	1354, 1360, 1375a
746.	37294-28-3	Glucoxylan		429b, 4248	
747.	66369-21-9	Glucuronoarabinoxylan		5811	
748.	576-37-4 6556-12-3	Glucuronic acid 	312, 4249	120, 2070, 2939, 3973, 4249, 4360a, 5079, 5478, 5706, 5785	
749.	6556-12-3	*D*-Glucuronic acid		5811	
750.	14984-34-0	*D*-Glucuronic acid, monosodium salt		5811b	
751.	28905-07-9	α-*D*-Glucuronic acid, methyl ester		4249	
752.	32449-92-6	*D*-Glucurono-3,6-lactone 	1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249		1360, 1375a
753.	62930-75-0	Glucuronomannan		2042a, 2618a	
754.	77272-02-7	Glucuronomannoarabinan		4249, 4428	
755.	37317-38-7	Glucuronoxylan		5811	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

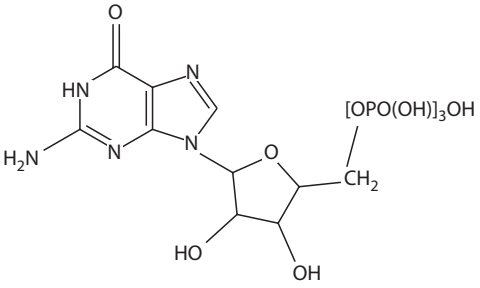
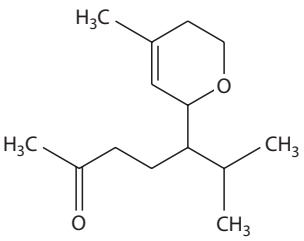
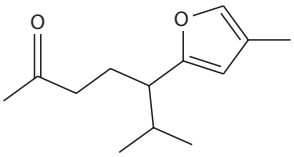
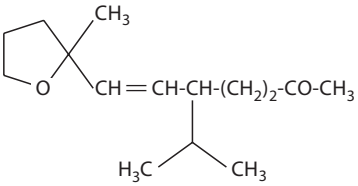
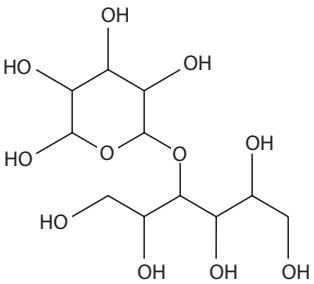
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
756.	4429-05-4	Glycine, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
757.	73360-07-3	Glycine, *N*-[2-(2-aminoethoxy)ethenyl]-		4249	
758.	86-01-1	Guanosine 5′-(tetrahydrogen triphosphate)		4249	86-01-1
					
759.	9034-32-6	Hemicellulose		120, 385, 385a, 842, 1838, 1887, 2056, 2154, 2283, 2850, 2939, 3059, 3372, 3665a, 3702, 3973, 4249, 5079, 5189, 5344, 5811b	
760.	63100-39-0	Hemicellulose A		120, 3973, 4249	
761.	63100-40-3	Hemicellulose B		120, 3973, 4249	
	65058-12-0	Hemicellulose C		3973, 4249, 4805	
762.		4,6-Heptadien-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methylfuranyl)-		3547, 4249	
763.	98188-02-4	Heptanoic acid, 7-(2-furanyl)-, methyl ester		2917a	
764.	52812-43-8	2-Heptanone, 5-[3-(1-hydroxy-1-methylethyl)oxiranyl]-6-methyl-	2545	940, 942, 4249	
765.		2-Heptanone, 5-(2,3-dihydro-4-methyl-6-pyranyl)-6-methyl-		943, 944	
766.		2-Heptanone, 5-(5,6-dihydro-4-methyl-2-pyranyl)-6-methyl-		943, 944	
					
767.	121269-00-9	2-Heptanone, 6-(5-methyl-2-furanyl)-		941, 1256, 3547, 4249, 4780, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
768.	41059-93-2	2-Heptanone, 6-methyl-5-(4-methyl-2-furanyl)- {solanofuran} 		943, 1087, 1662, 3547, 5811b	
769.	34098-52-7	*D*-xylo-Hept-2-enaric acid, 2,6-anhydro-3-deoxy- {2*H*-pyran-2,4-dicarboxylic acid, 3,4-dihydro-3,4-dihydroxy-}		4249	
770.	57782-61-3	6-Hepten-2-ol, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)-		943, 944, 1156, 4090, 4249, 5811b	
771.	152209-54-6	3-Hepten-2-one, 5-(1-methylethyl)-7-[2-methyl-3-(3-methyl-5-oxo-3-hexenyl)oxiranyl]-, [2S-[2α(3E,5R*),3β(*E*)]]-		4249	
772.	57782-60-2	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)- 		568b, 944, 3545, 3547, 4098a, 4249, 5811b	
773.	104669-35-4	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-4-hydroxy-2-methyl-2-furanyl)-		232, 943, 944, 1156, 3852, 4090, 4249, 4780, 5811b	
774.	160115-55-9	6-Hepten-2-one, 7-[4-(acetyloxy)tetrahydro-5-hydroxy-2-methyl-2-furanyl]-5-(1-methylethyl)-		4249	
775.	117210-48-7	6-Hepten-2-one,7-[tetrahydro-2-methyl-5-(1-methylethyl)-2-furanyl]-		4249, 5811b	
776.	90-65-3	2,5-Hexadienoic acid, 3-methoxy-5-methyl-4-oxo-	3760, 4249	3760, 4249, 5811b	
777.		Hexane, hexahydroxy-, 2,6-di-*O*-methyl-		3669	
778.		Hexane, hexahydroxy-, 2,3,6-tri-*O*-methyl-		3669	
779.		Hexane, hexahydroxy-, 2,3,4,6-tetra-*O*-methyl-		3669	
780.	585-88-6	Hexane, hexahydroxy-, 4-*O*-β-*D*-glucopyranosyl- {maltitol; 4-*O*-β-*D*-glucopyranosyl-*D*-glucitol} 		3163	
781.	14360-50-0	1-Hexanone, 1-(2-furanyl)-	2767, 2769, 4249		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

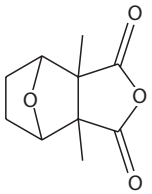
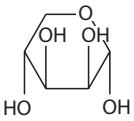
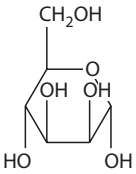
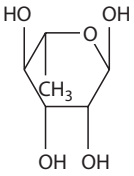
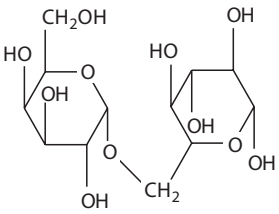
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
782.	72692-69-4	1*H*-Inden-1-one, 2,3-dihydro(methoxymethyl)-	1586, 2767, 3557, 4249		
783.	71608-14-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]octadecyl hydrogen phosphate], disodium salt		429b, 1838, 4249	
784.	71608-17-8	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-1-[(2-hydroxy-1-oxopentacosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
785.	71608-15-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
786.	71608-16-7	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
787.	71608-19-0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
788.	71608-20-3	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
789.	71608-21-4	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
790.	71608-22-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxopentacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
791.	71608-23-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxohexacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
792.	89194-80-9	myo-Inositol, *O*-*D*-glucopyranosyl-		3667, 4249	
793.	49741-70-0	*D*-myo-Inositol, *O*-*D*-glucopyranosyl-		429b, 3667, 4249	
794.	56-25-7	1,3-Isobenzofurandione, 3a,7a-dimethyl-4,7-epoxy-hexahydro {cantharidin} 		2917a	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
795.	61010-32-0	Isoquinoline, 1-[(4-methoxy-3-nitrophenyl)methyl]-, mononitrate		4249	
796.	63-42-3	Lactose		933, 1361, 1835b, 3075, 5079, 5811b	
797.	1114-34-7	Lyxose 	5580	3075	
798.	31103-86-3	Mannose 	1587, 2761, 2762, 2765, 2766, 2777, 3266, 3555, 4249, 5580	1053, 2070, 3266, 3555, 3797, 3973, 3974a, 4249, 5768	
799.	3458-28-4	*D*-Mannose {seminose}	1360, 1375a, 2765, 2766, 4249	3797, 4249, 5811b	1360, 1375a
800.	14307-02-9	*D*-Mannose, 2-amino-2-deoxy-		1063–1066, 1068–1074, 1370, 4249, 4422, 5811b	
801.	3615-41-6	*L*-Mannose, 6-deoxy- {α-rhamnose} 	3555, 5580	71, 120, 158, 344a, 2070, 2079, 2270, 2338, 2704a, 2939, 3075, 3555, 3655b, 3797, 3973, 3974a, 4249, 5079, 5698, 5768, 5811b, 5831	
802.	585-99-9	Melibiose 		3075	
803.	115-10-6	Methane, oxybis- {dimethyl ether}	2950, 4249	984, 4249	
804.	19870-75-8	1*H*-3a,7-Methanoazulene, 6-methoxy-octahydro-3,6,8,8-tetramethyl- {cedryl methyl ether}		568b, 4249	
805.	105300-09-2	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 1a-[(β-*D*-glucopyranosyloxy)methyl]octahydro-5,7b-dimethyl-, [1aR-(1aa,2b,4ab,5a,7aa,7ba)]-		4249, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

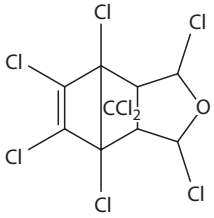
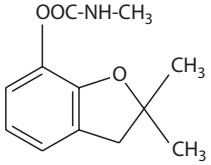
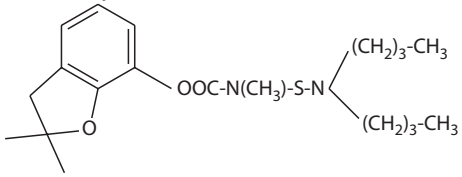
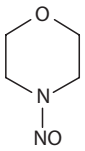
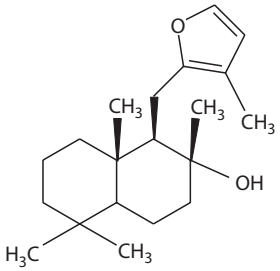
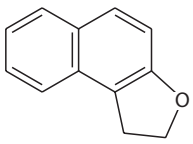
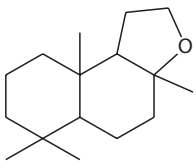
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
806.	125537-96-4	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 3-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,3β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
807.	125537-95-3	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 4-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
808.	105300-10-5	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 5-[(β-*D*-glucopyranosyloxy)methyl]octahydro-1a,7b-dimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		4249, 4717, 5811b	
809.	88848-60-6	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 6-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,6β,7aα,7bα)]-		4249, 4717, 5811b	
810.	1024-57-3	2,5-Methano-2*H*-indeno[1,2-*b*]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)- {Heptachlor® epoxide}	606	1219, 1219a, 1219b, 3188a, 3633, 3770	
811.	297-78-9	4,7-Methanoisobenzofuran, 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro- {Telodrin®} 	937, 1457, 1458, 4249, 21A19	1457, 1458, 3797, 4249, 21A19	
812.	1563-66-2	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester: see 7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate {Furadan®; Carbofuran®} 	1553, 21A19	1280, 1553, 2650b, 3481, 3633, 3973, 4249, 4271a, 5811b, 21A19	
813.	55285-14-8	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl [(di-*N*-butylamino)thio] ester {Carbosulfan®} 		3633	
814.	16709-30-1	Methylcarbamic acid, 2,2-dimethyl-3(2*H*)-oxobenzofuran-7-yl ester		5811, 5811b	
815.	110-91-8	Morpholine		568b, 3973, 4249	
816.	110488-70-5	Morpholine, 3-(3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl)- {Dimethomorph®; Acrobat®}		2892a, 3633	
817.	147688-58-2	Morpholine, 2,2-dimethyl-		3951	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
818.	59-89-2	Morpholine, 4-nitroso- {NMOR} 	31, 126a, 203, 471, 478, 485, 510, 746c, 1058, 1059, 1727, 1842, 2442, 2443, 3255, 3257, 4010, 4011, 5811b	468, 478, 498, 510, 1217, 1727, 1740, 1741, 1773, 3256, 3265, 3300, 3973, 3974b, 4010, 4011, 4249, 5001, 5496, 5811b	
819.	70699-77-3	3-Morpholinepropanamide, 2-oxo-6-(1,2,3,4-tetrahydroxybutyl)-, [3S-[3α,6α(1R*,2S*,3S*)]]-		1863a	
820.	93-18-5	Naphthalene, 2-ethoxy- {β-naphthyl ethyl ether}	5811b	1053, 1248, 3266, 4249, 5811b	
821.	2216-69-5	Naphthalene, 1-methoxy-	5811, 5811a, 5811b		
822.	93-04-9	Naphthalene, 2-methoxy-	5811b	1256, 3547, 4249, 5811b	
823.	62121-32-8	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-[(3-methyl-2-furanyl)methyl]-, [1R-(1α,2β,4aβ,8aα)]- 		1156, 4090, 4101	
824.	64083-16-5	Naphthofuran	3514, 3619, 3620, 5811, 5811a, 5811b		
825.		Naphthofuran, dimethyl-	3619, 3620		
826.		Naphthofuran, methyl-	3619, 3620		
827.	234-03-7	Naphtho[1,2-*b*]furan	3619, 4249		
828.	71607-62-0	Naphtho[1,2-*b*]furan, dimethyl-	3619, 4249		
829.	25826-63-5	Naphtho[1,2-*b*]furan, 2-methyl-	3615, 4249		
830.	232-95-1	Naphtho[2,1-*b*]furan 	3514, 3619, 3758, 3759, 4249, 5811b		
831.	3738-00-9	Naphthalene, decahydro-1-ethoxido-2,5,5,8a-tetramethyl- {amberlyn, ambroxide *DL*} 		174b, 3266	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

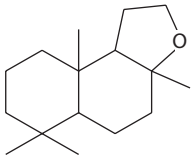
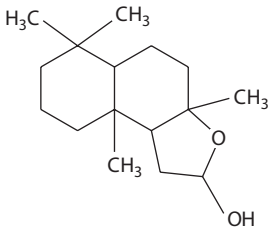
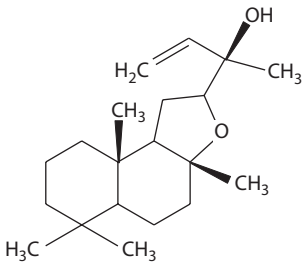
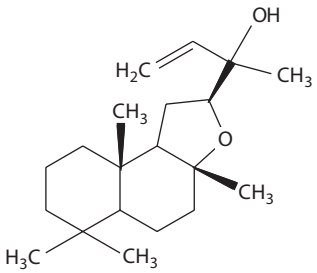
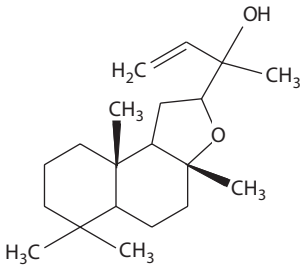
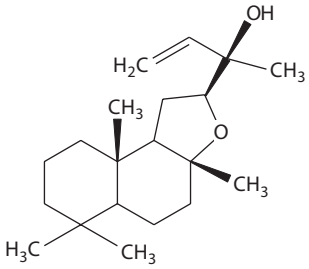
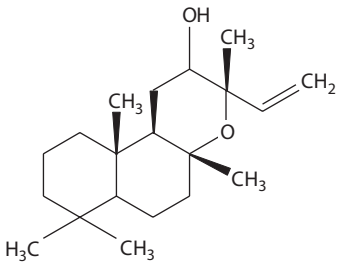
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
832.	6790-58-5 65588-69-4	Naphtho[2,1-*b*]furan, dodecahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {ambroxyl} 		568b, 2338, 3534, 3547, 3560, 3561, 3905, 4249, 5811b	
833.	52811-62-8	Naphtho[2,1-*b*]furan-2-ol, dodecahydro-3a,6,6,9a-tetramethyl- {sclaral} 	5811b	2338, 3547	
834.	30450-17-0	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aS-(3aα,5aα,9aβ,9bα)]-		4249	
835.	56682-25-8	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2R-[2α(R*), 3aβ,5aα,9aβ,9bα]]- 		6, 7, 1156, 4090	
836.	56711-38-7	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2R-[2α(S*),3aβ,5aα,9aβ,9bα]]- 		6, 7, 1156, 2386, 4086, 4090, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
837.	56711-39-8	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(S*), 3aα,5aβ,9aα,9bβ]]-		6, 7, 1156, 4086, 4090, 4249	
					
838.	56711-40-1	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(R*),3aα, 5aβ,9aα,9bβ]]-		6, 7, 1156, 4086, 4090, 4249	
					
839.	5153-92-4	1*H*-Naphtho[2,1-*b*]pyran, 4a,5,6,6a,7,8,9,10,10a,10b-decahydro-3,4a,7,7,10a-pentamethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]-	5811b	947, 4249, 5811b	
840.	6252-26-2	1*H*-Naphtho[2,1-*b*]pyran, dodecahydro-3,4a,7,7,10a-pentamethyl-		947, 3560, 3561, 4249	
841.	596-84-9	1*H*-Naphtho[2,1-*b*]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aβ,6aα,10aβ,10bα)]-		1157, 4249	
842.	59170-14-8	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3β,4aβ,6aα,10aβ,10bα)]- {labd-14-ene, 8,13-epoxy-12α-hydroxy-; 12α-hydroxy-13-epimanoyl oxide}	323, 568b, 800, 3251, 3281, 3286, 3971, 5811b	6, 568b, 1156, 1298, 2308, 2386, 3971, 3974a, 4090, 4101	
					

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

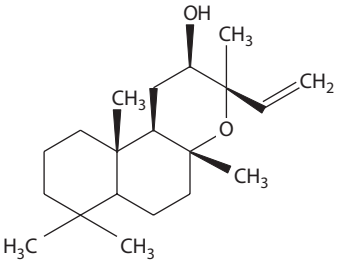
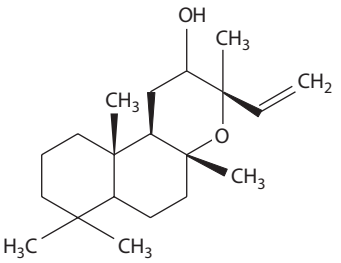
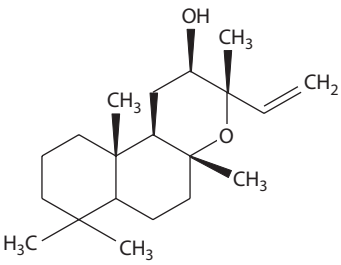
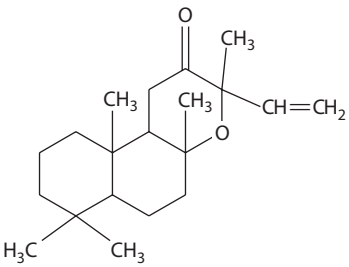
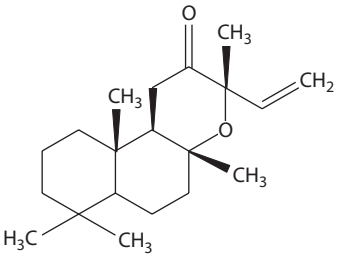
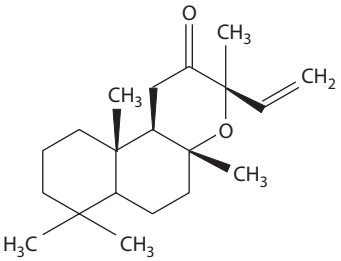
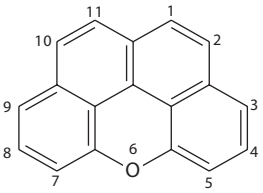
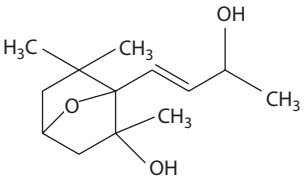
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
843.	64681-69-2	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2R-(2α,3α,4aα,6aβ,10aα,10bβ)]- 		6, 1156, 2308, 2565, 4090, 4101, 4249	
844.	64681-70-5	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3α,4aβ,6aα,10aβ,10bα)]- 		6, 1156, 2565, 4090, 4101, 4249	
845.	67528-84-1	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2R-(2α,3β,4aα,6aβ,10aα,10bβ)]- 		6, 1156, 4090, 4101	
846.	38017-17-3	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-{8,13-epoxylabd-14-en-12-one} 		5811, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
847.	37551-73-8	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]-		11, 1156, 2308, 4090, 4249	
					
848.	37551-74-9	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aα,6aβ,10aα,10bβ)]-		11, 1156, 4090, 4249, 5811b	
					
849.	68985-12-6	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-		2094, 4249	
850.	191-37-7	Naphtho[2,1,8,7-*klmn*]xanthene	2939, 3302, 3999, 4020, 4249		
					
851.	58002-07-6	2-Nonanone, 6,7-epoxy-8-hydroxy-5-(1-methylethyl)-		2917a	
852.		5-Nonanone, 2,8-dimethyl-7,8-epoxy-		3545	
853.	124354-88-7	Octen-4-one, 2,6-dimethyl-, monoepoxy derivative		4249, 5811b	
854.	38284-11-6	7-Oxabicyclo[4.1.0]heptane-2,5-dione, 1,3,3-trimethyl-		1157, 4249, 5811b	
855.	73051-73-7	7-Oxabicyclo[2.2.1]heptan-2-ol,1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-		1, 234, 1156, 4090, 4249	
					
856.	102518-80-9	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-[1R[1AL]]		5811, 5811b	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

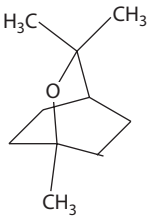
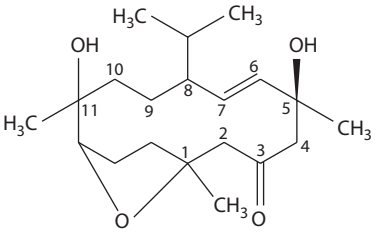
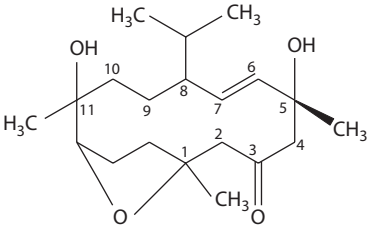
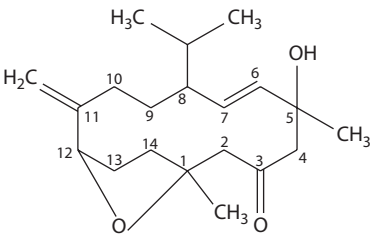
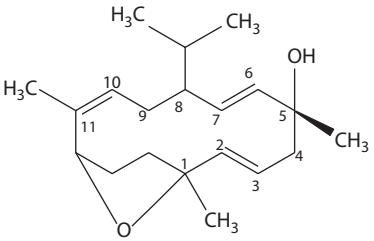
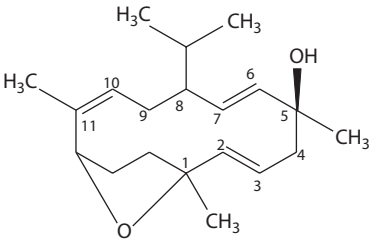
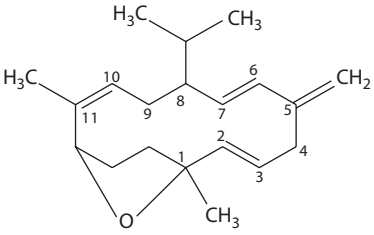
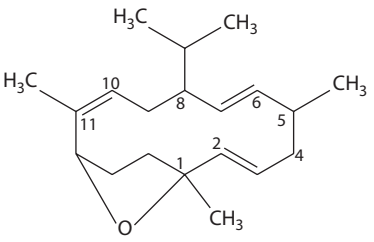
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
857.	72777-88-9	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-		234, 1156, 1251, 4090, 5811b	
858.	10276-21-8	7-Oxabicyclo[4.1.0]heptan-2-one, 4,4,6-trimethyl-	568b, 4249		
859.	17024-44-1	6-Oxabicyclo[3.1.0]hexan-4-one, 1-methyl-	568b, 4249		
860.	470-82-6	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- {eucalyptol; 1,8-cineole} 	568b, 3193, 3266, 3302, 4249	172a, 174b, 568b, 1053, 1247, 1254, 1256, 1662, 2339a, 2389, 2544, 3266, 3370, 4249, 5811b	
861.		6-Oxabicyclo[3.2.1]octan-7-one, 6-hydroxy-3-methyl-	568b, 4249		
862.	665-27-0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy-, [1S-(exo,exo)]-	4249, 5811b		
863.	98064-77-8	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,11R*)]- 		4089, 4091, 4249, 5811b	
864.	98167-33-0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,11S*,12S*)]- 		4089, 4098, 4249	
865.	98064-76-7	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5-hydroxy-1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*] 		943, 3352, 4089, 4091, 4098, 4249, 5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
866.	121927-14-8	15-Oxabicyclo[10.2.1]pentadec-6-ene-2,3,5-triol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2S*,3R*,5S*,6E,8*)]		4249	
867.	57760-48-2	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2E,5S*,6E,8S*,10E,12S*)]- 	568b, 809, 909, 2767, 3285, 3361, 4089, 4249, 4570a	235, 568b, 943, 3352, 3361, 3547, 3804, 3973, 3974a, 4089, 4249	
868.	60047-18-9	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)- 	2767, 3361, 4089, 4249, 4570a	9, 236, 1149, 1149a, 2386, 2389, 3352, 3361, 3547, 3804, 3973, 3974a, 4089, 4249, 5811b	
869.	60026-18-8	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,11-dimethyl-5-methylene-8-(1-methylethyl)-	4249	4249	
870.	69010-30-6	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,11-dimethyl-5-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,6*E*,8S*,10*Z*,12S*)]- 	568b, 2767, 3557, 4249	568b, 2386, 2389, 2544, 3547, 4089, 4249	
871.		15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,5,11-trimethyl-8-(1-methylethyl)- 	1586	3547	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

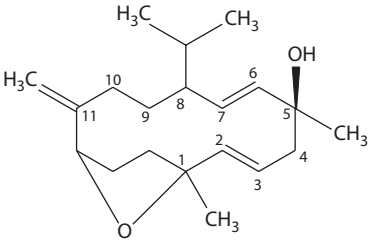
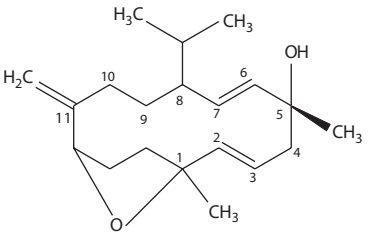
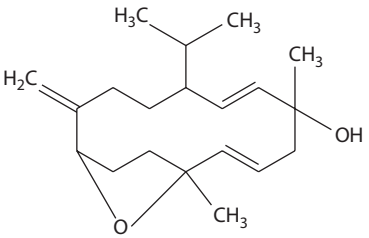
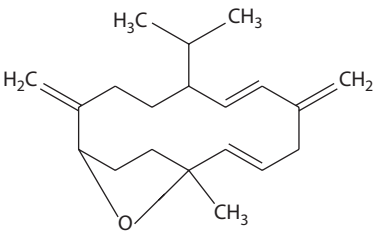
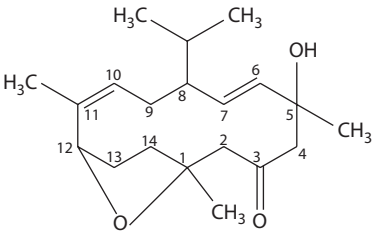
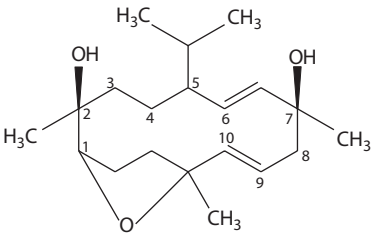
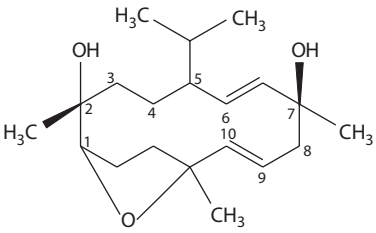
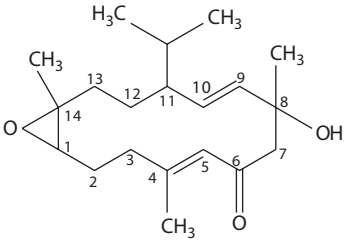
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
872.	57688-98-9	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8R*,10S*)]- 	327, 1063–1066, 1068–1074, 1586, 2726, 2767, 3361, 4249, 5811b	9, 235, 327, 404, 671, 1591, 2389, 2544, 3361, 3973, 3974a, 4089, 5811b	
873.	57760-47-1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-,[1R-(1R*,2*E*,5R*,6*E*,8S*,12S*)]- 	1063–1066, 1068–1074, 1352, 3361, 4249, 5811b	9, 235, 1352, 1591, 2389, 3222, 3361, 3543, 3545, 3547, 4089, 4249, 5811b	
874.	60047-16-7	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)- 	1063–1066, 1068–1074, 1352, 3361	9, 235, 671, 1352, 1591, 3222, 3547	
875.	102977-88-8	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 5-methyl-11-methylene-8-(1-methylethyl)-		4159b, 5811b	
876.	72693-05-1	15-Oxabicyclo[10.2.1]pentadeca-2,6-diene, 1-methyl-5,11-bis(methylene)-8-(1-methylethyl)- 	4249	9, 671, 2767, 3547	
877.	58947-96-9	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-2-one, 8-hydroxy-8,12-dimethyl-5-(1-methylethyl)-		4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
878.	98064-75-6	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-3-one, 5-hydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6E,8S*,10E)]- 		3219, 3971, 4089, 4091, 5811b	
879.	66890-76-4	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol, 2,8,12-trimethyl-5-(1-methylethyl)-, [1S-(1R*,2S*,5R*,6E,8R*,10E,12S*)]- 		235, 327, 404, 1156, 3219, 3547, 3971, 4089, 4090, 4249	
880.	66966-04-9	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol, 2,8,12-trimethyl-5-(1-methylethyl)-, [1S-(1R*,2R*,5R*,6E,8R*,10E,12S*)]- 		235, 404, 1156, 3219, 3547, 3971, 4084, 4089, 4090, 4249, 4573	
881.	119613-99-9	15-Oxabicyclo[12.1.0]pentadec-9-en-5-one, 11,13-dihydroxy-1,11-dimethyl-8-(1-methylethyl)-, [1S-(1R*,8R*,9E,11R*,13S*,14S*)]-		4249, 5811b	
882.	98064-73-4	15-Oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one, 8-hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4E,8R*,9E,11R*)]- 		9, 12, 235, 236, 1156, 3971, 4089–4091, 5811b	
883.	152209-53-5	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 11-(1-hydroxy-1-methylethyl)-4,8,14-trimethyl-, [1S-(1R*,4E,6S*,8R*,9E,11S*,14R*)]-		4249	
884.	70969-36-7	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol,4,8,14-trimethyl-11-(1-methylethyl)-		4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

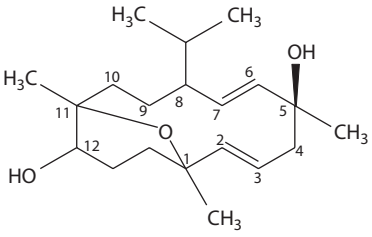
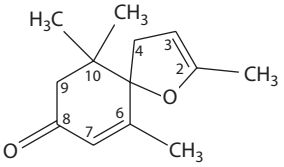
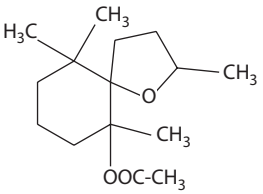
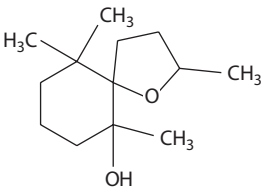
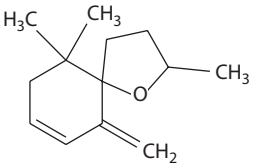
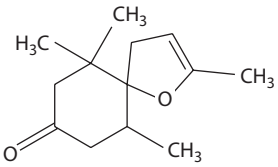
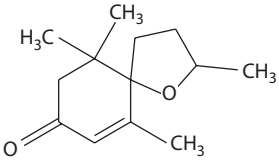
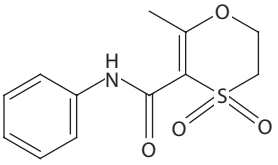
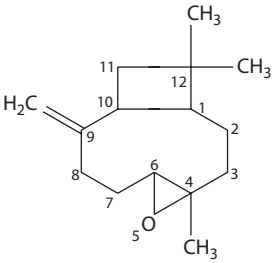
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
885.	75281-93-5	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4E,6S*,8S*,9E,11R*,14R*)]-		4100, 4249	
886.	75281-99-1	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4E,6S*,8R*,9E,11R*,14R*)]-		227, 236, 4249, 5811b	
887.	75282-00-7	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1R-(1R*,4E,6R*,8S*,9E,11S*,14R*)]-		4089, 4249, 5811b	
888.	62498-80-0	15-Oxabicyclo[9.3.1]pentadeca-2,6-diene-5,12-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2E,5S*,6E,8R*,11S*,12S*)]- 		12, 4089, 4249	
889.	80722-28-7	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl- 		4249, 5811b	
890.	85248-56-2	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-, (*S*)- {8,9-dehydrotheaspirone}		5811, 5811b	
891.	57893-27-3	1-Oxaspiro[4.5]decane, 6-acetoxy-2,6,10,10-tetramethyl- {6-acetoxydihydrotheaspirane} 		1053, 3266	
892.	65620-50-0	1-Oxaspiro[4.5]decane, 6-hydroxy-2,6,10,10-tetramethyl- {6-hydroxydihydrotheaspirane} 		1053, 3266	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
893.	65416-59-3	1-Oxaspiro[4.5]dec-7-ene, 6-methylene-2,10,10-trimethyl- {vitispirane} 		2339a	
894.	38713-26-7	1-Oxaspiro[4.5]dec-2-en-8-one, 2,6,6,10-tetramethyl- 		937, 4249	
895.	19377-59-4	1-Oxaspiro[4.5]dec-6-en-8-one, 2,6,10,10-tetramethyl- 		937, 4249	
896.	5259-88-1	1,4-Oxathiin-3-carboxamide 4,4-dioxide, 5,6-dihydro-2-methyl-*N*-phenyl- {Oxycarboxin®} 		2650b	
897.	1139-30-6	5-Oxatricyclo[8.2.0.04,6]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- {β-caryophyllene oxide} 		172a, 174b, 568b, 1053, 1156, 1157, 1662, 3266, 4090, 4249, 5811b	
898.	75-21-8	Oxirane {ethylene oxide}	126a, 333, 1037b, 1325, 1740, 1741, 1743, 1744, 3265, 3300, 3714, 3882, 4249, 4612, 4998, 5508, 5512, 5811b, 5869a		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

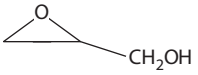
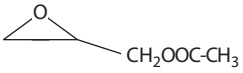
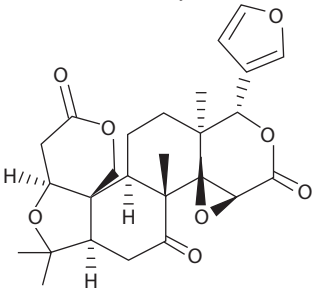
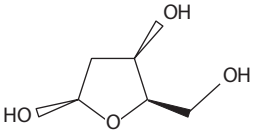
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
899.	106-89-8	Oxirane, (chloromethyl)-		642a, 4249, 4795	
900.	558-30-5	Oxirane, 2,2-dimethyl- {isobutylene oxide}	5770		
901.	7200-26-2	Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-, (all-*E*)-	4249, 4936		
902.	3234-28-4	Oxirane, dodecyl- {tetradecane, 1,2-epoxy}-	5811, 5811a, 5811b		
903.	75-56-9	Oxirane, methyl- {propylene oxide}	126a, 968, 1037b, 1325, 1743, 1744, 2009, 2825, 3265, 3300, 4998, 5512, 5869a		
904.	96-09-3	Oxirane, phenyl- {phenylethylene oxide}	5811b	429b, 568b, 4249, 5811b	
905.	77341-24-3	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-		5811, 5811b	
906.	77288-97-2	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-, [2α(αS*,δR*),3α]-		4249, 4948	
907.	77288-94-9	Oxiranebutanol, 3-(1-hydroxyethyl)-α-methyl-δ-(1-methylethyl)-		4249, 4948, 5811b	
908.	77-83-8	Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester {ethyl methylphenylglycidate}		174b, 3266	
909.	61892-62-4	2,3-Oxiranedimethanol, monopropanoate	568b, 3553, 4249, 5811b		
910.	556-52-5	Oxiranemethanol {glycidol} 	568b, 3553, 4249, 5811b		
911.	6387-89-9	Oxiranemethanol, acetate {glycidyl acetate} 		568b, 2917a, 4249	
912.	51297-34-8	Oxiranemethanol, 3-(1-ethyl-2-methylpropyl)-α,α-dimethyl-		1660, 4249, 5811b	
913.	1180-71-8	11*H*,13*H*-Oxireno[*d*]pyrano[4′,3′:3,3a]isobenzofuro[5,4-*f*][2]benzopyran-4,6,13(2*H*,5a*H*)-trione,8-(3-furyl)decahydro-2,2,4a,8a-tetramethyl- {limonin} 	5811, 5811a, 5811b		
914.	52786-29-5	1,4-Pentanedione, 1-(2-furanyl)-	568b, 2570, 3553, 4249, 5811b		
915.	60026-13-3	4-Penten-2-ol, 5-(tetrahydro-2-methyl-2-furanyl)-		2544, 4249	
916.	104-27-8	1-Penten-3-one, 1-(4-methoxyphenyl)-		1053, 3266	
917.		Pentose		1971, 5079, 5189, 5306, 5344, 5777	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
918.	533-67-5	*D*-erythro-Pentose, 2-deoxy- {deoxyribose} 		1351, 3079, 3973, 3974a, 4249, 5811b	
919.	61128-87-8	Phenanthrene, methoxy-	2570, 4249		
920.		Phenol, alkyldimethoxy-	1586, 2767, 3557		
921.	25155-26-4	Phenol, dimethoxy-	3753, 5034		
922.		Phenol, dimethoxy-4-ethenyl-	2767		
923.		Phenol, dimethyl-ethenyl-2-methoxy-	3746, 3747, 4249		
924.	1329-97-1	Phenol, dimethyl-methoxy-	1884, 3712, 4249		
925.		Phenol, dimethyl-2-methoxy-	1884, 3746, 3747, 4249		
926.		Phenol, dimethyl-4-methoxy-	1884, 3746, 3747		
927.		Phenol, ethenyl-2-methoxy-trimethyl-	3746, 3747, 4249		
928.	80652-16-0	Phenol, ethyl-methoxy-	1884, 4249		
929.		Phenol, ethyl-2-methoxy-	1884, 3746, 3747		
930.	26638-03-9	Phenol, methoxy-	152, 157, 2767, 4249		
931.	32391-38-1	Phenol, methoxymethyl-	1884, 3712	5811b	
932.	25013-16-5	Phenol, 2-(1,1-dimethylethyl)-4-methoxy-	568b, 4249		
933.	120550-69-8	Phenol, 2-ethenyl-6-methoxy-	90a, 3712, 5811b		
934.	94-86-0	Phenol, 2-ethoxy-5-propenyl- {5-propenylguaethol}		172a, 174b, 1053, 3266, 3370	
935.	13391-32-7	Phenol, 2-ethyl-4-methoxy-	1884, 2769, 3712, 5811, 5811b	5811, 5811b	
936.	90534-46-6	Phenol, 2-ethyl-6-methoxy-	90a, 3712, 5811b		
937.	90-05-1	Phenol, 2-methoxy- {guaiacol}	50, 376, 568b, 615, 723, 765, 789, 789a, 804, 830a, 851, 859, 966, 1063–1066, 1068–1074, 1089a, 1099, 1140, 1232, 1235, 1236, 1292, 1360, 1364, 1371, 1375, 1375a, 1375b, 1427, 1586, 1626, 1882, 1884, 1887a, 1906, 1928, 1963, 1995, 2042–2045, 2079, 2142, 2195, 2270, 2298, 2302, 2307, 2311, 2327c, 2379a,	120, 172a, 174a, 174b, 404, 568b, 937, 952, 1053, 1063–1066, 1068–1074, 1102, 1590a, 1825, 1876, 1877a, 1980, 2338, 2379a, 2611, 2862, 2917a, 2939, 3059, 3090, 3194, 3266, 3350, 3430,	50, 1360, 1375a, 2387, 3395

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Phenol, 2-methoxy- {guaiacol} (cont.)	2387, 2524a, 2545, 2577, 2598, 2601a, 2761, 2762, 2765–2767, 2777, 2858, 2939, 3059, 3090, 3255, 3266, 3302, 3308, 3394, 3410, 3453, 3457, 3462, 3555, 3557, 3559, 3719, 3746, 3747, 3764, 3767, 3797, 3876, 3952, 4248, 4249, 4313, 4317, 4319, 4414, 4796, 4999, 5011, 5034, 5079, 5811b	3543, 3547, 3555, 3560, 3561, 3797, 3973, 3974a, 4202, 4249, 5079, 5811b	
938.	60825-46-9	Phenol-$^{14}C_6$, 2-methoxy- {guaiacol-$^{14}C_6$}	2769, 2777, 4249		
939.		Phenol, 2-methoxymethyl-	1884, 3746, 3747		
940.	18102-31-3	Phenol, 2-methoxy-3-methyl-	90a, 3712, 5811b		
941.	53587-16-9	Phenol, 2-methoxy-4-(1-methylethyl)-	90a, 3712, 4249, 5811b		
942.	97-54-1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}	127, 568b, 1063–1066, 1068–1074,1375, 1375b, 1426, 1427, 1649, 2270, 2327c, 2543, 2545, 2761, 2762, 2767, 2773, 2777, 3251, 3280, 3300, 3302, 3462, 3557, 3712, 3797, 4005–4007, 4248, 4249, 5537, 5811b	120, 568b, 1063–1066, 1068–1074, 1091, 1221, 1626, 1649, 2079, 2270, 2283, 2917a, 2939, 3059, 3430, 3797, 3974a, 4249, 5079, 5180, 5811b	
943.	5932-68-3	Phenol, 2-methoxy-4-(1-propenyl)-, (*E*)- {*trans*-isoeugenol}	101, 3712, 3746, 3747, 5811b	1877a, 3430, 5811b	
944.	5912-86-7	Phenol, 2-methoxy-4-(1-propenyl)-, (*Z*)- {*cis*-isoeugenol}	101, 3712, 3746, 3747, 4249, 5811b	1877a, 3430, 5811b	
945.	97-53-0	Phenol, 2-methoxy-4-(2-propenyl)- {eugenol}	101, 127, 497, 568b, 1063–1066, 1068–1074, 1360, 1375, 1375a, 1375b, 1427, 1586, 1884, 2270, 2487, 2543, 2545, 2570, 2628, 2629, 2636, 2765–2767, 2773, 2939, 3251, 3280, 3300, 3302, 3308, 3453, 3557, 3712, 3746, 3747, 3797, 4005–4007, 4028, 4037, 4113, 4248, 4249, 5537, 5811b	120, 568b, 1102, 1221, 1626, 1825, 1854, 1876, 1877a, 2014, 2079, 2270, 2283, 2338, 2339, 2611, 2862, 2917a, 3059, 3194, 3430, 3797, 3973, 3974a, 4249, 5079, 5180, 5363, 5811b	1360, 1375a

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
946.	93-15-2	Phenol, 2-methoxymethyl-4-(2-propenyl)- {eugenol, methyl-}	568b, 1741, 1743, 1744, 3265, 3300, 5512, 5537	5515	
947.	93-51-6	Phenol, 2-methoxy-4-methyl- {4-methylguaiacol}	568b, 1063–1066, 1068–1074, 1360, 1364, 1371, 1375, 1375a, 1375b, 1586, 2327c, 2543, 2767, 2773, 2775, 3266, 3410, 3553, 3557, 3712, 4249, 4796, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877a, 2014, 3266, 3370, 3430, 4249, 5811b	1360, 1375a
948.	2785-87-7	Phenol, 2-methoxy-4-propyl-	90a, 2570, 3712, 5811b	1876, 1877a, 4249, 5811b	
949.	19784-98-6	Phenol, 2-methoxy-5-(1-propenyl)-, (*E*)-	90a, 3712, 5811b		
950.	1195-09-1	Phenol, 2-methoxy-5-methyl-	90a, 3712	1876, 1877	
951.	58539-27-8	Phenol, 2-methoxy-5-propyl-	90a, 3712, 5811b		
952.	29275-83-0	Phenol, 2-methoxy-6-(1-propenyl)-, (*E*)-	3712		
953.	29275-82-9	Phenol, 2-methoxy-6-(1-propenyl)-, (*Z*)-	90a, 3712, 5811b		
954.	2896-67-5	Phenol, 2-methoxy-6-methyl-	90a, 3712, 5811b		
955.	32073-24-8	Phenol, 2-methoxy-propyl-	1884, 3746, 3747		
956.	93526-86-4	Phenol, 2-methoxy-trimethyl-	101, 1884, 3746, 3747, 4249, 5811b	5811b	
957.	114-26-1	Phenol, 2-(1-methylethoxy)-, methylcarbamate {Undene®; Propoxur®}		1280, 2698, 3633, 4249, 4271a	
958.	2417-10-9	Phenol, 2-phenoxy-	1884, 3712, 3744		
959.	88-32-4	Phenol, 3-(1,1-dimethyethyl)-4-methoxy-	4570a		
960.	621-34-1	Phenol, 3-ethoxy-		2917a	
961.	29760-89-2	Phenol, 3-ethyl-2-methoxy-	5811, 5811a, 5811b		
962.	150-19-6	Phenol, 3-methoxy-	1626, 1879, 1882, 1884, 2598, 3308, 3712, 3764, 3765, 3797, 4414, 4796, 5011, 5811b	952, 1876, 1877a, 4249, 5811b	3395
963.	5451-83-2	Phenol, 3-methoxy-, acetate	2601a		
964.	713-68-8	Phenol, 3-phenoxy-	568b, 1587, 1884, 3108, 3712, 3745, 4249, 5811b		
965.	537-33-7	Phenol, 4-(3-hydroxy-1-propenyl)-2,6-dimethoxy- {sinapyl alcohol}		1102, 2338,3973, 4249, 4438a, 5811b	
966.	458-35-5	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy- {coniferyl alcohol}	596, 1879, 1881, 1883, 1884, 3712, 3828, 4249, 5811b	1102, 2338, 3973	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
967.	32811-40-8	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*E*)-		1879, 4249	
968.	69056-21-9	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*Z*)-		1879, 4249, 5811b	
969.	59832-96-1	Phenol, 4-butyl-2-methoxy-	90a, 3712, 5811b		
970.	7786-61-0	Phenol, 4-ethenyl-2-methoxy- {4-vinylguaiacol}	101, 1063–1066, 1068–1075, 1089a, 1364, 1586, 1879, 1881, 1883, 1884, 1887a, 2524a, 2545, 2570, 2767, 3255, 3266, 3397, 3410, 3557, 3712, 3746, 3747, 4159, 4249, 5811b	172a, 174b, 937, 1053, 1587a, 1590a, 1876, 1877a, 1878, 2338, 2389, 2544, 2917a, 3266, 3430, 3547, 3549, 4249, 5811b	
971.	2785-89-9	Phenol, 4-ethyl-2-methoxy- {ethylguaiacol}	568b, 1063–1066, 1068–1074, 1364, 1371, 1375, 1375b, 1586, 1587, 1884, 2327c, 2543, 2765–2767, 2769, 3266, 3410, 3557, 3559, 3712, 3746, 3747, 4249, 5034, 5811b	568b, 1876, 1877a, 2014, 2338, 3266, 3430, 4249, 5811b	
972.	120550-71-2	Phenol, 4-ethyl-2-methoxy-5-methyl-	90a, 3712, 5811b		
973.	120550-70-1	Phenol, 4-ethyl-2-methoxy-6-methyl-	90a, 3712, 5811b		
974.	150-76-5	Phenol, 4-methoxy-	414, 1586, 1626, 2387, 2570, 2598, 2767, 3255, 3257, 3265, 3555, 3712, 3764, 3797, 4319, 4414, 4796, 5011, 5811b	1876, 1877a, 2389, 2544, 3555, 5811b	2387, 3395
975.	831-82-3	Phenol, 4-phenoxy-	4249		
976.	2785-88-8	Phenol, 5-ethyl-2-methoxy-	90a, 3712, 5811b		
977.	5150-42-5	Phenol, 2,3-dimethoxy-	568b, 2570, 3712, 4249	568b, 1877a, 4249	
978.	20578-97-6	Phenol, 2,3-dimethoxy-4-ethyl-	3712	1876, 1877a	
979.	34883-01-7	Phenol, 2,3-dimethyl-5-methoxy-	3712		
980.	91-10-1	Phenol, 2,6-dimethoxy- {syringol}	568b, 1063–1066, 1068–1074, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1879, 1884, 2043, 2045, 2327c, 2387, 2543, 2545, 2598, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 3266, 3302, 3394, 3410, 3553, 3557, 3712, 3797, 4249, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877, 2339, 2386, 2917a, 3266, 3430, 4249, 5811b	1360, 1375a, 2387, 3395

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
981.		Phenol, 2,6-dimethoxy-ethenyl-	3557, 4249		
982.	28343-22-8	Phenol, 2,6-dimethoxy-4-ethenyl-	1364, 1884, 2767, 2769, 3255, 3712	2338, 3430, 5811b	
983.	14059-92-8	Phenol, 2,6-dimethoxy-4-ethyl-	1879, 1884, 2543, 2773, 3712	3430, 5811b	
984.	6638-05-7	Phenol, 2,6-dimethoxy-4-methyl-	1586, 1884, 2543, 2570, 2769, 2767, 2773, 3557, 3712	1877a, 2386, 3430, 4249, 5811b	
985.	20675-95-0	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*E*)-	3712, 3557, 4249	2339, 3430	
986.	26624-13-5	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*Z*)-	3712	3430, 5811b	
987.	6627-88-9	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	1586, 1884, 2601a, 2767, 2769, 3557, 3712, 5811b	2338, 2339, 3430, 5811b	
988.	2033-89-8	Phenol, 3,4-dimethoxy-	568b, 3952, 4249		
989.	500-99-2	Phenol, 3,5-dimethoxy-	568b, 3712, 4249	568b, 1877, 4249	
990.	2785-85-5	Phenol, 3,5-dimethyl-2-methoxy-	90a, 1884, 3712, 5811b		
991.	72312-07-3	Phenol, 4,5-dimethoxy-2-methyl-		2917a	
992.	7771-25-7	Phenol, 4,5-dimethyl-2-methoxy-	90a, 3712, 5811b		
993.	2896-66-4	Phenol, 4,6-dimethyl-2-methoxy-	90a, 3712, 3746, 3747, 4249, 5811b		
994.	123844-48-4	Phenol, 5,6-dimethyl-2-methoxy-	90a		
995.	31105-03-0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
996.		2,6-Piperidinedione, methoxy-	1371, 1586, 4249		
997.		2,6-Piperidinedione, 3-methoxy-	568b, 4249		
998.	61892-70-4	2,6-Piperidinedione, 4-methoxy-	1365, 2773, 2775, 3553, 4249, 5811b		
999.	24946-64-3	Plastochromenol {solanachromene isomer}		840	
1000.		*L*-Proline, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
1001.	62137-28-4	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-		4249, 4429	
1002.	62137-29-5	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-ar abinofuranosyl) oxy]-, *trans*-		4249, 4429	
1003.	7778-85-0	Propane, 1,2-dimethoxy-	568b, 4249		
1004.	77-76-9	Propane, 2,2-dimethoxy-	568b, 4249		
1005.	505-84-0	Propane, 1,1′-[methylenebis(oxy)]bis- {dipropoxymethane} $(C_3H_7O)_2{=}CH_2$	1371, 4249		
1006.	111-43-3	Propane, 1,1′-oxybis- {dipropyl ether} $[H_3C\text{-}(CH_2)_2]_2{=}O$	642, 4249		
1007.	20390-21-0	1,2-Propanediol, 3-(furfuryloxy)-	568b, 1586, 2767, 3553, 4249		
1008.	2034-60-8	1,2-Propanedione, 1-(4-hydroxy-3-methoxyphenyl)-	4249	5811b	
1009.	1438-92-2	1,2-Propanedione, 1-(2-furanyl)-	568b, 2765, 2766, 3553, 4249, 5811b	568b, 3547, 4249, 5811b	
1010.	1197-20-2	1,2-Propanedione, 1-(5-methyl-2-furanyl)-	568b, 3553, 3555, 4249	568b, 3547, 3555, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

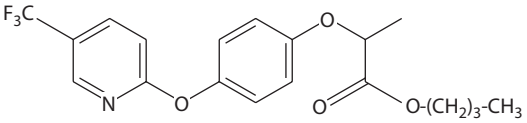
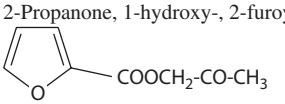
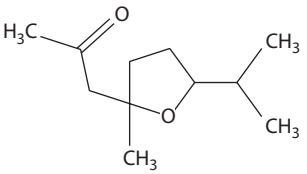
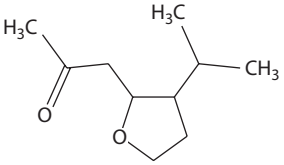
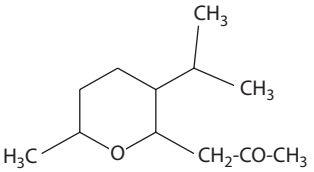
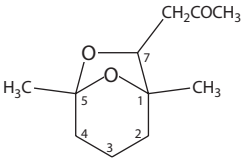
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1011.	65416-14-0	Propanoic acid, 2-methyl-, 2-methyl-4-oxo-4*H*-pyran-3-yl ester		1053, 3266, 3370	
1012.	69806-50-4	Propanoic acid, 2-(4-(5-trifluoromethyl-2-pyridyloxy)phenoxy)-, butyl ester {Fluazifop-butyl®} 		3633, 4271a	
1013.	935-13-7	Propanoic acid, 3-(2-furanyl)-	91b, 5811b		
1014.	2544-06-1	Propanoic acid, 3-methoxy-		1948, 4249	
1015.	1456-08-2	Propanoic acid, 3-(5-methyl-2-furanyl)-	91b, 5811b		
1016.	110053-58-2	1-Propanol, 2,2-bis(1-hydroxypropoxy)- $HOCH_2$-$C(CH_3)$= $(OCH_2CH_2CH_2OH)_2$	3553, 5811, 5811a, 5811b		
1017.	108-61-2	1-Propanol, 2,2′-oxybis- $[HOCH_2$-$CH(CH_3)]_2$=O	3553, 4249, 5811b		
1018.	2396-61-4	1-Propanol, 3,3′-oxybis- $(HOCH_2$-CH_2-$CH_2)_2$=O	3553, 4249		
1019.	110-98-5	2-Propanol, 1,1′-oxybis- $(CH_3$-$CHOH$-$CH_2)_2$=O	3553, 4249, 5811b		
1020.	110053-57-1	2-Propanol, 1,1-bis(2-hydroxypropoxy)- CH_3-$CHOH$-CH= $(OCH_2CHOHCH_3)_2$	3553, 5811, 5811a, 5811b		
1021.	107-98-2	2-Propanol, 1-methoxy-		3905, 4249	
1022.	3194-15-8	1-Propanone, 1-(2-furanyl)-	568b, 1587, 2570, 2767, 2773, 4249, 5770, 5811b		
1023.		1-Propanone, 1-(3-furanyl)-	2773, 4249		
1024.		2-Propanone, 1-hydroxy-, 2-furoyl ester 	1586		
1025.	122-84-9	2-Propanone, 1-(4-methoxyphenyl)-		172a, 174b, 174b, 568b, 1053, 3266	
1026.	20194-70-1	2-Propanone, 1-(tetrahydro-4-methyl-2*H*-pyran-2-yl)-	568b, 2761, 2762, 2765, 2766, 4249	568b, 937, 3188, 3543, 3547, 3560, 3561, 4048	
1027.		2-Propanone, 1-[tetrahydro-(2-methyl-5-methylethyl)-2-furanyl]- 		3219, 3545	
1028.	38713-24-5	2-Propanone, 1-[tetrahydro-3-(1-methylethyl)-2-furanyl]-, *trans*- 		404, 568b. 943, 1156, 3205, 3219, 3543, 3547, 3550, 4090, 4249	
1029.	39815-69-5	2-Propanone, 1-[tetrahydro-4-(1-methylethyl)-2-furanyl]-	5811b	3219, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1030.	39815-68-4	2-Propanone, 1-[tetrahydro-6-methyl-3-(1-methylethyl)-2*H*-pyran-2-yl]- {two isomers reported} 	568b, 2761, 4249, 5811b	404, 568b, 937, 1063–1066, 1068–1074, 1590a, 2386, 2389, 2544, 3188, 3219, 3356, 3543, 3545, 3547, 3550, 3561, 4098a, 4249, 5811b	
1031.		2-Propanone, 1-[tetrahydro-6-methyl-4-(1-methylethyl)-2*H*-pyran-2-yl]-		3217, 4249	
1032.		2-Propanone, 1-(1,5-dimethyl-6,8-dioxabicyclo[3.2.1]oct-7-yl)- 		3547, 4249	
1033.	6975-60-6	2-Propanone, 1-(2-furanyl)-	568b, 3555, 4249, 5811b	568b, 2917a, 3547, 3555, 4249, 5811b	3404
1034.	5211-62-1	2-Propanone, 1-(2-methoxyphenyl)-	1586, 3266, 4249		
1035.		2-Propanone, 1-(2-tetrahydrofuranyl)-	1360, 1375a		1360, 1375a
1036.		2-Propanone, 1-(3,4-dihydro-6-methylpyran-2-yl)-		3547, 4249	
1037.	19037-58-2	2-Propanone, 1-(3,5-dimethoxy-4-hydroxyphenyl)-	3553, 3712	5811b	
1038.	2503-46-0 110053-51-5	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	568b, 1364, 1586, 1884, 2570, 2767, 3553, 3557, 3712, 4249, 5811b	568b, 3430, 4249, 5811b	
1039.	13678-74-5	2-Propanone, 1-(5-methyl-2-furanyl)-	2570, 4249	2917a	
1040.	50672-03-2	2-Propanone, 1-[5-(hydroxymethyl)-2-furanyl]-	568b, 1375, 3553, 4249, 5811b		
1041.	31704-79-7	2-Propenal, 2-methyl-3-(5-methyl-2-furanyl)-	568b, 1587, 4249, 5811b		
1042.	874-66-8	2-Propenal, 3-(2-furanyl)-2-methyl-	1587, 4249, 5811b		
1043.	1504-74-1	2-Propenal, 3-(2-methoxyphenyl)-		568b, 4249	
1044.	42369-86-8	2-Propenamide, *N,N′*-1,4-butanediylbis[3-(4-hydroxy-3-methoxyphenyl)]-		4249, 4769, 5811b	
1045.	557-31-3	1-Propene, 3-ethoxy- {allyl ethyl ether}	2506, 2507, 4249, 4964, 5811b	3186, 3188, 4249	2506, 2507
1046.	2316-26-9	2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-		2389, 2544, 4249, 5811b	
1047.	539-47-9	2-Propenoic acid, 3-(2-furanyl)-	91b, 5811b		
1048.	82826-13-9	2-Propenoic acid, 3-(2-furanyl)-2-methyl-, ethyl ester		568b, 4249	
1049.		2-Propenoic acid, 3-(2-furanylmethyl)-2-methyl-, ethyl ester		568b, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

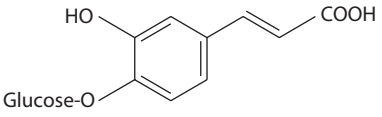
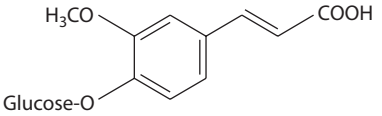
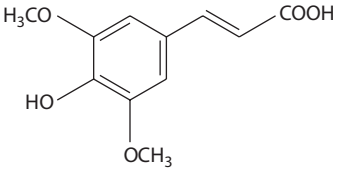
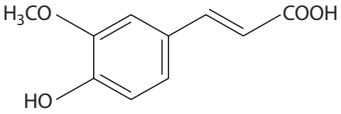
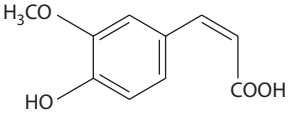
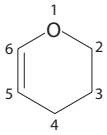
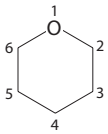
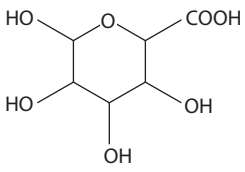
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1050.	17093-82-2	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]- {1-*O*-caffeoylglucose} 		3797, 3974a, 4402	
1051.	7196-71-6 14364-12-6	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-methoxyphenyl]- {1-*O*-feruloylglucose} 		3797, 3974a, 4249, 4402, 5811, 5811b	
1052.	14364-05-7	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)phenyl]-		2023, 4249	
1053.	7361-90-2	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*Z*)- {*cis*-sinapic acid}	1626	1102, 3748, 3749, 3751, 4249, 4624	
1054.	7362-37-0	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*E*)- {*trans*-sinapic acid} 	1626, 1884, 3302, 3712, 3797, 4249, 4377	1102, 3748, 3749, 3751, 4249	
1055.	537-73-5	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-	3712, 4113, 4249		
1056.	25522-33-2	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-, (*E*)-	3712, 5811b		
1057.	1782-55-4	2-Propenoic acid, 3-(4,5-dihydroxy-3-methoxyphenyl)- {5-hydroxyferulic acid}		1102	
1058.	1135-24-6	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)- {cinnamic acid, 3-hydroxy-4-methoxy-; ferulic acid}	3712, 5811b	5811b	
1059.	530-59-6	2-Propenoic acid, 3-(4-hydroxy-3,5-dimethoxyphenyl)-	5811, 5811b		
1060.	537-98-4	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid} 	1626, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3555, 3749, 3797, 4249, 4377, 5811b	404, 1102, 1626, 1884, 2216, 2389, 2544, 2939, 2954, 3103, 3161, 3555, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 4377	
1061.	1014-83-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid} 	1626, 1842, 2216, 2939, 3255, 3257, 3302, 3712, 3741, 3743, 3749, 4249, 4377	1102, 1626, 2216, 2389, 2544, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3797, 3973, 3974a	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1062.	2309-07-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester {ferulic acid, methyl ester}	3712, 4249, 4553a	5811b	
1063.	17570-26-2	2-Propenoic acid, 3-(3-methoxyphenyl)-, (*E*)-	2388, 4249	3561, 3797	
1064.	14779-25-0	2-Propenoic acid, 3-(5-methyl-2-furanyl)-	91b, 5811b		
1065.	90-50-6	2-Propenoic acid, 3-(3,4,5-trimethoxyphenyl)-		2389, 2544, 5811b	
1066.	2983-65-5	2-Propen-1-one, 1-(4-hydroxy-3-methoxyphenyl)-	4249	5811b	
1067.	525-79-1	1*H*-Purin-6-amine, *N*-(2-furanylmethyl)-		3973, 4249, 4509	
1068.	56159-42-3	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-		4249, 4603	
1069.	38477-23-5	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-		4249, 4603	
1070.	54538-20-4	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-		4249, 4620	
1071.	25512-65-6	2*H*-Pyran, dihydro-	157, 2767, 2799a, 4249	3973, 4249, 4807	
1072.	110-87-2	2*H*-Pyran, 3,4-dihydro- 	4249	5811b	
1073.	10141-72-7	2*H*-Pyran, 2-methyltetrahydro-		3186, 4249	
1074.	142-68-7	2*H*-Pyran, tetrahydro- 	1140, 1374, 1375a, 1377, 1378, 1413, 1416, 2767, 3302, 3308, 3557, 3797, 4249, 4319, 5811b	3561	1375a, 1377, 1378
1075.	16409-43-1	Pyran, tetrahydro-4-methyl-2-(2-methylpropen-1-yl)- {rose oxide}		174b, 568b, 3266, 4249	
1076.	100-73-2	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro- {acrolein dimer}	568b, 1587, 3169, 4249, 5811b	404, 568b, 4249	
1077.	70898-35-0	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro-6-hydroxy-3-oxo-	1378	2939, 3797, 4249	1378
1078.	9046-38-2	2-Pyrancarboxylic acid, 3,4,5,6-tetrahydroxytetrahydro- {oxane-2-carboxylic acid, 3,4,5,6-tetrahydroxy-; *D*-galacturonan} 		5811, 5811b	
1079.	85373-77-9	4*H*-Pyran-3-carboxylic acid, 5,6-dihydro-2,6-dimethyl-, methyl ester	568b, 4249		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

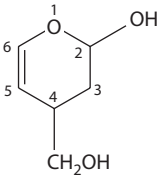
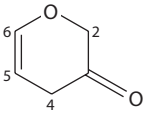
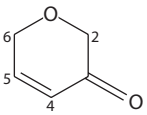
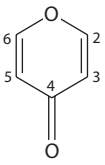
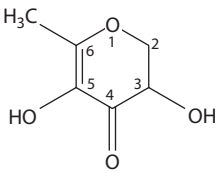
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1080.		2*H*-Pyran-4-methanol, 3,4-dihydro-2-hydroxy-	3553		
					
1081.	61892-96-4	2*H*-Pyran-6-methanol, 3,4-dihydro-3-hydroxy-	568b, 3553, 4249		
1082.	19752-84-2	2*H*-Pyran-3-ol, tetrahydro-	568b, 3553, 4249, 5811b		3405
1083.	121198-47-8	Pyranone, dimethyl-	4249		
1084.		2*H*-Pyran-2-one, tetrahydro-3,4-epoxy-5-hydroxy-	1375a (0), 1377 (0)		1375a, 1377
1085.		2*H*-Pyran-2-one, tetrahydro-methoxy-	1375a (0), 1377 (0)		1375a, 1377
1086.	28743-04-6	2*H*-Pyran-3(4*H*)-one	4054, 4249	5811b	
					
1087.	23462-75-1	2*H*-Pyran-3(4*H*)-one, dihydro-	4249, 5811b		3402, 3404, 4249
1088.	121197-11-3	2*H*-Pyran-3(4*H*)-one, dihydro-4-(hydroxymethyl)-	4249	5811b	
1089.	65712-87-0	2*H*-Pyran-3(4*H*)-one, dihydro-6-methoxy-	4249, 5811b		3404, 4249
1090.	43152-89-2	2*H*-Pyran-3(4*H*)-one, dihydro-6-methyl-	3404, 4249		
1091.	98166-23-5	2*H*-Pyran-3(6*H*)-one	4249	5811b	
					
1092.	108-97-4	4*H*-Pyran-4-one	1352, 5811b		
					
1093.	84302-42-1	4*H*-Pyran-4-one, 2,3-dihydro-	4249	5811b	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

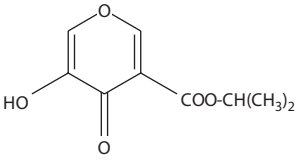
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1094.	28564-83-2	4*H*-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- 	568b, 1089a, 1134, 1138, 1351, 1352, 1360, 1375, 1375a, 1375b, 1882, 1887a, 2337, 2493, 2524a, 2543, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2857, 3394, 3397, 3553, 3557, 3828, 4249, 5811b	568b, 2339b, 2917a, 3549, 4249, 5811b	1360, 1375a, 3402, 3405
1095.	6380-97-8	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-2-(hydroxymethyl)-	3553, 4249	3430, 5811b	
1096.	38877-21-3	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-6-methyl-	1134, 1138, 4249		
1097.	131524-09-9	4*H*-Pyran-4-one, 2,6-diethyl-3-hydroxy-	90b, 4249, 5811b		
1098.	1004-36-0	4*H*-Pyran-4-one, 2,6-dimethyl-	2507, 4249		
1099.	4940-17-4	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-	90b, 4249, 5811b		
1100.	131524-16-8	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-6-methyl-	90b, 4249, 5811b		
1101.	4940-11-8	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy- {ethylmaltol}	90b, 568b, 3266, 4249, 5811b	172a, 174b, 568b, 1053, 3219, 3266, 3370, 4249	
1102.	131524-08-8	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5,6-dimethyl-	90b, 4249, 5811b		
1103.	131524-04-4	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5-methyl-	90b, 4249, 5811b		
1104.	22639-24-3	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-6-methyl-	90b, 4249, 5811b		
1105.	61892-88-4	4*H*-Pyran-4-one, 2-hydroxy-3-methyl-	3410, 3553, 4249		
1106.	61892-87-3	4*H*-Pyran-4-one, 2-hydroxy-5-methyl-	1351, 1352, 3553, 4249		
1107.		4*H*-Pyran-4-one, 2-hydroxymethyl-3,5,6-trihydroxy-	1375a (0), 1377 (0), 4249		1375a, 1377, 4249
1108.		4*H*-Pyran-4-one, 2-methyl-3,5,6-trihydroxy-	1375a (0), 1377 (0)		1375a, 1377
1109.	29943-42-8	4*H*-Pyran-4-one, 2,3,5,6-tetrahydro-; 4*H*-pyran-4-one, tetrahydro-	568b, 4249		
1110.	488-18-6	4*H*-Pyran-4-one, 3,5-dihydroxy-	568b, 1351, 1375a, 1377, 1586, 2769, 4249		1375a, 1377
1111.		4*H*-Pyran-4-one, 2,5-dihydroxy-3-methyl-	1351, 1352		
1112.	61892-86-2	4*H*-Pyran-4-one, 3,5-dihydroxy-2,6-dimethyl-	568b, 1375, 1375b, 2767, 3553, 3557, 4249		

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1113.	1073-96-7	4*H*-Pyran-4-one, 3,5-dihydroxy-2-methyl- {5-hydroxymaltol}	568b, 1089a, 1351, 1352, 1360, 1375, 1375a, 1375b, 1377, 1882, 1856, 1887a, 2524a, 2761, 2762, 2765–2767, 2777, 3394, 3410, 3553, 3557, 4249, 5811b	568b, 2389, 2544, 3430, 4249, 5811b	1360, 1375a, 1377, 3402, 3404, 3405
1114.		4*H*-Pyran-4-one, 3,5-dihydroxymethyl-2,6-dimethyl-	1375, 1375b, 2767, 4249		
1115.	496-63-9	4*H*-Pyran-4-one, 3-hydroxy-	568b, 1351, 1352, 1375, 1375a, 1375b, 1377, 1586, 2767, 3553, 3557, 4249, 5811b		1375a, 1377, 3401, 3402, 3404, 3405, 4249
1116.	40311-00-0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylethyl)-	90b, 4249, 5811b		
1117.	4940-18-5	4H-Pyran-4-one, 3-hydroxy-2-(1-methylpropyl)-	90b, 4249, 5811b		
1118.	131524-11-3	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylbutyl)-	90b, 4249, 5811b		
1119.	76015-10-6	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylpropyl)-	90b, 4249, 5811b		
1120.	131524-12-4	4*H*-Pyran-4-one, 3-hydroxy-2-(3-methylbutyl)-	90b, 4249, 5811b		
1121.	131524-05-5	4*H*-Pyran-4-one, 3-hydroxy-2,5,6-trimethyl-	90b, 4249, 5811b		
1122.	131524-02-2	4*H*-Pyran-4-one, 3-hydroxy-2,5-dimethyl-	90b, 4249, 5811b		
1123.	2298-99-9	4*H*-Pyran-4-one, 3-hydroxy-2,6-dimethyl-	90b, 4249, 5811b		
1124.		4*H*-Pyran-4-one, 3-hydroxymethyl-	1582		
1125.	118-71-8	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}	568b, 1131, 1351, 1352, 1375, 1375a, 1375b, 1377, 1378, 1586, 1881, 1884, 2570, 2767, 2777, 3266, 3397, 3553, 3555, 3557, 4249, 5811b	172a, 174d, 568b, 965, 1053, 1590a, 2337, 2339b, 2386, 2389, 2544, 2917a, 3266, 3430, 3543, 3555, 3560, 3561, 5811b	1375a, 1377, 1378, 3401, 3402, 3404, 3405
1126.	131524-10-2	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-6-propyl-	90b, 4249, 5811b		
1127.	131524-13-5	4*H*-Pyran-4-one, 3-hydroxy-2-pentyl-	90b, 4249, 5811b		
1128.	4940-16-3	4*H*-Pyran-4-one, 3-hydroxy-2-propyl-	90b, 4249, 5811b		
1129.	42508-10-1	4*H*-Pyran-4-one, 3-hydroxy-5-methyl-	568b, 4249		
1130.	131524-07-7	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylethyl)-	90b, 4249, 5811b		
1131.	131524-14-6	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylpropyl)-	90b, 4249, 5811b		

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1132.	131524-15-7	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(2-methylpropyl)-	90b, 4249, 5811b		
1133.	40861-87-8	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-propyl-	90b, 4249, 5811b		
1134.	50671-50-6	4*H*-Pyran-4-one, 3-methyl-	1375, 1375b, 4249		
1135.	131524-03-3	4*H*-Pyran-4-one, 5-hydroxy-2,3-dimethyl-	90b, 5811b		
1136.	644-46-2	4*H*-Pyran-4-one, 5-hydroxy-2-methyl-; 4*H*-pyran-4-one, 3-hydroxy-6-methyl- {allomaltol}	568b, 1351, 1352, 1364, 2601a, 3553, 4249, 5811b		
1137.	131524-06-6	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-methyl-	90b, 4249, 5811b		
1138.	131524-17-9	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-propyl-	90b, 4249, 5811b		
1139.	499-78-5	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-	1375a (0), 1377 (0)	2544, 4249	1375a, 1377
1140.		4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-, (1-methylethyl) ester 	1375a (0), 1377 (0)		1375a, 1377
1141.	25680-58-4	Pyrazine, 2-ethyl-3-methoxy-		1053, 3266	
1142.		Pyrazine, 2-ethyl-5-methoxy-		1053, 3266	
1143.	67845-38-9	Pyrazine, 2-ethyl-6-methoxy-		1053, 3266	
1144.	32736-95-1	Pyrazine, 2-furanyl-	568b, 1351, 1587a, 2727, 2731, 2735, 2799a, 3410, 3491, 4249, 5811b	568b, 3547, 4249	
1145.	32737-01-2	Pyrazine, 2-(2-furanyl)-3-methyl-	568b, 4249		
1146.	29460-98-8	Pyrazine, 3-furanyl-	1587, 2799a, 4249, 5811b		
1147.	36238-34-3	Pyrazine, 5-(2-furanyl)-2,3-dimethyl-; pyrazine, 2-(2-furanyl)-5,6-dimethyl-	1351, 2731, 2735, 4249, 5811b		
1148.	27610-38-4	Pyrazine, 2-(2-furanyl)-5-methyl-	568b, 1351, 1587a, 2543, 2545, 2724, 2727, 2731, 2732, 2735, 2773, 2775, 3255, 3410, 3491, 3553, 4249, 5811b	568b, 2724, 3491, 3547, 4249	
1149.	32737-03-4	Pyrazine, 2-(2-furanyl)-6-methyl-	568b, 1075, 1351, 1587a, 2727, 2731, 2735, 3410, 3491, 4249, 5811b	568b, 3547, 4249	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1150.	29461-10-7	Pyrazine, 2-(3-furanyl)-5-methyl-	2775, 4249		
1151.	3149-28-8	Pyrazine, methoxy-		1053, 3266, 4249	
1152.	2847-30-5	Pyrazine, 3-methoxy-2-methyl-		172a, 174b, 568b, 1053, 3266, 3370, 4249	
1153.	2882-22-6	Pyrazine, 5-methoxy-2-methyl-		172a, 174b, 1053, 3266, 4249	
1154.	2882-21-5	Pyrazine, 6-methoxy-2-methyl-		172a, 174b, 1053, 3266, 4249	
1155.	24683-00-9	Pyrazine, 2-methoxy-3-methylpropyl-		568b, 1053, 3266, 4249	
1156.		Pyrazinecarboxaldehyde, 5-(2-furanyl)-3-methyl-		568b, 3547, 4249	
1157.	61771-67-3	3-Pyridinamine, 6-methoxy-*N*-methyl-	568b, 3553, 4249		
1158.	14529-53-4	Pyridine, 2-ethoxy-	568b, 4249		
1159.	1628-89-3	Pyridine, 2-methoxy-	568b, 2775, 4249, 4570a		
1160.	114-91-0	Pyridine, 2-(2-methoxyethyl)-	568b, 4249		
1161.	7295-76-3	Pyridine, 3-methoxy-	568b, 1371, 1587, 4249, 5034, 5811b	568b, 2917a, 4249, 5811b	
1162.	78210-42-1	Pyridine, 3-methoxy-5-methyl-	568b, 1587, 4249, 5811b		
1163.	78210-88-5	Pyridine, 3-[1-(5-ethyl-2-furanyl)-1*H*-pyrrol-2-yl]-	568b, 1587, 4249, 5811b		
1164.	78210-87-4	Pyridine, 3-[1-[2-(2-furanyl)ethyl]-2-pyrrolidinyl]-, (S)-	568b, 1587, 4249, 5811b		
1165.	78210-85-2	Pyridine, 3-[1-(2-furanylmethyl)-2-pyrrolidinyl]-, (S)-	568b, 1371, 1587, 2773, 2775, 3410, 4249, 5811b		
1166.	88111-63-1	Pyridine, 3-(1-methylethoxy)-	568b, 4249		
1167.	78210-86-3	Pyridine, 3-[1-[(5-methyl-2-furanyl)methyl]-2-pyrrolidinyl]-, (S)-	568b, 1587, 4249, 5811b		
1168.	78210-89-6	Pyridine, 3-[1-(5-propyl-2-furanyl)-1*H*-pyrrol-2-yl]-	568b, 1587, 4249, 5811b		
1169.	78210-45-4	Pyridine, 3-[2,5-dihydro-1-[(5-methyl-2-furanyl)methyl]-1*H*-pyrrol-2-yl]-	568b, 1587, 4249, 5811b		
1170.	78210-46-5	Pyridine, 3-[(5-methyl-2-furanyl)methyl]-	568b, 1587, 4249, 5811b		
1171.	78210-50-1	Pyridine, 3-(tetrahydro-2-furanyl)-	1587, 4249, 5811b		
1172.	70199-60-9	Pyridine, 4-(methoxymethyl)-	568b, 1587, 4249, 5811b		
1173.	55270-47-8	Pyridine, 5-methoxy-2-methyl-	568b, 1587, 4249, 5811b		
1174.	60655-87-0	Pyridinium, 1-α-*L*-arabinopyranosyl-3-carboxy-		4249, 4738	
1175.	35323-45-6	Pyridinium, 3-carboxy-1-β-*D*-glucopyranosyl-, hydroxide {trigonelline}		1858a, 4249	
1176.	3589-73-9	3*H*-Pyrido[3,4-*b*]indole, 4,9-dihydro-6-methoxy-1-methyl-	5811		
1177.	304-21-2	3*H*-Pyrido[3,4-*b*]indole, 4,9-dihydro-7-methoxy-1-methyl- {harmaline}	5811		

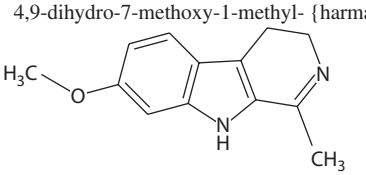
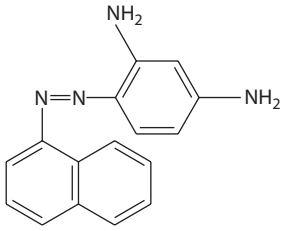
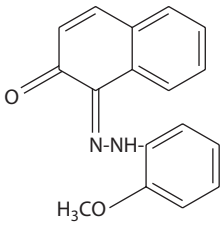
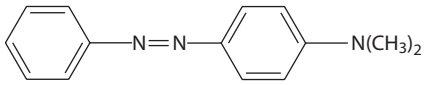


TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1178.	3589-72-8	9*H*-Pyrido[3,4-*b*]indole, 6-methoxy-1-methyl-	5811a		
1179.	442-51-5	9*H*-Pyrido[3,4-*b*]indole, 7-methoxy-1-methyl- {harmine}	5811, 5811a, 5811b		
1180.		1*H*-Pyrrole, 1-(2-furanyl)-	2731, 2735, 4249		
1181.	13678-52-9	1*H*-Pyrrole, 1-[(5-methyl-2-furanyl)methyl]-	568b, 1386, 4249		
1182.	1438-94-4	1*H*-Pyrrole, 1-(2-furanylmethyl)-	568b, 1587a, 2727, 3410, 3491, 4249, 5811b	568b, 2336, 4249	
1183.	84499-92-3	1*H*-Pyrrole-1-acetic acid, 2-(ethoxymethyl)-5-formyl-		4249, 4573a, 5811b	
1184.	13788-32-4	1*H*-Pyrrole-2-carboxaldehyde, 1-(2-furanylmethyl)-		404, 568b, 3547, 3555, 4249	
1185.	61893-12-7	Pyrrolidine, 1-(2-furanylmethyl)-	568b, 3410, 3553, 3559, 4249		
1186.	78504-05-9	Pyrrolidine, 1-(2-furoyl)-	568b, 4249		
1187.		Pyrrolidine, 1-(2-furoyl-5-methyl)-	568b, 4249		
1188.	61480-99-7	Pyrrolidine, 1-[(5-methyl-2-furanyl)methyl]-	568b, 3410, 3553, 3559, 4249		
1189.		Quinoline, 5-amino-6,8-dimethoxy-		2917a	
1190.		Quinoline, 5-amino-2-hydroxymethyl-6-methoxy-		2917a	
1191.	6931-16-4	Quinoline, 2-methoxy-	568b, 4249		
1192.	6931-17-5	Quinoline, 3-methoxy-	568b, 4249		
1193.	5263-87-6	Quinoline, 6-methoxy-	568b, 4249, 5811		
1194.	4964-76-5	Quinoline, 7-methoxy-	568b, 4249		
1195.	938-33-0	Quinoline, 8-methoxy-	568b, 4249		
1196.	6416-57-5 69772-40-3 60-11-7	Resinol, brown  Resinol Resinol, red  Resinol, yellow 		5079, 5381	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1197.		Rhamnitol, 2,4-di-*O*-methyl-		3669	
1198.		Rhamnitol, 3,4-di-*O*-methyl-		3669	
1199.		Rhamnitol, 3-*O*-methyl-		3669	
1200.		Rhamnitol, 2,3,4-tri-*O*-methyl-		3669	
1201.	39280-21-2	(1→2)-*L*-Rhamno-(1→4)-α-*D*-galacturonan		5811, 5811b	
1202.	2718-25-4	Rheadan, 8-β-methoxy-6-methyl-2,3,10,11-[methylenebis(oxy)]- {rhoeadine}		3763, 5079	
1203.	62574-27-0	Spiro[4.5]dec-6-en-8-one, 2-[1-[(β-*D*-glucopyranosyloxy)methyl]ethenyl]-6,10-dimethyl-		77, 1156, 4090, 4249	
1204.	62574-29-2	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-		77, 1156, 4090, 4249	
1205.	62623-87-4	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-		77, 1156, 4090, 4249	
1206.	62574-25-8	Spiro[4.5]dec-6-en-8-one, 9-(β-*D*-glucopyranosyloxy)-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]-		77, 1156, 4090, 4249	

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1207.	162188-94-5	Spiro[benzofuran-6(2*H*),2′-[1,3]dioxolan]-2-one, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-, (±)-		4249	
1208.	5989-24-2 30987-48-5	Spiro[furan-2(3*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5(4*H*)-one, decahydro-3,3′a,6′,6′,9′a-pentamethyl-{α-levantenolide}	323, 799, 801, 1173, 1352, 1373, 2722, 3251, 3302, 3308, 3797, 3971, 4341, 5811b	1149, 1149a, 1156, 1173, 1290, 1299, 1300, 1352, 2308, 2939, 3797, 3804, 3971, 3973, 3974a, 4090, 4319, 4341, 5811b	
1209.	1235-78-5	Spiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one, 3′a,4′,5′,5′a,6′,7′,8′,9′,9′a,9′b-decahydro-3,3′a,6′,6′,9′a-pentamethyl-, [2′S-(2′α,3′aα,5′aβ,9′aα,9′bβ)]-{β-levantenolide}	323, 799, 801, 1173, 1373, 3251, 3302, 3308, 3797, 3971,4319, 4341, 5811b	1149, 1149a, 1156, 1173, 1290, 1299, 1300, 2308, 2939, 3797, 3804, 3971, 3973, 3974a, 4090, 4319, 4341, 5811b	
1210.		Spiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one, dodecahydro-3,3′a,6′,6′,9′a-pentamethyl-{α_2-levantanolide}		1149, 1149a, 1156, 1300, 2308, 3973, 3974a, 4090	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1211.	9005-25-8	Starch	5811b	69, 120, 248, 385, 385a, 420, 535, 677b, 722, 963, 1063–1066, 1068–1074, 1266, 1267, 1289, 1329, 1330, 1333, 1933a, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2394a, 2395, 2529, 2543, 2545, 2688, 2761, 2762, 2764–2766, 2914, 2939, 2947c, 3059, 3087, 3334, 3372, 3450, 3551, 3592, 3797, 3871, 3973, 3974a, 3974b, 4249, 4261, 4262, 4275, 5079, 5108, 5109, 5126, 5189, 5194, 5298, 5344, 5449, 5468, 5767, 5811b, 5831, 5843, 5866, 5896	
1212.	39341-47-4	Starch, labeled with ^{13}C {starch-^{13}C}		976a, 4249, 4720	
1213.	70226-57-2	Starch, labeled with ^{14}C {starch-^{14}C}		2764	
1214.		Tergitol ether I[a]	1378 (0)		1378
1215.		Tergitol ether II[a]	1378 (0)		1378
1216.		Tergitol ether III[a]	1378 (0)		1378
1217.		Tergitol ether IV[a]	1378 (0)		
1218.		*L*-Threonine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337	
1219.	50-89-5	Thymidine		3973, 4249	

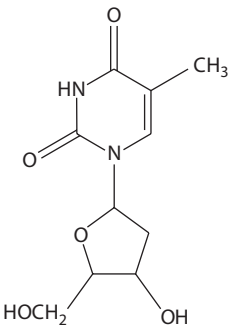
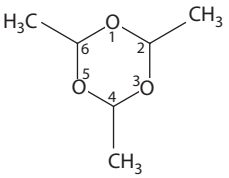
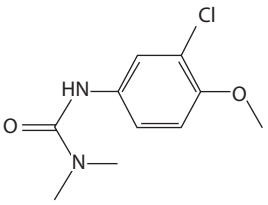
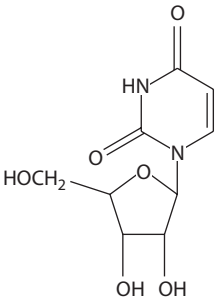
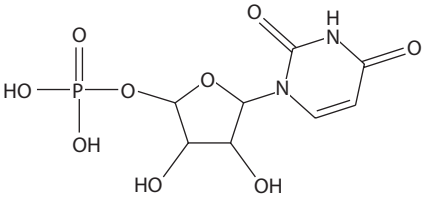
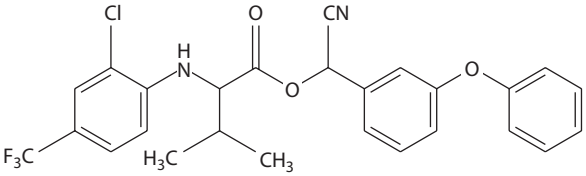
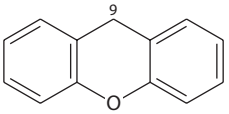
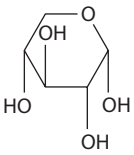


TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

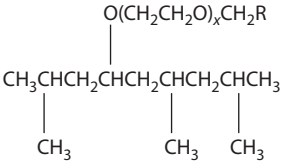
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1220.	55219-65-3	1*H*-1,2,4-Triazol-1-ethanol, 8-(4-chlorophenoxy)-α-(1,1-dimethylethyl)- {Triadimenol®}		928a	
1221.	123-63-7	1,3,5-Trioxane, 2,4,6-trimethyl- {paraldehyde; acetaldehyde trimer} 	156, 157, 568b, 4249		
1222.	34393-22-1	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
1223.	152209-56-8	6,10-Undecadien-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-2-methyl-2-furanyl)-		4249	
1224.	160115-56-0	6-Undecen-2-one, 10-(acetyloxy)-8,11-dihydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-5-hydroxy-2-methyl-2-furanyl)-		4249	
1225.	3060-89-7	Urea, *N*′-(4-bromophenyl)-*N*′-methoxy-*N*′-methyl- {Patoran®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
1226.	19937-59-8	Urea, *N*′-(3-chloro-4-methoxyphenyl)-*N,N*-dimethyl- {Metoxuron®} 		622, 3633, 4249, 4271a	
1227.	1746-81-2	Urea, *N*′-(4-chlorophenyl)-*N*-methoxy-*N*-methyl- {Linuron®, 30% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
1228.	330-55-2	Urea, *N*′-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methyl- {Monolinuron®, 20% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
1229.	58-96-8	Uridine 		3973, 4249	
1230.	133-89-1	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-glucopyranosyl ester		4249, 4489, 4580	
1231.	3616-06-6	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester		429b, 4249	
1232.	19253-25-9	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester		4249, 4458	

(*continued*)

TABLE 10.2 (continued)
Ethers in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1233.	58-97-9	5′-Uridylic acid 		429b, 4249, 4474	
1234.		*L*-Valine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
1235.	102851-06-9	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®} 		904, 2346, 3585e	
1236.	92-83-1	9*H*-Xanthene {dibenzopyran} 	2114, 2767, 3514, 4249, 5811b	4249, 4788	
1237.	6279-07-8	9*H*-Xanthene, 2-methyl-	1508, 4249	3541, 4249	
1238.	90-47-1	9*H*-Xanthen-9-one {xanthone}		246, 247, 4249	
1239.	9014-63-5	Xylan		842, 2070, 2850, 2939, 3371, 3666, 3797, 3973, 3974a, 4249, 5811b	
1240.		Xylan, 4′-*O*-methylglucuronyloxy-		4249, 4584	
1241.	58-86-6 25990-60-7	Xylose 	2145, 2939, 3302, 4249, 5580, 5811, 5811a, 5811b	120, 2070, 2270, 3079, 3797, 3973, 3974a, 4249, 5768, 5785, 5811, 5811a, 5811b	
1242.	31178-70-8	α-*D*-Xylose		3075, 3667, 3973, 3974a, 4249	
1243.	31178-71-9	β-*D*-Xylose		3667, 3973, 3974a, 4249	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke.

[a] The Tergitol ethers possessed the following structures: 

Tergitol ether I: R=CH_3, x = 1
Tergitol ether II: R=CH_3, x = 2
Tergitol ether III: R=CH_3, x = 3
Tergitol ether IV: R=H, x = 1

TABLE 10.3
Distribution of Identified Oxygen-Containing Components between Tobacco and Tobacco Smoke

Component	Table	Total[a]	Smoke	Tobacco	Smoke and Tobacco
Alcohols	Table 2.5	1722	675	1360	313
Phytosterols and derivatives	Table 2.7	134	54	123	43
Aldehydes	Table 3.12	297	187	217	107
Ketones	Table 3.13	1254	737	800	283
Carboxylic acids	Table 4.3	787	380	656	249
Amino acids	Table 4.10	117	36	117	36
Esters	Table 5.3	1143	670	1026	553
Lactones	Table 6.3	336	201	213	78
Anhydrides	Table 7.1	24	17	16	9
Carbohydrates	Table 8.3	316	44	310	38
Phenols	Table 9.22	607	468	305	166
Quinones	Table 9.24	50	38	19	7
Ethers	Table 10.2	1243	654	847	258
Totals		8029	4160	6008	2139

[a] Polyfunctional *O*-containing compounds are counted in each functional group; e.g., propanoic acid, 2-hydroxy- (lactic acid) appears in the alcohol catalog and the acid catalog; benzoic acid, 4-hydroxy-3-methoxy- (vanillic acid) appears in the acid catalog, the phenol catalog, and the ether catalog.

11 Nitriles

The nitriles in tobacco and/or tobacco smoke provide another excellent example of the escalation of the number of identified components. From the listing in 1954 by Kosak (2170) who recorded only HCN, in tobacco smoke to those cataloged in Table 11.2 which includes the simplest "nitrile," hydrocyanic acid (HCN) plus 155 nitriles identified to date in tobacco and/or tobacco smoke. HCN was first identified in tobacco smoke in 1828 by Vogler (4062). Examination of Table 11.2 indicates the listing of seven partially identified nitrile isomers plus 13 cyano group-containing pesticides used in tobacco agronomy. In the latter case, many were identified in tobacco only, but several identified in tobacco were also found to transfer intact to smoke, e.g., Cypermethrin® (52315-07-8).

In their 1959 review of tobacco and tobacco smoke components, Johnstone and Plimmer (1971) listed the following four components containing a -C≡N group: hydrogen cyanide, cyanogen, thiocyanic acid, and thiocyanogen. No alkyl nitriles were listed.

With the advent of gas chromatography, Grob used his gas chromatographic knowledge and skill to identify a series of nitriles in tobacco smoke in 1962 (1413) and 1965 (1416, 1417). His 1965 findings were accompanied by similar findings reported in 1965 by Newsome et al. (2782). Many of the nitriles identified in the Grob and Newsome et al. studies were discussed by Wynder and Hoffmann in their 1967 book [see pp. 450–451 in (4332)]. They also discussed the reports by Campbell et al. (582) and McKee et al. (2519b) on the indication that acetonitrile in the body fluids was indicative of exposure to tobacco smoke because no other respiratory exposure was known. Table 11.1 lists some of the nitriles identified in the early 1960s.

In his 1968 review on tobacco and tobacco smoke composition, Stedman (3797) listed 15 nitriles, including HCN, as chemical components of tobacco smoke. Many of the listed nitriles were those identified by Grob (1412, 1413, 1416, 1416a, 1419) in his gas chromatographic studies of tobacco smoke. Stedman also listed 2-pyridinecarbonitrile and 3-pyridinecarbonitrile (nicotinonitrile) as pyrolysis products of various alkaloids.

In addition to HCN, cyanogen, thiocyanic acid, and thiocyanogen, Schmeltz and Hoffmann in their 1977 review of *N*-containing components of tobacco and tobacco smoke listed 31 nitriles [see Table IX in (3491)]. Ishiguro and Sugawara in their 1980 catalog (1884) of the chemical components of tobacco smoke listed 30 nitriles in addition to HCN, cyanogen, thiocyanogen, and thiocyanic acid.

In its 1986 monograph on tobacco smoking, the International Agency for Research on Cancer (IARC) wrote very little about nitriles in tobacco smoke. IARC categorized HCN as one of the most toxic agents in the vapor phase of tobacco smoke and noted its presence in smoke was dependent on the level of nitrate, proteins, and amino acids in tobacco [see p. 96 in (1870)]. IARC also listed cyanogen as a tobacco smoke component. In its summary of its evaluation for carcinogenicity of chemical components identified in tobacco smoke, IARC did classify 2-propenenitrile (acrylonitrile) with sufficient evidence for carcinogenicity in animals but limited evidence in humans [see p. 392 in (1870)]. The per cigarette MSS yield of 2-propenenitrile (acrylonitrile) was listed at 3.2–15 µg, based on data provided by Wynder and Hoffmann from their 1982 publication (4348a). In a publication issued shortly after the IARC 1986 monograph on tobacco smoking, Hoffmann and Wynder estimated the number of tobacco smoke components to be approximately 3900, of which the number of nitriles was listed at 105 [see Table 1 in (1808)]. They listed HCN as a major toxic agent in nonfiltered cigarette smoke [see Table 2 in (1808)] and 2-propenenitrile (acrylonitrile) as a biologically active agent in MSS [see Table 13 in (1808)]. It is interesting to note that, despite the considerable contribution of Wynder and Hoffmann to the subject of smoke components and their biological properties in the IARC 1986 monograph on tobacco smoking, only HCN, cyanogen, and 2-propenenitrile (acrylonitrile) of the 105 nitriles noted by Hoffmann and Wynder (1808) appeared in the IARC monograph (1870).

In many of the publications issued between 1990 and 2001 in which various tumorigens in tobacco smoke, particularly cigarette smoke, were listed, 2-propenenitrile (acrylonitrile) was included [Hoffmann et al. (1727, 1740, 1741, 1743, 1744, 1783), Fowles and Bates (1217), OSHA (2825)]. In 2003, these lists were discussed in detail by Rodgman (3265).

HCN and cyanogen, while not listed as tumorigens, were listed in many instances as biologically active toxicants. In many cases, acetonitrile was listed as a vapor-phase component of tobacco smoke. For example, in their 1997 and 2001 articles, Hoffmann and Hoffmann (1740, 1743) and Hoffmann et al. (1744) listed HCN, acetonitrile,

TABLE 11.1
Nitriles Identified and/or Discussed in Tobacco Smoke by the Mid-1960s

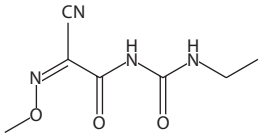
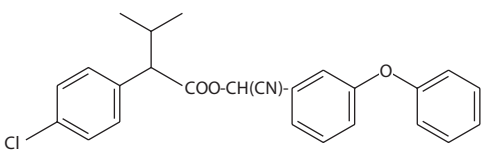
CAS No.	Nitrile	References by Mid-1960s
75-05-8	Acetonitrile	Grob (1413, 1416), Newsome et al. (2782), Wynder and Hoffmann (4319, 4332)
140-29-4	Benzeneacetonitrile {α-tolunitrile}	Grob (1427)
100-47-0	Benzonitrile	Grob (1426)
109-74-0	Butanenitrile	Grob (1416, 1417, 1422), Wynder and Hoffmann (4332)
625-28-5	Butanenitrile, 3-methyl- {isovaleronitrile}	Grob (1416, 1417), Wynder and Hoffmann (4332)
4786-20-3	2-Butenenitrile {crotononitrile}	Newsome et al. (2782), Wynder and Hoffmann (4332)
628-73-9	Hexanenitrile {capronitrile}	Grob (1416, 1417, 1422), Wynder and Hoffmann (4332)
107-12-0	Propanenitrile	Grob (1413, 1416, 1422), Newsome et al. (2782), Wynder and Hoffmann (4319, 4332)
78-82-0	Propanenitrile, 2-methyl- {isobutyronitrile}	Grob (1413, 1416, 1422), Newsome et al. (2782), Wynder and Hoffmann (4319, 4332)
107-13-1	2-Propenenitrile {acrylonitrile}	Grob (1413, 1416, 1422), Newsome et al. (2782), Wynder and Hoffmann (4319, 4332)
126-98-7	2-Propenenitrile, 2-methyl- {methacrylonitrile}	Grob (1413, 1416, 1422), Newsome et al. (2782), Wynder and Hoffmann 4319, 4332
110-59-8	Pentanenitrile {valeronitrile}	Grob (1416, 1417, 1422), Wynder and Hoffmann (4332)
542-54-1	Pentanenitrile, 4-methyl- {isocapronitrile}	Grob(1416, 1417), Wynder and Hoffmann (4332)
100-54-9	3-Pyridinecarbonitrile {nicotinonitrile}	Grob (1426)

2-propenenitrile (acrylonitrile), and 10 unnamed nitriles as cigarette MSS vapor-phase components, but they listed only 2-propenenitrile (acrylonitrile) as a carcinogen. HCN was listed as a major toxic agent in cigarette smoke in their 2001 article (1743).

Because of its inclusion in so many of the Hoffmann et al. lists, 2-propenenitrile (acrylonitrile) was among the 40 or so smoke components that subsequently became classified as a "Hoffmann analyte." While it did not use the term "Hoffmann analyte" in its 2000 report, the Department of Health (Canada) proposed that analytical data on over 40 components from tobacco smoke should be a requirement (11A01). In its list, the Department of Health (Canada) included 2-propenenitrile (acrylonitrile) and HCN. Examination of the Department of Health (Canada) list reveals that most of its components appear in the biologically active component lists in the publications coauthored by Hoffmann (1727, 1773, 1808, 1740, 1741, 1743, 1744).

Table 11.2 lists the 156 nitriles identified to date in tobacco products. Of the 156, 145 have been identified in tobacco smoke, 30 in tobacco, and 19 in both tobacco and tobacco smoke.

TABLE 11.2
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	107-91-5	Acetamide, 2-cyano- $NC\text{-}CH_2\text{-}CO\text{-}NH_2$	2141, 4249		
2.	57966-95-7	Acetamide, 2-cyano-2-methoxyimino-*N*-(ethylcarbamoyl)- {Cymoxanil®} 		3633	
3.	75-05-8	Acetonitrile $CH_3\text{-}CN$	37, 38, 111, 112, 167, 172, 173a, 199, 239, 298, 299, 480, 568b, 582, 643, 645, 892, 893, 1050, 1063–1066, 1068–1074, 1099, 1140, 1348–1351, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1413, 1416, 1418, 1419, 1437, 1445, 1449, 1586, 1589, 1632, 1634, 1639, 1643, 1744, 1842, 1947, 1966, 2004, 2133, 2134a, 2142, 2252, 2310, 2313a, 2520, 2543, 2545, 2570, 2634, 2724, 2765, 2767, 2777, 2781, 2782, 2799a, 2804, 2822, 2857, 2939, 3254, 3255, 3257, 3300, 3302, 3308, 3373, 3441a, 3482, 3491, 3530, 3557, 3583, 3584, 3692, 3880, 3882, 3883, 3901, 3976, 4005–4007, 4052, 4056, 4162, 4249, 4257, 4319, 4332, 4394, 5512, 5554, 5770, 5811b, 5869a, 4A02		1354, 1375a, 1377, 1378, 4052, 4056
4.	926-64-7	Acetonitrile, (dimethylamino)- $(H_3C)_2{=}N\text{-}CH_2\text{-}CN$	299, 568b, 1063–1066, 1068–1074, 1364, 1365, 1371, 1587, 2506, 2507, 2775, 3255, 3410, 3559, 4249, 5811b		2506 (0), 2507 (0)
5.	107-16-4	Acetonitrile, hydroxy- $HOCH_2\text{-}CN$	568b, 1371, 2543, 2773, 3410, 4249, 5770		
6.	4471-47-0	Acetonitrile, oxo- $O{=}CH\text{-}CN$	314, 568b, 1367, 2545, 4249		
7.	51630-58-1	Benzeneacetic acid, 4-chloro-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®} 	21A19	3585e, 21A19	

(*continued*)

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

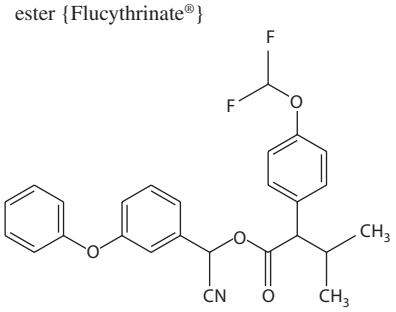
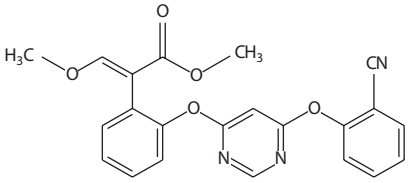
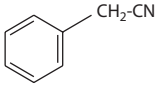
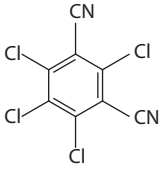
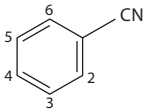
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
8.	70124-77-5	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Flucythrinate®} 		904	
9.	131860-33-8	Benzeneacetic acid, methyl (α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)- {Azoxystrobin®} 		5568	
10.	140-29-4	Benzeneacetonitrile {benzyl cyanide} 	568b, 662, 1360, 1371, 1375, 1375a, 1375b, 1426, 1427, 1586, 2543, 2545, 2724, 2727, 2731, 2735, 2743, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3410, 3491, 3557, 4249, 5811b	568b, 984, 2339a, 3547, 4249, 5811b	1360, 1375a
11.	14191-95-8	Benzeneacetonitrile, 4-hydroxy-	568b, 1375, 1375b, 1586, 2270, 2327c, 3712, 3737, 3741, 3743, 4249		
12.	21850-61-3	Benzeneacetonitrile, 4-hydroxy-α-methyl-	3712		
13.		Benzeneacetonitrile, methyl-	1371		
14.	22364-68-7	Benzeneacetonitrile, 2-methyl-	1371, 2570, 2769, 4249		
15.	2947-61-7	Benzeneacetonitrile, 4-methyl-	1371		
16.	91-15-6	1,2-Benzenedicarbonitrile	568b, 2908, 4249		
17.	626-17-5	1,3-Benzenedicarbonitrile	568b, 2908, 4249		
18.	1897-45-6	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro {Chlorothalonil®} 		3585c, 3633	
19.	623-26-7	1,4-Benzenedicarbonitrile	568b, 2908, 4249		
20.	645-59-0	Benzenepropanenitrile	568b, 666, 1360, 1371, 1375a, 1244, 1586, 1899, 2543, 2545, 2570, 2724, 2727, 2761, 2762, 2765–2767, 2773, 2871, 2939, 3308, 3410, 3491, 3557, 3797, 4249, 5811b		1360, 1375a

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

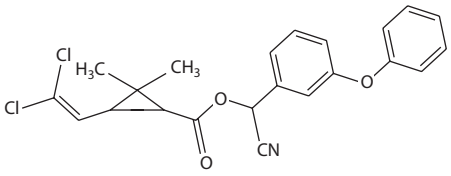
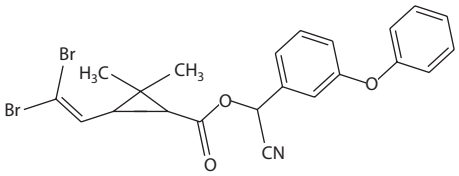
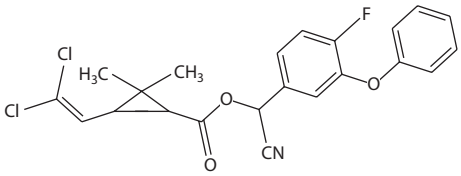
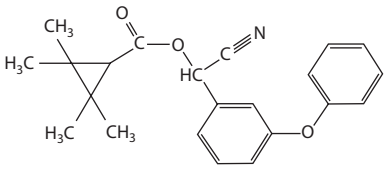
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
21.	100-47-0	Benzonitrile {phenyl cyanide} 	156, 157, 167, 172, 339, 480, 568b, 662, 1313, 1360, 1364, 1375a, 1426–1428, 1899, 2387, 2506, 2507, 2543, 2545, 2724, 2727, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2777, 2799a, 2908, 2912, 3255, 3397, 3410, 3491, 3559, 3729, 4249, 5034, 5811b	568b, 1157, 1248, 2339a, 3547, 4092, 4249	1360, 1375a, 2387, 2506, 2507
22.		Benzonitrile, C_2-alkyl- {two isomers detected}	568b, 2570, 4249		
23.		Benzonitrile, C_3-alkyl- {five isomers detected}	568b, 2570, 4249		
24.	6136-68-1	Benzonitrile, 3-acetyl-	2767, 4249		
25.	1885-29-6	Benzonitrile, 2-amino- {anthranilonitrile}	278, 568b, 4249		
26.	36541-24-9	Benzonitrile, dimethyl-	2726, 2727, 2731, 2735, 3491, 4249		
27.	5724-56-1	Benzonitrile, 2,3-dimethyl-	662, 1364, 1371, 3410, 3485, 3491, 3557, 4249, 5811b		
28.	21789-36-6	Benzonitrile, 2,4-dimethyl-	662, 3557, 4249, 5811b		
29.	13730-09-1	Benzonitrile, 2,5-dimethyl-	568b, 662, 2554, 3485, 3491, 4249, 5811b		
30.	6575-13-9	Benzonitrile, 2,6-dimethyl-	2767, 3485, 3491, 3557, 4249, 5811b		
31.	22884-95-3	Benzonitrile, 3,4-dimethyl-	662, 5811b		
32.	34136-59-9	Benzonitrile, 2-ethyl-	2570, 3485, 3491, 3557, 4249, 5811b		
33.	25550-22-5	Benzonitrile, methyl-	1371, 2543, 2773, 2799a, 3410, 4249, 5034, 5811b		
34.	529-19-1	Benzonitrile, 2-methyl-	37, 38, 568b, 662, 1360, 1375a, 1428, 1899, 2387, 2554, 2727, 2731, 2735, 2761, 2762, 2765, 2766, 2777, 3410, 3491, 3557, 3729, 4249, 4772, 5811b	5811b	1360, 1375a, 2387
35.	34136-57-7	Benzonitrile, 3-ethyl-	3485, 3491, 3557, 4249, 5811b		
36.	873-62-1	Benzonitrile, 3-hydroxy-	2327c, 2570		
37.	620-22-4	Benzonitrile, 3-methyl-	299, 662, 1899, 2727, 2731, 2735, 3491, 4249, 5811b		
38.	3435-51-6	Benzonitrile, 4-ethenyl-	3397, 4249		
39.	25309-65-3	Benzonitrile, 4-ethyl-	662, 2554, 3485, 3491, 3557, 4249, 5811b		
40.	767-00-0	Benzonitrile, 4-hydroxy-	568b, 2327c, 2767, 4249		
41.	104-85-8	Benzonitrile, 4-methyl-	299, 568b, 1428, 1899, 2387, 2545, 2727, 2731, 2735, 3410, 3491, 4249, 5811b		2387
42.	60484-66-4	Benzonitrile, 4-propyl-	3387, 4249		
43.	77417-06-2	Benzonitrile, trimethyl-	662, 2543, 2773		
44.	2571-52-0	Benzonitrile, 2,4,6-trimethyl-	5811, 5811a, 5811b		
45.	61892-66-8	Butanamide, 3-cyano-3-methyl- $(H_3C)_2{=}C(CN)\text{-}CH_2\text{-}CO\text{-}NH_2$	568b, 3553, 4249, 5811b		
46.	53897-27-1	Butanamide, 4-cyano- $NC\text{-}(CH_2)_3\text{-}CO\text{-}NH_2$	568b, 3553, 4249, 5811b		
47.	110-61-2	Butanedinitrile {succinonitrile} $NC\text{-}(CH_2)_2\text{-}CN$	568b, 3553, 4249		

(*continued*)

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
48.	16411-13-5	Butanedinitrile, 2,3-dimethyl- NC-CH(CH_3)-CH(CH_3)-CN		4249	
49.	109-74-0	Butanenitrile H_3C-$(CH_2)_2$-CN	37, 38, 112, 314, 348, 1063–1066, 1068–1074, 1140, 1348–1350, 1354, 1365, 1374, 1375a, 1413, 1416–1418, 1419, 1422, 1586, 1589, 1947, 2004, 2142, 2543, 2545, 2570, 2724, 2765, 2767, 2777, 2857, 3255, 3302, 3308, 3491, 3557, 3559, 4052, 4056, 4162, 4249, 4332, 5770, 5811b	5811b	1354, 1375a, 4052, 4056, 4249
50.	13989-82-7	Butanenitrile, 4-(dimethylamino)- $(H_3C)_2$═N-$(CH_2)_3$-CN	2773, 4249		
51.	4476-02-2	Butanenitrile, 2-hydroxy- H_3C-CH_2-CHOH-CN	172, 1067, 1075, 1364, 1365, 1371, 2545, 2773, 3553, 4249		
52.	15344-34-0	Butanenitrile, 2-hydroxy-3-methyl- $(H_3C)_2$═CH-CHOH-CN	172, 1067, 1075, 4249, 4578, 4579		
53.	18937-17-9	Butanenitrile, 2-methyl-	568b, 4249, 4570a, 5770		
54.	625-28-5	Butanenitrile, 3-methyl- $(H_3C)_2$═CH-CH_2-CN	112, 299, 314, 568b, 1140, 1313, 1365, 1418, 1419, 1587, 1947, 2142, 2543, 2545, 2724, 2765, 2767, 2773, 3255, 3308, 3491, 3797, 4249, 4332, 4570a, 5034, 5770, 5811b	568b, 2339a, 4249	
55.	4786-20-3	2-Butenenitrile {crotononitrile} H_3C-CH═CH-CN	299, 568b, 1063–1066, 1068–1074, 1140, 1365, 1419, 2724, 2733, 2782, 2804, 3302, 3308, 3491, 4249, 4332, 5770, 5811b		
56.	1190-76-7	2-Butenenitrile [*cis* or *trans*]	568b, 4249, 5770		
57.	4786-24-7	2-Butenenitrile, 3-methyl-	4570a		
58.	109-75-1	3-Butenenitrile {allyl cyanide} H_2C═CH-CH_2-CN	112, 299, 568b, 1140, 1365, 1419, 2387, 2724, 3302, 3491, 3557, 4249, 5811b		
59.	4786-19-0	3-Butenenitrile, 3-methyl-	4570a		
60.	156-62-7	Cyanamide, calcium salt Ca═N-CN		3633	
61.	1467-79-4	Cyanamide, dimethyl- $(CH_3)_2$═N-CN	4249	5811b	
62.	57-12-5	Cyanide ion CN^{-1}	2170, 2524, 2627, 5079		
63.		Cyanide radical CN	27A68, 27A99, 27A100		
64.		Cyanide radical {acrylonitrile radical} C_3H_2N	27A68		
65.		Cyanide radical C_3H_4N	27A68		
66.	91465-08-6	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {λ-Cyhalothrin®}	21A19	2650b, 21A19	

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
67.	52315-07-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {Cypermethrin®} 	21A19	904, 1219b, 1219c, 3188a, 3585e, 3633, 4249, 4271a, 5568, 21A19	
68.	67375-30-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {α-Cypermethrin®}	21A19	3633, 21A19	
69.	52918-63-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl)methyl ester {Deltamethrin®} 	21A19	904, 1219b, 1219c, 3585e, 3633, 4271a, 21A19	
70.	68359-37-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester {Cyfluthrin®} 		904, 3633	
71.	66841-25-6	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-, cyano(3-phenoxyphenyl)methyl ester {Tralomethrin®}		21A05	
72.	39515-41-8	Cyclopropanecarboxylic acid, 2,2,3,3-tetramethyl cyano(3-phenoxyphenyl)methyl ester {Fenpropathrin®, Danitol®} 	21A19	21A19	
73.	4616-73-3	Eicosanenitrile $H_3C\text{-}(CH_2)_{18}\text{-}CN$	2767, 4249		
74.	460-19-5	Ethanedinitrile {cyanogen} NC-CN	513, 1741, 1971, 1991, 2079, 2634, 2724, 2939, 3300, 3302, 3308, 3491, 3932, 4249, 4332, 5079, 5811b		

(*continued*)

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
75.	617-90-3	2-Furancarbonitrile	568b, 2726, 2731, 2735, 2777, 4249		
76.	13714-86-8	2-Furancarbonitrile, 5-methyl-	2726, 2727, 2731, 2735, 2777, 3491, 4249, 5811b		
77.	646-20-8	Heptanedinitrile $NC\text{-}(CH_2)_5\text{-}CN$	299, 1371, 4249		
78.	629-08-3	Heptanenitrile	5811, 5811a, 5811b		
79.	628-73-9	Hexanenitrile {capronitrile} $H_3C\text{-}(CH_2)_4\text{-}CN$	112, 568b, 1413, 1416–1419, 1422, 1428 2545, 2724, 2767, 3302, 3308, 3491, 3557, 4249, 4332, 4570a, 5034		
80.	64350-07-8	Hexanenitrile, 2-hydroxy-	1368, 4249		
81.	74-90-8	Hydrocyanic acid {hydrogen cyanide} HCN	80–83, 110, 112, 126b, 167, 172, 174a, 174b, 174c, 174e, 213, 237–239, 267, 269, 270, 314, 337, 402, 429a, 480, 491, 513, 577, 603, 631, 688, 722, 747, 748, 765, 779, 780, 804, 861, 916, 918a, 920, 966, 1051, 1063–1074, 1077a, 1091, 1092, 1099, 1119, 1140, 1202, 1235, 1276, 1283, 1284, 1292, 1329, 1330, 1332–1336, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1331, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1442, 1445, 1466, 1467, 1469, 1492, 1497, 1498, 1589, 1668, 1673, 1674, 1693, 1695, 1719, 1741, 1744, 1746, 1751, 1760, 1781, 1803, 1807a, 1842, 1932, 1956, 1966, 1967, 2059, 2062, 2067, 2068, 2079, 2083–2086, 2133, 2134a, 2142, 2157, 2159, 2170, 2252, 2270, 2293, 2310, 2313a, 2313c, 2313d, 2326, 2342, 2342a, 2343, 2344, 2502, 2506, 2507, 2537, 2543, 2545, 2570, 2607, 2608, 2628, 2634, 2679, 2683, 2724, 2761, 2762, 2775, 2777, 2780, 2782, 2799a, 2801, 2804, 2805, 2866, 2939, 2942, 2956, 2971, 2973, 3007, 3029, 3059, 3087, 3088, 3101, 3116, 3120, 3121, 3121a, 3132, 3135–3137, 3139, 3140, 3145, 3148, 3149, 3190, 3251, 3254, 3255, 3257, 3290, 3300–3302, 3306, 3308, 3370, 3482, 3491,	2607, 3290, 3633, 4064, 4271a, 5079, 5189, 5811b	1330 (0), 1332 (0) 1354, 1375a, 1377, 1378, 2506, 2507, 4052, 4056

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Hydrocyanic acid {hydrogen cyanide} HCN (cont.)	3493, 3524, 3525, 3530, 3557, 3690, 3724, 3729, 3844, 3872, 3876, 3880–3882, 3897, 3909–3911, 3917a, 3939, 3952, 3973, 3976, 3984, 3992, 3996, 4005–4007, 4010, 4011, 4052, 4053, 4056, 4063, 4064, 4109, 4143, 4162, 4202, 4249, 4259, 4260, 4301, 4319, 4342, 4360, 4365, 4398, 4418, 4502, 4743, 4745, 4816, 5042, 5079, 5140, 5189, 5208, 5219, 5263, 5512, 5531, 5546, 5547, 5554, 5587, 5811b, 5835, 5836, 5869a		
82.		1*H*-Indole-2-acetonitrile, 1-methyl-	2327c		
83.	771-51-7	1*H*-Indole-3-acetonitrile	1842, 1898, 3219, 3255, 3257, 3265, 3308, 3685, 4249, 5811b		
84.	64849-99-6	Isoquinolinecarbonitrile	1587, 4249		
85.	1198-30-7	1-Isoquinolinecarbonitrile	1587		
86.	132-75-2	1-Naphthaleneacetonitrile	278, 4249		
87.	25551-35-3	Naphthalenecarbonitrile	172, 480, 1897, 4249, 5034, 5811b		
88.		Naphthalenecarbonitrile, alkyl-	2141, 3491		
89.		Naphthalenecarbonitrile, methyl-{two isomers}	662		
90.	86-53-3	1-Naphthalenecarbonitrile	480, 642, 662, 1897, 2141, 3410, 3491, 4249, 5811b		
91.	77417-07-3	1-Naphthalenecarbonitrile, 3-methyl-	5811a		
92.	23245-64-9	1-Naphthalenecarbonitrile, 5-nitro-	4249		
93.	613-46-7	2-Naphthalenecarbonitrile	662, 1897, 2141, 3410, 3491, 3729, 4249		
94.	124-12-9	Octanenitrile	568b, 4249		
95.	110-59-8	Pentanenitrile {valeronitrile} H_3C-$(CH_2)_3$-CN	112, 172, 299, 314, 346, 568b, 1063–1066, 1068–1074, 1140, 1365, 1374, 1375a, 1377, 1413, 1416–1419, 1422, 1947, 2002, 2004, 2142, 2545, 2724, 2767, 3255, 3302, 3308, 3491, 3557, 4249, 4332, 4570a, 5034, 5811b		1375a, 1377
96.	69975-94-6	Pentanenitrile, 2,4-dimethyl- H_3C-$CH(CH_3)$-CH_2-$CH(CH_3)$-CN	4249		
97.		Pentanenitrile, 2-hydroxy-	1067		
98.		Pentanenitrile, 3-hydroxy-4-methyl-	1364		
99.		Pentanenitrile, methyl-	1418, 5034		
100.	6339-13-5	Pentanenitrile, 2-methyl- H_3C-$(CH_2)_2$-$CH(CH_3)$-CN	314, 1360, 1365, 1371, 1375a, 2761, 2762, 2765, 4249, 4570a		1360, 1375a
101.	21101-88-2	Pentanenitrile, 3-methyl-	4570a, 5034		
102.	542-54-1	Pentanenitrile, 4-methyl- $(H_3C)_2$ = $CH(CH_2)_2$-CN	112, 568b, 1140, 1416–1419, 2545, 2724, 3491, 3797, 4249, 4332, 4570a, 5770, 5811b		
103.	927-56-0	Pentanenitrile, 4-oxo- H_3C-CO-$(CH_2)_2$-CN	4249		
104.	592-51-8	4-Pentenenitrile	1365, 1587, 4249		

(*continued*)

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

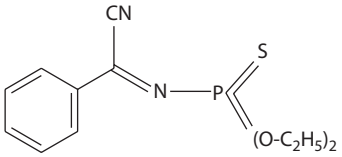
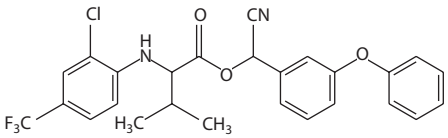
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
105.	14816-18-3	Phosphorothioic acid, *O,O*-diethyl *O*-(α-cyanobenzylideneamino)- {Phoxim®} 		1492a, 4271a	
106.		Piperidine, 1-(3-pyridinemethyl)-2-cyano-4, 5-didehydro-	4570a		
107.		Piperidine, 1-(3-pyridinemethyl)-2-cyano-4, 5-didehydro-	4570a		
108.	61892-68-0	Propanamide, 3-cyano- $NC\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}NH_2$	568b, 3553, 4249, 5811b		
109.	107-12-0	Propanenitrile $H_3C\text{-}CH_2\text{-}CN$	37, 38, 112, 172, 173a, 299, 314, 568b, 1063–1066, 1068–1074, 1140, 1348–1350, 1354, 1364, 1365, 1374, 1375a, 1375a, 1377, 1378, 1413, 1414, 1416, 1418, 1419, 1422, 1589, 1634, 1639, 1643, 1947, 2002, 2004, 2142, 2313a, 2543, 2545, 2559, 2559a, 2570, 2724, 2733, 2765–2767, 2773, 2777, 2782, 2804, 2857, 2939, 3255, 3302, 3308, 3491, 3530, 3557, 3797, 3901, 4052, 4056, 4162, 4249, 4290, 4319, 4332, 5770, 5811b	38, 568b, 4249, 5811b	1354, 1375a, 1377, 1378, 4052, 4056, 4249
110.	78-97-7	Propanenitrile, 2-hydroxy- $H_3C\text{-}CHOH\text{-}CN$	568b, 1067, 1360, 1371, 1375a, 2543, 2545, 2679, 2761, 2762, 2775, 2777, 3410, 3553, 4249, 5770, 5811b		1360, 1375a
111.	75-86-5	Propanenitrile, 2-hydroxy-2-methyl- $(H_3C)_2{=}COH\text{-}CN$	568b, 3553, 4249, 5770, 5811b		
112.	78-82-0	Propanenitrile, 2-methyl- {isobutyronitrile} $(H_3C)_2{=}CH\text{-}CN$	37, 38, 112, 299, 314, 348, 568b, 1063–1066, 1068–1074, 1140, 1348–1350, 1354, 1375a, 1377, 1412–1414, 1416, 1418, 1419, 1422, 1586, 1589, 1637, 2004, 2543, 2545, 2559, 2559a, 2570, 2724, 2765, 2767, 2777, 2782, 2804, 2857, 3302, 3308, 3491, 3901, 4052, 4056, 4162, 4249, 4319, 4332, 4570a, 5770, 5811b	568b, 2339a, 4249, 5811b	1354, 1375a, 1377, 4052, 4056
113.	78-67-1	Propanenitrile, 2-methyl-, 2,2′-azobis- {Porofor-57®}		3476	
114.	631-57-2	Propanenitrile, 2-oxo- $H_3C\text{-}CO\text{-}CN$	568b, 642, 4249		
115.	60153-49-3	Propanenitrile, 3-(methylnitrosoamino)- {MNPN} $CH_3\text{-}N(NO)\text{-}(CH_2)_2\text{-}CN$	3256	2994, 3947, 3948	
116.	1738-25-6	Propanenitrile, 3-(dimethylamino)-	2506, 3559, 4249		
117.	111-97-7	Propanenitrile, 3,3′-thiobis-	568b, 1587, 4249, 5811b		

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
118.	107-13-1	2-Propenenitrile {acrylonitrile} $H_2C{=}CH\text{-}CN$	73, 126a, 174b, 299, 314, 402, 566–568, 603, 688, 1140, 1148, 1217, 1262a, 1365, 1373, 1374, 1375a, 1377, 1386, 1413, 1416, 1422, 1445, 1634, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 2270, 2313a, 2520, 2545, 2634, 2645, 2724, 2767, 2781, 2782, 2804, 2825, 2857, 3007, 3190, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3491, 3530, 3557, 3692, 3714, 3882, 3897, 3992, 4005–4007, 4078, 4166, 4249, 4319, 4332, 4360, 4998, 5049, 5512, 5547, 5554, 5692a, 5770, 5811b, 5836, 5869a		1375a, 1377, 4249
119.	126-98-7	2-Propenenitrile, 2-methyl- {methacrylonitrile} $H_2C{=}C(CH_3)\text{-}CN$	605, 1140, 1374, 1412, 1413, 1416, 1422, 2724, 2782, 2804, 3302, 3308, 3491, 3557, 4249, 4319, 4332, 5770, 5811b		
120.	4360-47-8	2-Propenenitrile, 3-phenyl- {cinnamonitrile}	662, 1586, 2553, 2724, 2731, 2735, 2767, 3308, 3485, 3557, 4249, 4570a, 5811b		
121.	54356-27-3	2-Propenenitrile, 3-(3-pyridinyl)-, (*E*)-	568b, 1587, 4249, 5811b		
122.	54356-28-4	2-Propenenitrile, 3-(3-pyridinyl)-, (*Z*)-	568b, 1587, 4249, 5811b		
123.	36541-27-2	Pyridinecarbonitrile, dimethyl-	2731, 2735, 4249, 5811, 5811a, 5811b	5811, 5811a, 5811b	
124.	36541-26-1	Pyridinecarbonitrile, methyl-	1587, 2727, 2731, 2735, 3491, 4249, 5811, 5811a		
125.	55738-21-1	Pyridinedicarbonitrile	2908, 4249		
126.	100-70-9	2-Pyridinecarbonitrile	568b, 1587, 3190, 3499, 3992, 4249, 4570a, 5811b		
127.	20970-75-6	2-Pyridinecarbonitrile, 3-methyl-	568b, 1587, 4249		
128.	1620-76-4	2-Pyridinecarbonitrile, 4-methyl-	568b, 1587, 4249		
129.	35549-47-4	2-Pyridinepropanenitrile	568b, 1587, 4249, 5811b		
130.	100-54-9	3-Pyridinecarbonitrile {nicotinonitrile}	107, 299, 299, 480, 568b, 1078, 1099, 1140, 1371, 1426, 1427, 1568, 1587a, 2228, 2387, 2470, 2493, 2543, 2545, 2570, 2724, 2727, 2731, 2732, 2735, 2765, 2775, 3255, 3302, 3308, 3386, 3398, 3410, 3463, 3468, 3470, 3491, 3499, 3505, 4249, 4570a, 5034, 5079, 5811b, 25A84	568b, 937, 2339a, 3491, 4249, 5811b, 17B61	2387
131.	38076-78-7	3-Pyridinecarbonitrile, 2-amino-5-methyl-	1587, 4249, 5811b		
132.	71607-63-1	3-Pyridinecarbonitrile, dimethyl-	2727, 2735, 3491, 4249		
133.	61391-07-9	3-Pyridinecarbonitrile, 5-ethyl-	1587, 4249		
134.	3222-52-4	3-Pyridinecarbonitrile, 6-ethyl-; 5-pyridinecarbonitrile, 2-ethyl-	568b, 1587, 4249, 5811b		
135.	5444-01-9	3-Pyridinecarbonitrile, 4-methyl-	568b, 1587, 4249, 5811b		
136.	42885-14-3	3-Pyridinecarbonitrile, 5-methyl-	568b, 1371, 1587, 3729, 4249, 5811b		

(*continued*)

TABLE 11.2 (continued)
Nitriles in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
137.	13121-99-8	4-Pyridineacetonitrile	568b, 1568, 1587, 4249, 5811b		
138.	100-48-1	4-Pyridinecarbonitrile	568b, 3255, 3499, 3729, 4249, 5811b		
139.	71646-51-0	1*H*-Pyrrolecarbonitrile, methyl-	2761, 2767, 4249		
140.	4513-94-4	1*H*-Pyrrole-2-carbonitrile	1365, 1371, 1586, 1587a, 2761, 2762, 2765, 2766, 2773, 3410, 3491, 3650, 4249, 5811b		
141.	133829-71-7	1*H*-Pyrrole-2-carbonitrile, methyl- {two isomers}	1587a, 2761, 2762, 2765, 2766, 4249		
142.	26173-92-2	1*H*-Pyrrole-2-carbonitrile, 5-methyl-	568b, 1587, 2543, 2761, 2765, 2766, 2773, 2775, 3491, 3650, 4249, 5811b		
143.		1*H*-Pyrrole-3-acetonitrile	1586, 2767, 4249		
144.	7126-38-7	1*H*-Pyrrole-3-carbonitrile	568b, 1375, 1375b, 1586, 2543, 2545, 2761, 2762, 2765, 2766, 2773, 2775, 3557, 4249		
145.		Pyrrolidine, 1-(3-pyridinemethyl)-2-cyano-	4570a		
146.	29134-29-0	1-Pyrrolidineacetonitrile	568b, 1063–1066, 1068–1074, 1371, 1587, 3410, 3559, 4249, 5811b		
147.	35543-25-0	1-Pyrrolidinebuyronitrile	568b, 4249		
148.	1530-88-7	1-Pyrrolidinecarbonitrile	568b, 4249		
149.	64850-00-6	Quinolinecarbonitrile	1587, 2132, 4249, 5811b		
150.	59551-02-9	5-Quinolinecarbonitrile	568b, 1587, 4249, 5811b		
151.	23395-72-4	6-Quinolinecarbonitrile	568b, 1587, 4249, 5811b		
152.	67360-38-7	7-Quinolinecarbonitrile	568b, 1587, 3226, 3280, 4160, 4249		
153.	463-56-9	Thiocyanic acid HSCN	1140, 1971, 2170, 2270, 2607, 2724, 2939, 2940, 3302, 3491, 3525, 3797, 4249, 4319, 4332, 5079, 5811b	2607, 3525, 5079	
154.	556-64-9	Thiocyanic acid, methyl ester CH_3-SCN	1587, 4249, 5039, 5770		
155.	505-14-6 15941-77-2	Thiocyanogen $(SCN)_2$	1140, 1971, 2724, 2939, 2940, 3302, 3491, 3797, 3931, 4249, 5079, 5811b		
156.	102851-06-9	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®} 		904, 2346, 3585e	

12 Acyclic Amines

The great diversity and number of the *N*-containing components in tobacco and tobacco smoke make it difficult to categorize them and catalog the members in each category. Examination of past reviews indicates that their authors had the same problems even when the numbers of components in the various categories were much fewer than they are now. The categorization used herein is an attempt to present a simplified but complete system for the reader. Because of its nature, tobacco and its smoke contain a multitude of *N*-containing components distributed among various categories. The simplest categories, of course, are the nitriles and the acyclic or aliphatic amines. The latter category also includes individual amino acids and their complexes (proteins, polypeptides), many of which possess a nonsubstituted amino group. More complex are the pentacyclic and hexacyclic *N*-containing components plus those that are combinations of more than one of each type, i.e., linked pentacyclic structures (porphyrin), linked hexacyclic structures (2,3′-bipyridine), or a linked pentacyclic and hexacyclic structure [3-(1-methyl-2-pyrrolidinyl)-pyridine (nicotine)]. Even more complex are those structures in which two or more cyclic units are fused with at least one containing *N* in its cycle, i.e., the aza-arenes. Also pertinent to tobacco smoke chemistry are the components possessing a combination of an amino group with an aza-arene structure such as occurs in the *N*-heterocyclic amines.

All categories mentioned, except the amino acids, include components comprising carbon, hydrogen, and nitrogen. However, several other categories, like the amino acids and the *N*-nitrosamines, include oxygen in the molecule, e.g., the amides {I}, imides {II}, and lactams {III} (Figure 12.1). Herein, the amines will be discussed and cataloged. Subsequently, the other categories mentioned will be discussed and cataloged, i.e., amides, imides, and lactams, components with five-member *N*-containing rings, six-member *N*-containing rings, and combinations of them, the aza-arenes, and the *N*-heterocyclic amines. The amino acids were discussed and cataloged previously. Other components, similar to the *N*-heterocyclic amines in which an amino group is attached to a fused *N*-containing system, have been identified in tobacco and/or smoke, e.g., 1*H*-purin-6-amine (adenine).

Because of the multitude of nicotine-related alkaloids, amino acids, and proteins in tobacco, diligent research eventually led to the identification of a host of alkyl amines in tobacco and smoke. In addition to ammonia, the only alkylamine listed as a tobacco smoke component in 1954 by Kosak (2170) was methylamine, but he questioned its identification even though he cited the 1904 report by Thoms (3912) and the 1930 report by Koperina (2161) on its identification. A similar Koperina report (2162) appeared in a 1931 monograph edited by Shmuk on tobacco research (3655c).

In their 1959 review, Johnstone and Plimmer (1971) listed ammonia and trimethylamine as identified tobacco and smoke components and methylamine, dimethylamine, and ethylamine as identified tobacco smoke components. Nearly a decade later, in addition to the amino acids, Stedman listed over 40 components with either a free or substituted amino group [see Table XI in (3797)]. In their 1977 tabulations of aliphatic and aromatic amines, Schmeltz and Hoffmann listed nearly 80 components almost equally divided between aliphatic and aromatic amines [see Tables I and II in (3491)]. Many of those they listed were identified in tobacco in the late 1960s by Irvine and Saxby (1877) and in tobacco smoke by Pailer et al. (2882, 2883, 2889).

Ishiguro and Sugawara (1884) had a few more amines than those listed in the Schmeltz–Hoffmann compilation because they included as aliphatic amines several cyclic amines and their alkyl derivatives, e.g., pyrrolidine and piperidine. However, this need not be considered a discrepancy. Examination of the structures of *N*-ethylethanamine (diethylamine) {IV} *vs.* pyrrolidine {V} or *N*-(1-methylethyl)-2-propanamine {VI} *vs.* 2,5-dimethylpyrrolidine {VII} reveals the structural similarities (Figure 12.2).

While Tso (3973) in his 1990 book listed numerous nicotine alkaloid-related amines as identified tobacco components, his list also included ammonia but very few alkylamines and no aromatic aniline-related amines in tobacco [see Table 27-1, Part IV in (3973)].

In addition to the simplest amine of all, ammonia, included in Table 12.1 for the sake of completeness are hydroxylamine and hydrazine and several alkylhydrazine derivatives.

The source of many of the amines, including the alkylamines in tobacco and/or its smoke, is the disintegration of various proteins, individual amino acids, and nicotine-related alkaloids (2001, 3477, 4275a) during tobacco growth or the smoking process (3972). Obviously, a portion of those amines identified in both tobacco and tobacco smoke occur in the smoke because of their transfer from the tobacco during the smoking process. The various benzenamine (aniline)-related components in tobacco are considered to arise from

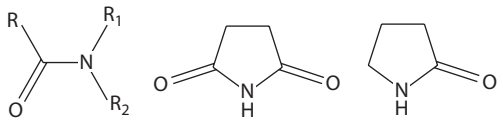


FIGURE 12.1 Oxygenated *N*-containing components of tobacco and tobacco smoke.

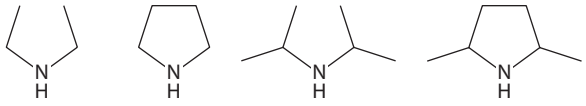


FIGURE 12.2 Structural similarities of alkylamines and pyrrolidines.

enzymatic or microbial disintegration of the amino acids phenylalanine or tyrosine (3491). Schmeltz et al. (3499) reported that the benzenamine-related amines were not generated from nicotine during the tobacco smoking process.

In its 1986 monograph on tobacco smoking, the International Agency for Research on Cancer (IARC) [see pp. 107–109 in (1870)] noted that about 200 amines had been identified in tobacco smoke, based on its citation of the 1977 review by Schmeltz and Hoffmann (3491) and the 1982 review by Dube and Green (1067) and the report by Heckman and Best (1587). IARC described the per cigarette smoke yield of several alkylamines, noting that the most plentiful was methylamine. Citing the data presented by Patrianakos and Hoffmann (2900), IARC also discussed the per cigarette

TABLE 12.1
IARC Evaluation of Carcinogenicity of Various Aromatic Amines in Tobacco Smoke (1870)

CAS No.	Amine	Yield, ng/cig	Degree of Evidence in	
			Animals	Humans
62-53-3	Benzenamine {aniline}	102, 364[a]	Limited evidence	—
95-53-4	Benzenamine, 2-methyl- {*o*-toluidine; 2-toluidine}	30–337[b] 32, 162[a]	Sufficient evidence	Inadequate evidence
104-94-9	Benzenamine, 4-methoxy- {*p*-anisidine}	Present	Sufficient evidence	—
92-67-1	[1,1′-Biphenyl]-4-amine {4-aminobiphenyl}	2–5.6[c] 2.4, 4.6[a]	Sufficient evidence	Sufficient evidence
302-01-2	Hydrazine	24–43[b]	Sufficient evidence	Inadequate evidence
57-14-7	Hydrazine, 1,1-dimethyl-	Present[b]	Sufficient evidence	—
134-32-7	1-Naphthalenamine	4.3, 2.5[a]	Inadequate evidence	Inadequate evidence
91-59-8	2-Naphthalenamine	1–334[b] 1.0, 1.7[a]	Sufficient evidence	Inadequate evidence
135-88-6	2-Naphthalenamine, *N*-phenyl-	Present	Inadequate evidence	Inadequate evidence

[a] Data cited by IARC (1870) from Patrianakos and Hoffmann (2900): first value is for a U.S. 85-mm nonfiltered cigarette; second value is for a French 70-mm nonfiltered cigarette.

[b] Data cited by Hoffmann and Hoffmann (1741, 1743, 1744).

[c] Data cited by Hoffmann and Hoffmann (1743, 1744).

mainstream and sidestream smoke yields of several aromatic amines including 11 benzenamines, the 1- and 2-naphthalenamines, and the [1,1′-biphenyl]-2-, 3-, and 4-amines (the aminobiphenyls). IARC noted that it had previously evaluated the carcinogenicity of several tobacco smoke aromatic amines, namely, 1- and 2-naphthalenamine, [1,1′-biphenyl]-4-amine, benzenamine (aniline), 2-methylbenzenamine (*o*-toluidine), *N*-phenyl-2-naphthalenamine, and 2-methoxybenzeneamine (*o*-anisidine). Table 12.1 summarizes the IARC categorization of several amines, including hydrazine and 1,1-dimethylhydrazine, identified in tobacco smoke [see Appendix 2 in (1870)].

The IARC monograph (1870) is based on the findings of its 1985 working group. Despite its review of the literature to 1985, the IARC had no comment about the numerous reports (1835a, 2491a, 2492, 2849, 2849a, 2949b, 3829a, 3862b, 3862c, 3862d, 3865b, 4365a, 4388) issued from 1975 to 1985 on the isolation initially from cooked food and subsequently from tobacco smoke of the tumorigenic and highly mutagenic *N*-heterocyclic amines.

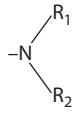
There are several interesting aspects to the Searle-edited American Chemical Society 1984 monograph on chemical carcinogens (3568):

- Despite a voluminous review by Dipple et al. (983) on PAHs and the tumorigenicity of many of them, no mention was made of a tumorigenic or carcinogenic PAH in tobacco smoke.
- The only significantly tumorigenic, carcinogenic, or biologically active tobacco and tobacco smoke components discussed in the 1400-page monograph were the *N*-nitrosamines [see pp. 839–844 in Preussmann and Eisenbrand (2990)]. Much of the data cited by Dipple et al. were those previously presented by Hoffmann et al. (514, 1680, 1685).
- In two chapters on the tumorigenicity of aromatic amines, neither Garner et al. (1275a) nor Parkes and Evans (12A02) mention the presence in tobacco smoke of the aromatic amines categorized as significant tumorigens or carcinogens, namely, 2-naphthalenamine, [1,1′-biphenyl]-4-amine, and 2-methylbenzenamine (*o*-toluene). Garner et al. [see Table I in (1275a)] tabulated the tumorigenicity results of studies on many substituted benzenamines (anilines). The data indicated that several appeared to be as tumorigenic as or even more tumorigenic than 2-methylbenzenamine (*o*-toluidine), a tobacco smoke component listed as a significant tumorigen (1217, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 2825). Each of them has been identified as a tobacco smoke component, e.g., 3-methylbenzeneamine (*m*-toluidine), 4-methylbenzeneamine (*p*-toluidine), and 2,4,6-trimethylbenzenamine (mesitylamine), but none was listed as a significant tumorigen.
- Despite the number of reports issued after 1975 on *N*-heterocyclic amines, Garner et al. (1275a) did not mention their presence in tobacco smoke. They commented as follows:

A multitude of new aromatic amine or heterocyclic amino compounds will most likely be discovered in the foreseeable future, such as those found in cooked foods [Yamazoe et al. (4370a), Takeda et al. (12A03)].

Several of the components listed in Table 12.1 have been included in many of the lists of carcinogens, tumorigens, or biologically active components in cigarette smoke presented by Fowles and Bates (1217), Hoffmann et al. (1727, 1740, 1741, 1743, 1744, 1773, 1808), and OSHA (the Occupational Safety and Health Administration) (2825). Based on these lists, the per cigarette yields proposed by some authorities, e.g., the Department of Health (Canada) (12A01), to be determined of the "Hoffmann analytes" among the amines include 1-naphthalenamine, 2-naphthalenamine, [1,1′-biphenyl]-3-amine, [1,1′-biphenyl]-4-amine, 2-methylbenzenamine (*o*-toluidine), and ammonia.

The primary goal in Table 12.2 is the listing of those tobacco and/or smoke components that are acyclic amines. In some cases, an amino group, either unsubstituted (-NH_2) or substituted {VIII}, may be linked to a cyclic *N*-containing structure, e.g., 2-pyridinamine, 2-amino-1,7-dihydro-6*H*-purin-6-one (guanine), but the reason for inclusion of the component in Table 12.2 is that part of the molecule is an acyclic amine.



VIII

For the sake of completeness, several components have been included in Table 12.2 because they possess the amine function (-NH_2) but are not linked to a carbon atom, e.g., ammonia, hydrazine, hydroxylamine. None of these fits the definition of an amide, imide, or lactam. Other components included in Table 12.2 for the sake of completeness are the amino acids with acyclic unsubstituted or substituted amine group, the acyclic *N*-nitrosamines, and the *N*-heterocyclic amines. With the inclusion in Table 12.2 of the various items just mentioned, the number of acyclic amines and their derivatives totals 510, with 295 identified in tobacco smoke, 354 in tobacco, and 139 in both tobacco and tobacco smoke.

TABLE 12.2
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

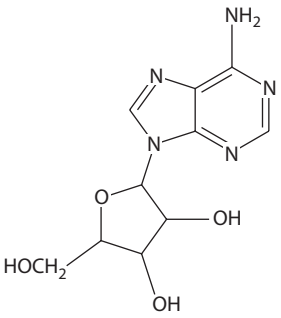
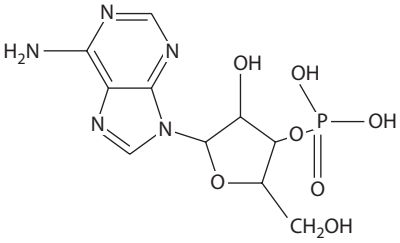
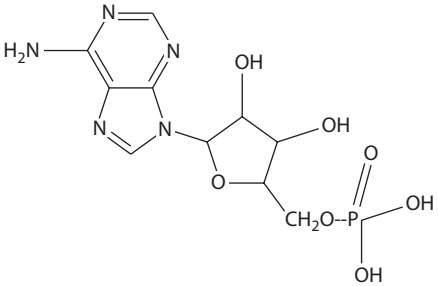
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	6542-88-7	Acetaldehyde, amino- H_2N-CH_2-CH═O	568b, 3410, 4249		
2.	926-64-7	Acetonitrile, (dimethylamino)- $(H_3C)_2$═N-CH_2-CN	299, 568b, 1063–1066, 1068–1074, 1364, 1365, 1371, 1587, 2506, 2507, 2775, 3255, 3410, 3559, 4249, 5811b		2506 (0), 2507 (0)
3.	58-61-7	Adenosine 		429b, 4249, 4828, 5540	
4.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P′* → 5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249	
5.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
6.	84-21-9	3′-Adenylic acid 		429b, 4249, 4758	
7.	61-19-8	5′-Adenylic acid 		429b, 4249	
8.	20268-93-3	5′-Adenylic acid, *N*-(3-methyl-2-butenyl)-		4249, 4536	
9.	13484-66-7	5′-Adenylic acid, *N*-(phenylmethyl)-		4249	
10.	6898-94-8	Alanine	1910, 1914, 2858, 2939, 3266, 3555, 3797	1053, 1086, 2079, 3266, 3555, 3797	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
11.	62-57-7	Alanine, 2-methyl-		429b, 4249, 4580, 4626, 5777	
12.	13100-82-8	Alanine, 3-sulfo-		3797, 3983b	
13.	107-95-9	β-Alanine $H_2N\text{-}(CH_2)_2\text{-}COOH$	1083, 1351, 1910, 1914, 2858, 2939, 3224, 3266, 3302, 3491, 3797, 4249, 4319	120, 158, 622, 749, 752-754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2270, 2337, 2338, 2359, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5603, 5785, 5811b, 5827, 5831, 5881, 5905	
14.	79-83-4 137-08-8	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- {pantothenic acid} $HO\text{-}CH_2\text{-}C(CH_3)_2\text{-}CHOH\text{-}CO\text{-}NH\text{-}(CH_2)_2\text{-}COOH$		429b, 1941, 4249, 4758, 5079	
15.	10478-42-9	β-Alanine, *N*-methyl-*N*-nitroso- {NMPA} {propanoic acid, 3-(methylnitrosamino)-} $H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOH$	3256, 3300, 3943a, 3944–3946	466, 485, 503, 982, 2852, 3943a, 3944–3946, 3971, 3973, 5001	
16.	133201-38-4	β-Alanine, *N*-(nitrosomethyl)-	4249	4249	
17.		β-Alanine, *N*-methyl-*N*-nitroso-, methyl ester $H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOCH_3$	4249	4249	
18.	923-16-0	*D*-Alanine, *N*-*D*-alanyl-		1351, 2337, 2797, 3491, 4249	
19.	56-41-7	*L*-α-Alanine $H_3C\text{-}CH(NH_2)\text{-}COOH$	1083, 1351, 1914, 2724, 3491	120, 158, 622, 749, 752–754, 826a, 1223, 1305a, 1351, 1493, 1918, 1919, 2799a, 2270, 2337, 2338, 2394a, 2453, 2529, 2532, 2597a, 2795, 2911a, 2911c, 3491, 3499, 3780, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4398c, 5079, 5603, 5699, 5785, 5881, 5905, 5907	
20.	16124-24-6 25127-16-6	*L*-Alanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1063–1066, 1068–1074, 1351, 2337, 3639, 3797, 3923, 4362, 5811b	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

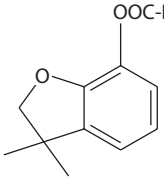
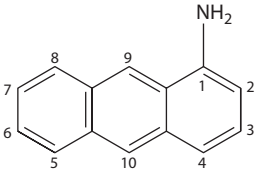
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
21.	82560-54-1	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy)carbonyl)methylamino)thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}  R═NH-S-N[CH(CH$_3$)$_2$]-(CH$_2$)$_2$-COOC$_2$H$_5$		3633	
22.	19701-89-4	*DL*-Alanine, *N,N*-dimethyl-	2882, 4249		
23.	7664-41-7	Ammonia NH_3	30, 31, 50, 126b, 129, 167, 172, 173a, 174a, 174b, 174c, 195, 197, 198, 213, 237, 239, 364, 365, 375, 376, 402, 407, 408, 424, 472, 473, 475, 480, 491, 688, 827, 916, 985–987, 989, 1051, 1063–1066, 1068–1075, 1091, 1099, 1100, 1128b, 1137, 1140, 1222, 1245, 1263, 1277, 1293, 1335, 1348–1351, 1354, 1369, 1375a, 1386, 1388–1390, 1437, 1442, 1445, 1469, 1489, 1492, 1522, 1524, 1531, 1532, 1539, 1580, 1589, 1673, 1674, 1709, 1741, 1744, 1808, 1841, 1842, 1853b, 1884, 1902, 1911, 1966, 2079, 2083–2085, 2133, 2134a, 2142, 2161, 2170, 2217, 2224, 2263, 2267, 2270, 2326, 2330, 2338, 2342, 2342a, 2343, 2368, 2480, 2524, 2529, 2541, 2543, 2545, 2607, 2627, 2688, 2691–2695, 2724, 2761, 2762, 2775, 2777, 2781, 2782, 2804, 2858, 2919, 2927, 2928, 2934, 2936, 2937, 2939, 2973, 2986–2988, 3007, 3022, 3029, 3059, 3140, 3187, 3190, 3213, 3214, 3251, 3254, 3255, 3257, 3266, 3300, 3302, 3306, 3308,	129, 174b, 212, 385, 555, 622, 677b, 826a, 856, 927, 989, 1053, 1063–1066, 1068–1074, 1128b, 1189, 1222, 1244, 1263, 1329, 1330, 1332, 1333, 1335, 1351, 1369, 1493, 1527, 1835b, 1941, 2079, 2313a, 2330, 2337, 2338, 2339b, 2356, 2381, 2394a, 2453, 2529, 2543, 2545, 2607, 2746, 2761, 2762, 2765, 2766, 2787, 2914, 2919, 2939, 2987, 3022, 3214, 3254, 3261, 3266, 3385, 3420, 3491, 3499, 3693, 3707, 3780, 3797, 3974a, 3974b, 4244, 4249, 4837a, 5018, 5079, 5126, 5165, 5186, 5189, 5194, 5298, 5382, 5389, 5396, 5669, 5712, 5803, 5811b, 5872, 5907, 17B40	50, 1354, 1375a, 4052, 4056

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

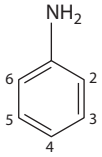
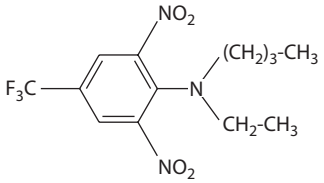
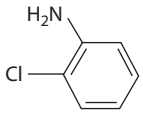
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Ammonia NH_3 (cont.)	3324, 3369, 3385, 3482, 3491, 3493, 3583, 3584, 3623, 3659, 3693, 3695, 3797, 3844, 3909, 3910, 3934, 3955, 3956, 3973, 3992, 4005–4007, 4009–4011, 4041, 4052, 4056, 4060–4062, 4064, 4065, 4136, 4226, 4245, 4249, 4301, 4319, 4332, 4406, 4636, 4686, 4743, 5042, 5049, 5082, 5079, 5099, 5100, 5129, 5189, 5263, 5359, 5382, 5389, 5512, 5548, 5811b, 5836, 5869a, 19A02		
24.	62813-37-0	Anthracenamine	5811		
25.	610-49-1	1-Anthracenamine  	1735, 4249	4249	
26.	613-13-8	2-Anthracenamine	5811	5811	
27.	779-03-3	9-Anthracenamine	1735, 4249		
28.	7004-12-8	Arginine H_2N-C(=NH)-NH-$(CH_2)_3$-CH(NH_2)-COOH		826a, 2911c, 2939, 3491, 3705, 3973, 3974b, 4224, 4226, 4244, 4398c, 5079, 5189, 5435, 5436, 5785, 5827	
29.	1069-09-6 34522-32-2	Arginine, *N*2-(1-carboxyethyl)- H_2N-C(=NH)-NH-$(CH_2)_3$-CH-[NH-CH(CH_3)-COOH]-COOH		3427a, 3973, 4249, 4688	
30.	74-79-3	*L*-Arginine H_2N-C(=NH)-NH-$(CH_2)_3$-CH(NH_2)-COOH	3797	120, 158, 555a, 555b, 622, 749, 751–756, 1053, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 1918, 1919, 2079, 2270, 2283, 2337, 2338, 2394a, 2453, 2532, 2597a, 2722, 2795, 2911c, 2939, 3266, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4244, 4249, 5811b	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	7006-34-0	Asparagine H_2N-CO-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 1965, 2724, 3266, 4159, 4249, 5811b	120, 480, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1223, 1305a, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2532, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4244, 4249, 4398c, 5048, 5079, 5126, 5189, 5437, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
32.	70-47-3	*L*-Asparagine		429b, 2338, 5811b	
33.	5794-13-8	*L*-Asparagine monohydrate		3973	
34.	6899-03-2	Aspartic acid	3555	3555, 3705, 5699, 5785, 5831, 5905, 5907, 17B17	
35	56-84-8	*L*-Aspartic acid HOOC-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3797, 4159, 4249	120, 158, 480, 555a, 555b, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4159, 4224, 4226, 4244, 4249, 4359, 4398b, 4422, 5079, 5699, 5785, 5811b, 5831, 5905, 5907	
36.	31105-02-9	*L*-Aspartic acid *N*-(1-deoxy-*D*-fructos-1-yl)-		5811	
37.	34441-14-0	1-Azetidinebutanoic acid, α-[(3-amino-3-carboxypropyl)amino]-2-carboxy-, [2S-[1[αR*(R*)],2R*]]- {nicotianamine}		3491, 4249, 4855, 5811b	
38.	2517-04-6	2-Azetidinecarboxylic acid		3491, 5811b	
39.	100-10-7	Benzaldehyde, 4-(dimethylamino)-	568b, 4249		

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
40.	62-53-3	Benzenamine {aniline} 	126b, 172, 237, 239, 414, 568b, 722, 1099, 1123, 1140, 1360, 1375a, 1378, 1419, 1426, 1427, 1437, 1442, 1445, 1674, 1741, 1842, 2133, 2134a, 2142, 2313a, 2387, 2543, 2724, 2734, 2761, 2762, 2765, 2766, 2773, 2799a, 2900, 3219, 3255, 3260, 3300, 3308, 3398, 3491, 3559, 3797, 3973, 4010, 4011, 4249, 5034, 5512, 5811b, 5869a	568b, 1877, 2722, 2724, 2746, 3491, 4249, 5811b	1360, 1375a, 1378, 2387
41.	106-40-1	Benzenamine, 4-bromo-	822, 4249		
42.	1861-40-1	Benzenamine,*N*-butyl-2,6-dinitro-*N*-ethyl-4-(trifluoromethyl)- {Benefin®; Benfluralin®} 		2892a, 3633	
43.	95-51-2	Benzenamine, 2-chloro- {2-chloroaniline} 	3491, 4249, 5811b	3797, 4249, 5811b	
44.	106-47-8	Benzenamine, 4-chloro-	822, 4249		
45.	46175-80-8	Benzenamine, 2-(cyclohexen-1-yl)-		2917a	
46.	95-76-1	Benzenamine, 3,4-dichloro-	822, 4249	4271a	
47.	99-30-9	Benzenamine, 2,6-dichloro-4-nitro- {Dicloran®}		3633	
48.	579-66-8	Benzenamine, 2,6-diethyl-	5811	5811	
49.		Benzenamine, dimethyl-	5034		
50.	87-59-2	Benzenamine, 2,3-dimethyl- {2,3-xylidine}	2142, 2313a, 2724, 2883, 2889, 3255, 3491, 3797, 4010, 4011, 4249, 5811b	1877, 3491, 4249	
51.	95-68-1	Benzenamine, 2,4-dimethyl- {2,4-xylidine}	568b, 2142, 2313a, 2724, 2883, 2889, 3255, 3491, 3797, 4010, 4011, 4249, 5811b		
52.	95-78-3	Benzenamine, 2,5-dimethyl- {25-xylidine}	2142, 2313a, 2724, 2883, 2889, 3255, 3491, 3797, 4010, 4011, 4249, 5811b	1877, 3491, 4249, 5811b	
53.	87-62-7	Benzenamine, 2,6-dimethyl- {2,6-xylidine}	1743, 1744, 2142, 2313a, 2724, 2883, 2889, 3255, 3265, 3300, 3491, 3714, 3797, 4010, 4011, 4249, 5512, 5811b	1877, 3491, 4249, 5811b	
54.	95-64-7	Benzenamine, 3,4-dimethyl- {3,4-xylidine}	822, 2313a, 2889, 4010, 4011, 4249	1877, 3491, 4249	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

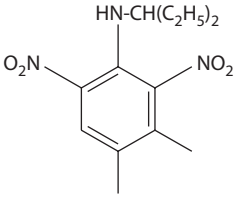
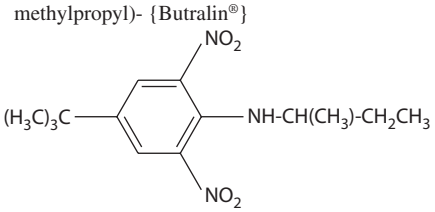
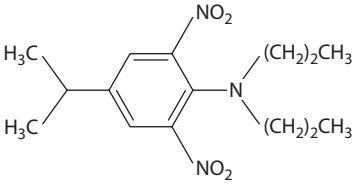
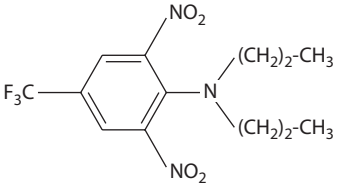
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
55.	40487-42-1	Benzenamine, 3,4-dimethyl-2,6-dinitro-*N*-(1-ethylpropyl)- {Pendimethalin®} 		2650b, 2913a, 3633, 3811a, 4271a	
56.	108-69-0	Benzenamine, 3,5-dimethyl- {3,5-xylidine}	2313a, 2724, 2883, 2889, 3491, 3797, 4010, 4011, 4249, 5811b	3491, 5811b	
57.	611-21-2	Benzenamine, *N*,2-dimethyl-	2889, 3491, 4249, 5811b	5811b	
58.	623-08-5	Benzenamine, *N*,4-dimethyl-	2889, 3491, 4249, 5811b	5811b	
59.	121-69-7	Benzenamine, *N*,*N*-dimethyl-	568b, 2882, 4249, 4570a		
60.	769-92-6	Benzenamine, 4-(1,1-dimethylethyl)- {parvoline}		4064, 5079	
61.	33629-47-9	Benzenamine, 4-(1,1-dimethylethyl)-2,6-dinitro-*N*-(1-methylpropyl)- {Butralin®} 		2913a, 3585c, 3633, 3811a, 3973, 5568	
62.	33820-53-0	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(1-methylethyl)- (Isopropalin®) 		2892a, 3633, 4271a	
63.	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)- (Trifluralin®) 		1219c, 2650a	
64.	1520-21-4	Benzenamine, 4-ethenyl- {4-aminostyrene}	5034	2359	
65.	578-54-1	Benzenamine, 2-ethyl-	2142, 2313a, 2724, 2883, 2889, 3255, 3491, 3797, 4010, 4011, 4249, 5811b	1877, 3491, 4249, 5811b	
66.	587-02-0	Benzenamine, 3-ethyl-	2142, 2313a, 2900, 3255, 4010, 4011, 4249, 5811b		

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
67.	589-16-2	Benzenamine, 4-ethyl-	2142, 2313a, 2724, 2883, 2889, 3255, 3491, 3797, 4010, 4011, 4249, 5811b		
68.	103-69-5	Benzenamine, *N*-ethyl- {*N*-ethylaniline}	568b, 2889, 3491, 4249, 5811b		
69.	1821-38-1	Benzenamine, 2-ethyl-*N*-methyl-	2724, 2889, 3491, 3797, 4249, 5811b	3797, 4249, 5811b	
70.	71265-20-8	Benzenamine, 3-ethyl-*N*-methyl-	2889, 3491, 4249, 5811b	5811b	
71.	37846-06-3	Benzenamine, 4-ethyl-*N*-methyl-	2889, 3491, 4249, 5811b	5811b	
72.	94-68-8	Benzenamine, *N*-ethyl-2-methyl-	2889, 4249		
73.	102-27-2	Benzenamine, *N*-ethyl-3-methyl-		2359, 2917a	
74.	71265-27-5	Benzenamine, ar-ethyl-ar-methyl-	2889, 4249		
75.	90-04-0	Benzenamine, 2-methoxy- {*o*-anisidine}	2889, 3300, 3491, 3781, 4249, 4763, 5811b	1248, 1254, 4249	
76.	50868-72-9	Benzenamine, 2-methoxy-5-methyl-	568b, 4249	568b, 4249	
77.	536-90-3	Benzenamine, 3-methoxy- {*m*-anisidine}	568b, 2724, 2883, 2889, 3491, 3797, 4010, 4011, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	
78.	104-94-9	Benzenamine, 4-methoxy- {*p*-anisidine}	2889, 3491, 4010, 4011, 4249, 5811b	5811b	
79.		Benzenamine, methyl-	5034		
80.	26915-12-8	Benzenamine, ar-methyl-	722, 2403, 3491, 4249		
81.	95-53-4	Benzenamine, 2-methyl- {*o*-toluidine; 2-toluidine}	126, 126a, 126b, 237, 239, 568b, 722, 1123, 1148, 1217, 1360, 1375a, 1410, 1445, 1674, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 2142, 2313a, 2724, 2734, 2761, 2762, 2765, 2766, 2773, 2777, 2825, 2882, 2883, 2889, 3255, 3257, 3260, 3265, 3300, 3491, 3714, 3729, 3781, 3797, 4010, 4011, 4249, 5512, 5811b, 5869a	568b, 1877, 3491, 4249, 5811b	1360, 1375a
82.	108-44-1	Benzenamine, 3-methyl- {*m*-toluidine; 3-toluidine}	239, 568b, 722, 1410, 1842, 2142, 2313a, 2724, 2889, 3255, 3491, 3729, 3797, 4010, 4011, 4249, 5512, 5811b		
83.	106-49-0	Benzenamine, 4-methyl- {*p*-toluidine; 4-toluidine}	239, 722, 414, 568b, 1410, 1842, 2142, 2313a, 2724, 2889, 3255, 3491, 3559, 3797, 4010, 4011, 4249, 5512, 5811b		
84.	100-61-8	Benzenamine, *N*-methyl- {*N*-methylaniline}	2724, 2883, 2889, 3491, 3797, 4249, 4570a, 5811b	5811b	
85.	5266-85-3	Benzenamine, 2-methyl-6-(1-methylethyl)-		2917a	
86.	614-00-6	Benzenamine, *N*-methyl-*N*-nitroso-	2884	2139	
87.		Benzenamine, (1-methylethyl)-*N*—(1-methylethylphenyl)-	2552, 3308		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

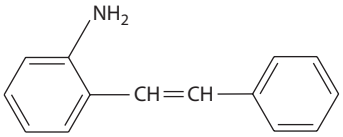
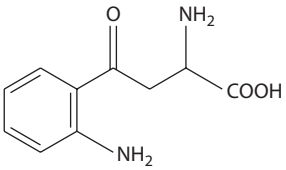
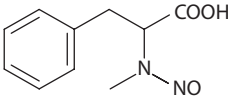
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
88.	5650-10-2	Benzenamine, 4-(1-methylethyl)-*N*-phenyl-	658, 2550, 2552, 2724, 2889, 3308, 3491, 4249, 5811b		
89.	552-82-9	Benzenamine, *N*-methyl-*N*-phenyl-	2141, 4249		
90.	86-30-6	Benzenamine, *N*-nitroso-*N*-phenyl-	746c		
91.	122-39-4	Benzenamine, *N*-phenyl- {diphenylamine}	329, 515, 568b, 658, 1360, 1375a, 2552, 2570, 2724, 2761, 2762, 2765, 2766, 2889, 3219, 3308, 3491, 3557, 3797, 4010, 4011, 4249, 5811b		1360, 1375a
92.	13066-19-8	Benzenamine, 2-(2-phenylethenyl)- {2-aminostilbene} 	568b, 1735, 1781, 2882, 2889, 3491, 4010, 4011, 4249, 5811b	5811b	
93.	14064-37-0	Benzenamine, 3-(2-phenylethenyl)-, (*Z*)-	1735, 4249		
94.	834-24-2	Benzenamine, 4-(2-phenylethenyl)-	1735		
95.	28059-64-5	Benzenamine, ?-phenylmethyl-	568b, 4249		
96.	71265-28-6	Benzenamine, ar,ar,ar,ar-tetramethyl-	2889, 3491, 4249		
97.	31093-11-5	Benzenamine, ar,ar,ar-trimethyl-	2889, 4249		
98.	88-05-1	Benzenamine, 2,4,6-trimethyl- {mesitylamine}	2724, 2889, 3491, 3797, 4010, 4011, 4249, 5811b	1877, 3491, 4249, 5811b	
99.	343-65-7	Benzenebutanoic acid, α,2-diamino-γ-oxo- {kynurenine} 		4249	
100.	71607-71-1	Benzenediamine, *N*-methyl-	2889, 3491		
101.	95-54-5	1,2-Benzenediamine {*o*-phenylenediamine}	93, 568b, 4249		
102.	3171-45-7	1,2-Benzenediamine, 4,5-dimethyl-	568b, 4249		
103.	496-72-0	1,2-Benzenediamine, ethyl-	5811, 5811a, 5811b		
104.	4760-34-3	1,2-Benzenediamine, *N*-methyl-	5811, 5811a, 5811b		
105.	823-40-5	1,3-Benzenediamine, 2-methyl-	568b, 4249, 5811b		
106.	95-80-7	1,3-Benzenediamine, 4-methyl-	568b, 4249		
107.	25376-45-8	1,3-Benzenediamine, ar-methyl-	2883, 3491, 4249		
108.	106-50-3	1,4-Benzenediamine	568b, 4249		
109.	623-09-6	1,4-Benzenediamine, *N*-methyl-	2889, 4249		
110.	101-54-2	1,4-Benzenediamine, *N*-phenyl-	2141, 4249		
111.	140-56-7	Benzenediazosulfonate, dimethylamino-, sodium salt {Fenaminosulf®}		3633	
112.	64-04-0	Benzeneethanamine C_6H_5-CH_2-CH_2-NH_2	2724, 2734, 2883, 2889, 3308, 3491, 3797, 4249, 5811b	1877, 2722, 2724, 2746, 3491, 3797, 3973, 3974a, 4249, 5811b	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

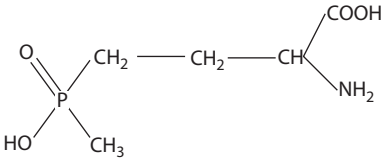
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
113.	582-22-9	Benzeneethanamine, β-methyl- C_6H_5-CH(CH_3)-CH_2-NH_2	4249, 4794		
114.	589-08-2	Benzeneethanamine, *N*-methyl- C_6H_5-CH_2-CH_2-NH-CH_3	1140, 2724, 2734, 2889, 3308, 3491, 5811b	2722, 2746, 3973, 3974a	
115.	100-46-9	Benzenemethanamine {benzylamine} C_6H_5-CH_2-NH_2	2889, 3491, 4249, 5811b	3491	
116.	62924-70-3	Benzenemethanamine, 2-chloro-*N*-(2,6-dinitro-4-(trifluoromethyl) phenyl)-*N*-ethyl-6-fluoro- {Flumetralin®}		2913a, 3633. 5568, 5811b	
117.	121850-61-1	Benzenepropanamide, *N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino] propyl]-3,4-dihydroxy-		4249, 5811b	
118.		Benzenepropanoic acid, 2-(methylnitrosamino)- 	1013	1008, 1009	
119.	19044-88-3	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro- {Oryzalin®}		4271a	
120.	118-92-3	Benzoic acid, 2-amino-		3797, 4249	
121.	7756-96-9	Benzoic acid, 2-amino-. butyl ester		5811	
122.	87-25-2	Benzoic acid, 2-aminoethyl ester		5811	
123.	134-20-3	Benzoic acid, 2-amino-, methyl ester {methyl anthranilate}		1053, 1254, 3266, 3370, 4249	
124.	85-91-6	Benzoic acid, 2-(methylamino)-, methyl ester		3905, 4249	
125.	1885-29-6	Benzonitrile, 2-amino- {anthranilonitrile}	278, 568b, 4249		
126.	26093-31-2	2*H*-Benzopyran-2-one, 7-amino-4-methyl-		2917a	
127.	92-87-5	1,1′-Biphenyl, 4,4′-diamino-	2313a		
128.	64850-01-7	[1,1′-Biphenyl]amine, *N*-methyl-	5811, 5811a, 5811b		
129.	90-41-5	[1,1′-Biphenyl]-2-amine	1410, 1735, 2142, 2313a, 3255, 4010, 4011, 4249, 5811b		
130.	2243-47-2	[1,1′-Biphenyl]-3-amine	174b, 174c, 688, 1386, 1735, 2142, 2313a, 2587, 3007, 3148a, 3255, 3300, 4010, 4011, 4249, 5022, 5049, 5516, 5811b, 5836		
131.	92-67-1	[1,1′-Biphenyl]-4-amine {4-aminobiphenyl}	126, 126a, 126b, 174b, 174c, 237, 239, 402, 688, 988a, 1099, 1148, 1212, 1217, 1373, 1386, 1410, 1445, 1674, 1727, 1735, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1870, 1871, 2142, 2313a, 2587, 2825, 3007, 3148a, 3255, 3257, 3265, 3300, 3441a, 3711, 3781, 4010, 4011, 4249, 4407, 4687, 4763, 4816, 5049, 5065, 5508, 5512, 5516, 5811b, 5836, 5869a		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
132.		2,2′-Bipyridine, amino-	442, 4249		
133.	4390-05-0	Butanal, 4-amino- H_2N-$(CH_2)_3$-CH═O		555b, 3973	
134.	7729-27-3	Butanal, 4-(methylamino)- H_3C-NH-$(CH_2)_3$-CHO		4249, 4707	
135.	64091-90-3	Butanal, 4-(methylnitrosamino)-4-3-(pyridyl)-	See 3-pyridinebutanal, γ-(methylnitrosoamino)-		
136.	109-73-9	1-Butanamine H_3C-$(CH_2)_3$-NH_2	172, 568b, 1140, 2724, 2734, 2882, 2883, 3255, 3308, 3398, 3491, 3797, 4052, 4056, 5811b	568b, 1877, 2092, 3491, 5811b	4052, 4056
137.	71277-84-4	1-Butanamine, methyl-	4249, 4810		
138.	96-15-1	1-Butanamine, 2-methyl- H_3C-CH_2-$CH(CH_3)$-CH_2-NH_2	2724, 2883, 2889, 3491, 3797, 4249, 5811b	5811b	
139.	107-85-7	1-Butanamine, 3-methyl- {isoamyl amine} $(H_3C)_2$═CH-$(CH_2)_2$-NH_2	568b, 1099, 1140, 2270, 2724, 2734, 2882, 2883, 2889, 3219, 3255, 3308, 3398, 3491, 3797, 4249, 5811b	120, 568b, 1877, 2746, 2939, 3491, 3797, 3974a, 4249, 5034, 5079, 5390a, 5135, 5136, 5811b, 5906	
140.	78579-58-5	1-Butanamine, 3-methyl-*N*-propyl- $(H_3C)_2$═CH-$(CH_2)_2$-NH-(CH_2)-CH_3	2724, 4249	2722	
141.	111-92-2	1-Butanamine, *N*-butyl- $[CH_3$-$(CH_2)_3]_2$═NH	5811b	568b, 1877, 3491, 3675, 4249, 5811b	
142.	924-16-3	1-Butanamine, *N*-butyl-*N*-nitroso- {NDBA} $[CH_3$-$(CH_2)_3]_2$═N-NO	203, 239, 486, 572, 573, 746c, 1058, 1217, 1740, 1741, 1743, 1744, 1781, 1870, 1871, 1952, 2442, 2443, 2516, 2561, 2724, 2751, 2825, 2884, 3219, 3257, 3265, 3300, 3308, 3491, 3711, 3713, 3714, 3994, 4010, 4011, 4249, 5512, 5811b 5869a	5811b	
143.	110-68-9	1-Butanamine, *N*-methyl- CH_3-$(CH_2)_3$-NH-CH_3	568b, 1140, 2724, 2734, 2883, 2889, 3308, 3491, 3797, 5811b	568b, 1877, 3491, 3675, 4249, 5811b	
144.	7068-83-9	1-Butanamine, *N*-methyl-*N*-nitroso- H_3C-$(CH_2)_3$-N(NO)-CH_3	486, 568b, 572, 573, 1058, 1428, 2205, 2724, 2750, 2751, 3123, 3300, 3308, 3491, 3994, 4332, 5811b	5811b	
145.	39099-23-5	1-Butanamine, *N*-(1-methylethyl)- H_3C-$(CH_2)_3$-NH-CH═$(CH_3)_2$	2889, 4249		
146.	20810-06-4	1-Butanamine, *N*-(2-methylpropyl)- H_3C-$(CH_2)_3$-NH-CH_2-CH═$(CH_3)_2$	2724, 2882, 2889, 3491, 4249, 5811b	5811b	
147.	56375-33-8	1-Butanamine, *N*-nitroso-	2041		
148.	20193-21-9	1-Butanamine, *N*-propyl-	568b, 4249	568b, 4249	
149.	4104-44-3	1-Butanamine, *N*,3-dimethyl-		3491, 3675, 4249, 5811b	
150.	13952-84-6	2-Butanamine H_3C-CH_2-$CH(NH_2)$-CH_3	568b, 1140, 2724, 2883, 2889, 3491, 3797, 4052, 4056, 4249, 5811b	568b, 2359, 2386, 3491, 4249, 5811b	4052, 4056

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
151.	7713-69-1	2-Butanamine, *N*-methyl- H_3C-CH_2-CH(NH-CH_3)-CH_3	2889, 3491, 5811b	1877	
152.	626-23-3	2-Butanamine, *N*-(1-methylpropyl)-	5811b	568b, 1877, 3491, 3675, 4249, 5811b	
153.	16748-73-5	Butanediamide, 2-amino-, (S)- {asparagine amide} H_2N-CO-CH_2-CH(NH_2)-CO-NH_2		826a, 2914	
154.	110-60-1	1,4-Butanediamine {putrescine} H_2N-$(CH_2)_4$-NH_2		555b, 568b, 3869, 3973, 4236, 4249, 5811b, 5869, 17B02, 17B63, 17B64	
155.	70185-59-0	1,4-Butanediamine, *N*-[3-(amino)-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy- {*p*-coumaroylspermidine}		5811, 5811b	
156.	124-20-9	1,4-Butanediamine, *N*-(3-aminopropyl)- {spermidine} H_2N-$(CH_2)_4$-NH-$(CH_2)_3$-NH_2		555b, 3869, 3973, 4236, 4249, 4450, 5811b	
157.	71-44-3	1,4-Butanediamine, *N,N′*-bis(3-aminopropyl)- {spermine} H_2N-$(CH_2)_3$-NH-$(CH_2)_4$-NH-$(CH_2)_3$-NH_2		4236, 4249, 4450, 5811b	
158.	15657-58-6	1,4-Butanediamine, 2-methyl- H_2N-$(CH_2)_2$-CH(CH_3)-CH_2-NH_2		4249, 4872	
159.	14475-60-6	1,4-Butanediamine, *N*-methyl- H_2N-$(CH_2)_4$-NH-CH_3		3973, 4685, 5811b	
160.		1,4-Butanediamine, 3-phenylpropenoyl-		17B02	
161.	13989-82-7	Butanenitrile, 4-(dimethylamino)- $(H_3C)_2$=N-$(CH_2)_3$-CN	2773, 4249		
162.		Butanimine CH_3-$(CH_2)_2$-CH=NH	2092, 3219, 3797, 4249	3491, 4249	
163.	80-60-4	Butanoic acid, 2-amino- H_3C-CH_2-CH(NH_2)-COOH	1580, 2939, 4249	480, 1329, 1351, 2337, 2597a, 2939, 3491, 3726, 3797, 3974a, 3978, 4249, 5785, 5811b, 5827, 5881, 5907	
164.	7004-04-8	Butanoic acid, 2-amino-3-hydroxy- H_3C-CHOH-CH(NH_2)-COOH	429b	429b, 4249	
165.	1927-25-9	Butanoic acid, 2-amino-4-hydroxy-		5777, 5905	
166.	51276-47-2 53369-07-6	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®} 		5521	
167.	454-41-1	Butanoic acid, 2-amino-4-(methylsulfinyl)-		172, 429b, 4249	
168.	1118-85-0 3226-65-1	Butanoic acid, 2-amino-4-(methylsulfonyl)- {methionine sulfone; methionine *S*-oxide} H_3C-SO-$(CH_2)_2$-CH(NH_2)-COOH		120, 172, 1305a, 1351, 2337, 3491, 3729, 3797, 3974a, 4224, 4249, 5811b	
169.	2338-03-6	Butanoic acid, 2-amino-4-oxo-, (S)-		4249	
170.	2835-82-7	Butanoic acid, 3-amino-		480	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

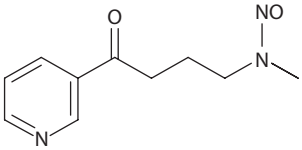
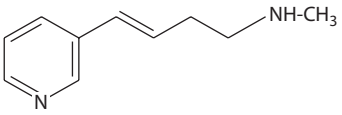
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
171.	56-12-2	Butanoic acid, 4-amino- H_2N-$(CH_2)_3$-COOH	1083, 1351, 1580, 1910, 1914, 2724, 2858, 2939, 3302, 3491, 3797, 4249, 5811b	120, 480, 555a, 555b, 622, 749, 752–754, 826a, 927, 1086, 1223, 1351, 2270, 2337, 2338, 2532, 2597a, 2795, 2911c, 2939, 3491, 3555, 3705, 3797, 3974a, 3978, 4224, 4244, 4249, 4398c, 5079, 5811b, 5699, 5905	
172.	61445-55-4 133201-39-5	Butanoic acid, 4-(methylnitrosoamino)- Butanoic acid, 4-[(nitrosomethyl)amino] {NMBA} CH_3-N(NO)-$(CH_2)_3$-COOH	466, 486, 982, 2852, 3256, 3300, 3943a, 3944–3946, 3973, 5811b	486, 982, 2852, 3943a, 3944–3946, 3947, 3948, 3973, 5001, 5811b	
173.	67557-56-6	Butanoic acid, 4-(methylnitrosoamino)-, methyl ester CH_3-N(NO)-$(CH_2)_3$-$COOCH_3$	466, 470, 3256, 3300		
174.	462-10-2	Butanoic acid, 4,4′-dithiobis-2-amino- {homocystine} $[S\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH]_2$		2337, 3491, 3729, 3797, 3974a, 4224, 4226, 4249	
175.	23599-75-9	1-Butanol, 2-methyl-4-(1*H*-purin-6-ylamino)- {dihydrozeatin}	2777	4249, 5811, 5811b	
176.	6291-17-4	2-Butanol, 3-amino-2-methyl-	1375, 1375b, 3557		
177.	155728-85-1	2-Butanol, 1-(4-bromophenoxy)-3-[(phenylmethyl) amino]-, (R*,R*)-		4249	
178.	71278-11-0	1-Butanone, 4-amino-1-(3-pyridinyl)- {poikiline}	3302, 3742, 4207, 4213, 4248	120, 2270, 4207, 4249, 5079	
179.		1-Butanone, 4-(methylamino)-1-(2,6-dihydroxy-3-pyridinyl)-		1101, 4249	
180.		1-Butanone, 4-(methylamino)-1-(6-hydroxy-pyridinyl)-		1101, 4249	
181.	2055-23-4	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)- {pseudooxynicotine}		553, 2221, 3974, 4236, 4249, 5079, 5222	
182.	64091-91-4 110053-55-9 121268-99-3 126165-82-0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}  {1-Butanone, 4-[(nitrosomethyl) amino]-1-(3-pyridinyl)-}	7, 23–26, 28–31, 34, 59, 70, 75, 97–99, 126, 126a, 126b, 172, 174b, 174c, 237, 239, 402, 458–460, 463, 478, 483, 484, 486, 501, 502, 508, 514, 568b, 572, 573, 595, 603, 688, 728, 772, 895, 998, 1001, 1002, 1004, 1006a, 1011, 1013–1016, 1016a, 1051, 1058, 1099, 1148, 1191–1200, 1373, 1386, 1445, 1557, 1564, 1566, 1567, 1567a, 1569–1571, 1571a, 1572, 1573a, 1580, 1584, 1674, 1679, 1685, 1692, 1696, 1702, 1710, 1725, 1727, 1728, 1730, 1731, 1736, 1741, 1746, 1750, 1751, 1768, 1769, 1781, 1842,	29, 33, 34, 64, 70, 97–99, 174c, 201, 324–326, 458, 463, 465, 468, 478, 483, 484, 486, 498, 501, 505, 508, 510, 548–550, 553, 554, 557, 568b, 595, 655, 720, 772, 895, 998, 1002, 1004, 1010, 1014, 1015, 1051, 1156, 1191–1200, 1385, 1564, 1566, 1567, 1567a, 1569–1571, 1573a, 1576, 1577, 1584, 1679, 1685, 1696, 1702, 1712, 1722, 1725, 1728, 1730, 1731, 1746, 1750, 1768, 1771,	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-{NNK} (cont.)	1870–1872, 1987, 1988, 2133, 2134a, 2142, 2168, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2879, 2949, 2991, 2992, 2993, 3007, 3094, 3178, 3179, 3180, 3181, 3182, 3184, 3190, 3255–3257, 3265, 3300, 3342, 3343, 3365, 3370, 3376, 3378, 3844, 3952, 3973, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5070, 5087, 5494, 5531, 5546, 5556, 5569, 5679, 5692, 5811, 5811a, 5811b, 5836	1870–1872, 1988, 2050–2052, 2169, 2235, 2326c, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2638, 2674, 2700, 2914-2917, 2949, 2992, 2996, 2997, 3144a, 3176a, 3177, 3183, 3441a, 3491, 3773, 3774, 3816, 3943b, 3947, 3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4090, 4128, 4161, 4236, 4247, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5531, 5579, 5584, 5589, 5811, 5811a, 5811b	
183.	76014-82-9	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-, *N*-oxide		4249	
184.	82806-40-4	Butenamine	5811, 5811a, 5811b	5811, 5811a, 5811b	
185.	692-31-9	2-Buten-1-amine, *N,N*-dimethyl- $H_3C\text{-}CH{=}CH\text{-}CH_2\text{-}N{=}(CH_3)_2$	2767, 4249		
186.	2524-49-4	3-Buten-1-amine $H_2C{=}CH\text{-}CH_2\text{-}CH_2\text{-}NH_2$	2883, 4249		
187.	20173-36-8	3-Buten-1-amine, *N,N*-dimethyl-4-(3-pyridinyl)-	2731, 2735, 2767, 4249		
188.	538-79-4	3-Buten-1-amine, *N*-methyl-4-(3-pyridinyl)-{metanicotine} 	568b, 761, 1078, 1084, 2724, 2734, 3054, 3302, 3499, 3557, 3797, 4249	120, 568b, 1087, 2270, 2349, 2746, 4249, 5079, 5382, 5390, 5804, 5811b	
189.		1-Buten-1-aminocarbonyl-(1*E*)-{[(1*E*)-1-but-1-en-1-yl]aminocarbonyl-} $CH_3CH_2\text{-}CH{=}CH\text{-}NH\text{-}C{=}O$	5044, 5503, 5504		
190.	1637-39-4	2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylamino)-, (*E*)-		2241a, 4249, 4514, 5811b	
191.	29736-33-2	2-Buten-1-ol, 2-methyl-4-[[2-(methylthio)-1*H*-purin-6-yl]amino]-, (*E*)-		4249, 4703	
192.	4539-51-9	9*H*-Carbazole, 2-amino-	933		
193.		9*H*-Carbazole, 2-amino-ethyl-	3226, 4249		
194.	2642-98-0	Chrysene, 6-amino- {6-chysenamine}	1410, 5811b		
195.	5220-49-5	2-Cyclohexen-1-one, 3-amino-	3553, 4249		
196.	22059-21-8	Cyclopropanecarboxylic acid, 1-amino-		4249, 5811b	
197.	498-40-8	Cysteic acid $HO\text{-}SO_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$		622, 1351, 2337, 3491, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

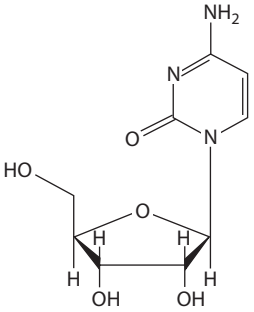
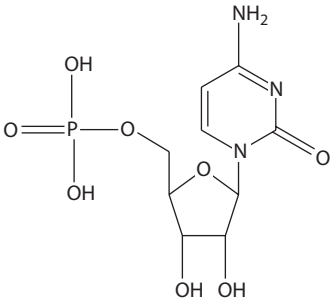
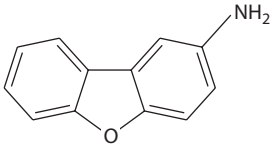
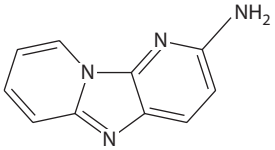
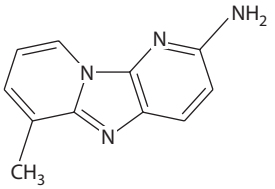
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
198.	52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto-(R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1274, 3265, 3266, 4249	120, 158, 172, 342, 722, 927, 1053, 1128b, 1305a, 1351, 1918, 2049, 2337, 2939, 3266, 3491, 3729, 3797, 3974a, 3978, 4224, 4249, 4398c, 5079, 5189, 5376, 5811b, 5874, 5881	
199.	636-58-8	*L*-Cysteine, *N*-*L*-γ-glutamyl-		4249	
200.	24645-67-8	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-} $\{S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH\}_2$		116, 120, 172, 622, 722, 749, 752–754, 1063–1066, 1068–1074, 1127b, 1329, 1330, 1332, 1351, 2049, 2079, 2270, 2337, 2453, 2597a, 2939, 3491, 3499, 3705, 3729, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079, 5189, 5376, 5603, 5881, 5907	
201.	56-89-3 13028-62-1	*L*-Cystine		5811, 5811b	
202.	65-46-3	Cytidine {2(1*H*)-pyrimidinone, 4-amino-1-β-*D*-ribofuranosyl-} 		429b, 4249, 4477, 4554a	
203.	65-47-4	Cytidine 5′-(tetrahydrogen triphosphate)		429b, 4249, 4474, 4505	
204.	63-37-6	5′-Cytidylic acid 		429b, 4249, 4299, 4774	
205.	2016-57-1	1-Decanamine	5811, 5811a, 5811b		

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

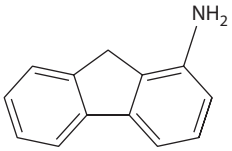
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
206.	3693-22-9	2-Dibenzofuranamine 	1735, 4249		
207.	4106-66-5	3-Dibenzofuranamine	568b, 642, 4249		
208.	67730-10-3	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine {Glu-P-2} 	751, 755, 756, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4249, 5002, 5512, 5811b, 5869a		
209.	67730-11-4	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 6-methyl- {Glu-P-1} 	751, 755, 756, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4249, 5512, 5869a		
210.	112-18-5	Dodecanamine, *N,N*-dimethyl-	5811, 5811a		
211.	75-04-7	Ethanamine {ethylamine} $H_3C\text{-}CH_2\text{-}NH_2$	568b, 1137, 1140, 1902, 1910, 2079, 2576, 2724, 2734, 2858, 2866, 2889, 2939, 3052, 3255, 3398, 3491, 4052, 4056, 4064, 4065, 4249, 5079, 5811b, 5869a	568b, 2722, 2746, 3491, 3974a, 4064, 4249, 5079, 5712, 5811b	4052, 4056
212.	51-75-2	Ethanamine, 2-chloro-*N*-(2-chloroethyl)-*N*-methyl- $(Cl\text{-}CH_2\text{-}CH_2)_2{=}N\text{-}CH_3$	703, 4249		
213.	121-44-8	Ethanamine, *N,N*-diethyl- {triethylamine} $(H_3C\text{-}CH_2)_3{\equiv}N$	568b, 1663a, 1667, 4249, 5869a	568b, 2001, 3491, 4249, 5811b	
214.	30533-08-5	Ethanamine, *N*,1-dimethyl-*N*-nitroso-	3256		
215.	109-89-7	Ethanamine, *N*-ethyl- {diethylamine} $(H_3C\text{-}CH_2)_2{=}NH$	568b, 1140, 1971, 2001, 2724, 2734, 2883, 2889, 3302, 3308, 3398, 3491, 3797, 4249, 4319, 5811b	558, 568b, 1877, 2001, 3476, 3491, 4249, 5811b	
216.	55-18-5	Ethanamine, *N*-ethyl-*N*-nitroso- {NDEA} $(H_3C\text{-}CH_2)_2{=}N\text{-}NO$	31, 126, 126a, 126b, 172, 203, 239, 379, 457, 470, 480, 486, 510, 568b, 572, 573, 649, 746c, 1058, 1148, 1217, 1236, 1428, 1445, 1557, 1580, 1674, 1727, 1736, 1740, 1741, 1743, 1744, 1761, 1773, 1808, 1842, 1870–1872, 1952, 2118, 2129, 2142, 2440–2443, 2516, 2635,	465, 468, 486, 568b, 1712, 1727, 1870–1872, 2516, 2655, 3973, 4010, 4010, 4011, 4249, 5496	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Ethanamine, *N*-ethyl-*N*-nitroso- {NDEA} $(H_3C\text{-}CH_2)_2{=}N\text{-}NO$ (cont.)	2686, 2722, 2724, 2825, 2884, 2990, 2991, 3123, 3255–3257, 3265, 3300, 3308, 3343, 3378, 3491, 3595–3598, 3713, 3994, 4010, 4011, 4249, 4332, 5512, 5811b, 5869a		
217.	624-78-2	Ethanamine, *N*-methyl- $H_3C\text{-}CH_2\text{-}NH\text{-}CH_3$	568b, 1140, 2724, 2734, 2883, 2889, 3219, 3308, 3491, 4249	558, 568b, 1877, 2722, 2746, 3491, 4249	
218.	10595-95-6	Ethanamine, *N*-methyl-*N*-nitroso- {NEMA} $H_3C\text{-}CH_2\text{-}N(NO)\text{-}CH_3$	31, 126a, 239, 457, 467, 470, 480, 486, 572, 573, 746c, 1058, 1148, 1217, 1236, 1428, 1445, 1580, 1725, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1784, 1808, 1842, 1870–1872, 1953, 2142, 2158, 2516, 2537, 2726, 2884, 2990, 2991, 3190, 3256, 3265, 3300, 2993, 3491, 3493, 3714, 3943a, 3944–3946, 3951, 3952, 3992, 3994, 4010, 4010, 4011, 4249, 5512, 5811b	486, 498, 1712, 1727, 1870–1872, 2516, 2655, 3943a, 3944–3948, 4249, 5496, 5811b	
219.	97190-07-3	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monooctadecadienoate monooctadecatrienoate, (all-*Z*)-		4249, 4570	
220.	97190-09-5	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecatrienoate, (*Z,Z,Z*)-		4249, 4570	
221.	97190-10-8	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecadienoate, (*Z,Z*)-		4249, 4570	
222.	97190-12-0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*- trimethyl-, hydroxide, inner salt, monooctadecadienoate		4249, 4570	
223.	62-49-7 123-41-1	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl- {choline} $HO\text{-}(CH_2)_2\text{-}N^+{\equiv}(CH_3)_3$		120, 1351, 2079, 2270, 2337, 2808a, 2939, 3491, 3555, 3797, 3973, 3974a, 4249, 5079, 5189, 5435, 5436	
224.	8002-43-5	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl-, phosphatidyl- {lecithin}		120, 328, 3973, 4249, 4976	
225.	107-35-7	Ethanesulfonic acid, 2-amino- {taurine} $H_2N\text{-}(CH_2)_2\text{-}SO_3H$		622, 1351, 2337, 3491, 3974a, 4224, 4226, 4249	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
226.	108-01-0	Ethanol, 2-(dimethylamino)- $(H_3C)_2$═N-$(CH_2)_2$-OH	1371, 3410, 3559, 4249		
227.	109-83-1	Ethanol, 2-(methylamino)- H_3C-NH-$(CH_2)_2$-OH		4249, 4829	
228.	1116-54-7	Ethanol, 2,2′-(nitrosoimino)bis- {NDELA} $(HO\text{-}CH_2CH_2)_2$═N-NO	126, 126a, 126b, 172, 237, 239, 458, 471, 477–479, 481, 482, 485, 486, 510, 603, 1058, 1148, 1159, 1217, 1445, 1674, 1704, 1705, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1867, 1870–1872, 2516, 2825, 2655, 3190, 3255–3257, 3265, 3300, 3370, 3480, 3714, 3973, 3992, 4010, 4011, 5512, 5869a	458, 468, 471, 477–479, 481, 482, 485, 486, 490, 498, 1704, 1705, 1727, 1867, 1870–1872, 2990, 3265, 3300, 3480, 3481, 3491, 3947, 3948, 3973, 4010, 4011, 4249, 5001, 5811b	
229.	111-42-2	Ethanol, 2,2′-iminobis- {diethanolamine} $(HO\text{-}CH_2CH_2)_2$═NH	479, 490	479, 490, 3973	
230.	141-43-5	Ethanol, 2-amino- {ethanolamine} HO-CH_2CH_2-NH_2		568b, 622, 749, 752–754, 3705, 4249	
231.	1071-23-4	Ethanol, 2-amino-, dihydrogen phosphate (ester)		908, 4249, 4670	
232.	593-67-9	Ethenamine H_2C═CH-NH_2	2889, 3491, 4249, 5811b	5811b	
233.	2693-46-1	3-Fluoranthenamine	1410, 5811b		
234.		Fluorenamine	1735, 4249		
235.	64294-96-8	9*H*-Fluorenamine	1781, 2883, 3491		
236.	6344-63-4	9*H*-Fluoren-1-amine 	1410		
237.	153-78-6	9*H*-Fluoren-2-amine	1410, 1735, 4249, 5811b		
238.	7083-63-8	9*H*-Fluoren-4-amine	1410		
239.	525-03-1	9*H*-Fluoren-9-amine	1735, 4249		
240.	70954-04-0	*D*-Fructose, 1-[(1-carboxy-2-hydroxypropyl) amino]-1-deoxy-, [R-(R*,S*)]-		434, 1351, 3555, 3973, 3974a	
241.	34393-27-6	*D*-Fructose, 1-[(3-amino-1-carboxy-3-oxopropyl) amino]-1-deoxy-, (S)-		1351, 2337, 4362	
242.	10003-63-1	*D*-Fructose, 1-[(3-carboxypropyl)amino]-1-deoxy-		1351, 2337, 3639, 3923, 3973, 3974a, 5811b	
243.	1192-20-7	2(3*H*)-Furanone, 3-aminodihydro-	2767, 3557, 4249		
244.	1948-54-5	Galactose, 2-amino-2-deoxy-		3797, 3974a, 4249	
245.	7535-00-4	*D*-Galactose, 2-amino-2-deoxy- {galactosamine}		3973, 4224, 4226, 4422, 5811b	
246.	75039-16-6	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl, mono(dihydrogen phosphate) (ester), (*E*)-		4249, 4813	
247.	62512-96-3	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)butyl		4249	

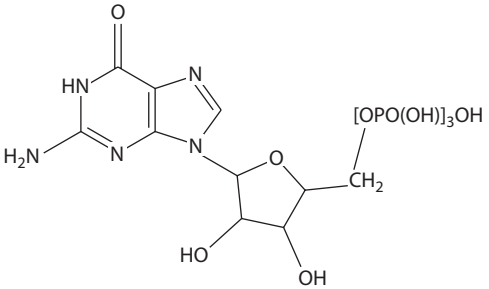
(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
248	3416-24-8	*D*-Glucose, 2-deoxy-, 2-amino- {glucosamine}		1032, 1063–1066, 1068–1074, 2445a, 3705, 3797, 3973, 3974a, 4224, 4226, 4249, 4422, 5540, 5811b	
249.	6899-05-4	Glutamic acid $HOOC-(CH_2)_2-CH(NH_2)-COOH$	562, 563, 1083, 1351, 1910, 1914, 2079, 2724, 2858, 2939, 3059, 3061, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 563, 622, 749, 751–756, 826a, 927, 966, 1033, 1034, 1053, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2026, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 4422, 5079, 5699, 5785, 5827, 5896, 5905, 5907	
250.	56-86-0	*L*-Glutamic acid	5811b	1053, 3266, 3973, 5811b	
251.	997-68-2	*L*-Glutamic acid, *N*-(5-amino-5-carboxypentyl)-, (S)-		429b, 4249, 4698	
252.	58-05-9	*L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl] amino]benzoyl]-		429b	
253.	1116-22-9	*L*-Glutamic acid, *N*-*L*-γ-glutamyl-		1351, 2027, 2337, 4249	
254.	3929-61-1	*L*-Glutamic acid, *N*-*L*-α-glutamyl-		2027, 2337, 3491, 4249, 4573	
255.	6899-04-3	Glutamine $H_2N-CO-(CH_2)_2-CH(NH_2)-COOH$	562, 1910, 1914, 2939	1971, 2939, 3705	
256.	56-85-9	*L*-Glutamine	480, 562, 563, 1351, 1668, 1910, 1914, 1965, 2079, 2724, 2858, 2939, 3059, 3266, 3302, 3491, 3797, 4159, 4249	120, 480, 563, 622, 749, 751–756, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2529, 2532, 2939, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 5079, 5189, 5434, 5437, 5699, 5785, 5811b, 5827, 5831, 5881, 5905, 5907	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
257.	56-40-6	Glycine $H_2N\text{-}CH_2\text{-}COOH$	1083, 1351, 1914, 2724, 2939, 3302, 3491, 3797, 4249, 5811b	120, 158, 480, 622, 722, 749, 751–756, 826a, 927, 1063–1066, 1068–1074, 1086, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5905, 17B59	
258.	18875-39-3	Glycine, labeled with ^{14}C		2099b	
259.	4429-05-4	Glycine, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
260.	88476-94-2	Glycine, *N*-(1-nitroso-*L*-prolyl)-		3951, 4249	
261.	70-18-8	Glycine, *N*-(*N*-*L*-γ-glutamyl-*L*-cysteinyl)- {glutathione}		120, 1351, 1668, 2337, 2939, 3491, 3797, 3974a, 4249, 5079, 5220, 5572, 5811b	
262.	1071-83-6	Glycine, *N*-(phosphonomethyl)-		1121a	
263.	1118-68-9	Glycine, *N,N*-dimethyl- $(H_3C)_2{=}N\text{-}CH_2\text{-}COOH$		4249, 4528	
264.	73360-07-3	Glycine, *N*-[2-(2-aminoethoxy)ethenyl]-		4249	
265.	19246-18-5	Glycine, *N*-*L*-cysteinyl-		429b	
266.	20661-60-3	Glycine, *N*-methyl-*N*-nitro-		992	
267.	13256-22-9	Glycine, *N*-methyl-*N*-nitroso- {NSAR} $H_3C\text{-}N(NO)\text{-}CH_2\text{-}COOH$	1058, 2442, 3256	466, 485, 486, 498, 2442, 3947, 3948, 5001, 5811b	
268.		Glycine, *N*-methyl-*N*-nitroso-, methyl ester $H_3C\text{-}N(NO)\text{-}CH_2\text{-}COOCH_3$	3256	466	
269.	306-60-5	Guanidine, (4-aminobutyl)-		429b, 4249, 4982	
270.	86-01-1	Guanosine 5′-(tetrahydrogen triphosphate)		4249	
271.	111-68-2	1-Heptanamine $H_3C\text{-}(CH_2)_6\text{-}NH_2$	568b, 2889, 3491, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	
272.	535-24-0	Heptanedioic acid, 2,6-diamino-3-hydroxy- $HOOC\text{-}CH(NH_2)\text{-}(CH_2)_2\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$		4249, 4602	



(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

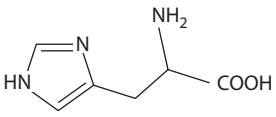
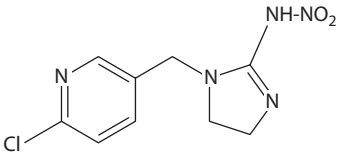
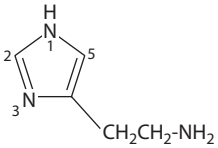
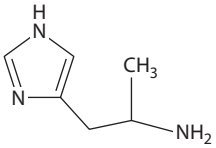
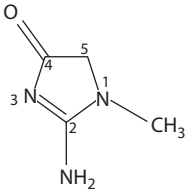
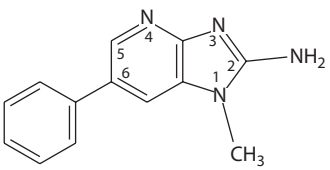
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
273.	111-26-2	1-Hexanamine $H_3C\text{-}(CH_2)_5\text{-}NH_2$	568b, 1140, 2724, 2882, 2883, 2889, 3491, 3559, 3797, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	
274.	28056-87-3	1-Hexanamine, 2-ethyl-*N,N*-dimethyl-	4249		
275.	542-32-5	Hexanedioic acid, 2-amino-		2337, 2597a, 3491, 3797, 3974a, 4224, 4226, 4249	
276.		Hexanoic acid, 2,6-di-(methylnitrosamino)- $R\text{-}(CH_2)_4\text{-}CH(R)\text{-}COOH$ where $R{=}CH_3N(NO)$-	1008, 1009, 1012, 3256, 3300	1008, 1009	
277.		Hexene, diamino-	2883, 4249		
278.		1-Hexen-1-aminocarbonyl- (1*E*)-{[(1*E*)-1-hex-1-en-1-yl]aminocarbonyl-} $CH_3(CH_2)_3\text{-}CH{=}CH\text{-}NH\text{-}C{=}O$	5044, 5503, 5504,		
279.	7006-35-1	Histidine		429b, 3797, 4249, 5699, 5785, 5831	
280.	71-00-1	*L*-Histidine  		120, 158, 553, 622, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5478, 5699, 5785, 5811b, 5831	
281.	332-80-9	*L*-Histidine, 1-methyl-	1083, 4249	1086, 1351, 2337, 2597a, 3491, 3797, 3974a, 3972, 4249	
282.	368-16-1	*L*-Histidine, 3-methyl-	1083, 4249	1086, 2597a, 4249	
283.	62504-27-2	*L*-Histidine, *N*-(1-carboxyethyl)-, (R)-		3565, 4249	
284.	454-29-5	*DL*-Homocysteine $HS\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		172	
285.	498-19-1 672-15-1	Homoserine {2-amino-4-hydroxybutanoic acid} $HO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	3557	1351, 2337, 2939, 3491, 3797, 3974a	
286.	302-01-2	Hydrazine $H_2N\text{-}NH_2$	126, 126a, 126b, 172, 237, 239, 427, 1148, 1217, 1373, 1437, 1445, 1507, 1557, 1571a, 1580, 1674, 1706, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1781, 1808, 1870, 1871, 2133, 2384, 2385, 2825, 3255, 3257, 3260, 3265, 3300, 3491, 3493, 3714, 3811a, 4010, 4011, 4249, 5512, 5811b, 5869a	1571a, 1580, 1581, 2385, 3481, 3491, 3493, 3811a, 3973, 3974b, 4249	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
287.	57-14-7	Hydrazine, 1,1-dimethyl- $H_2N\text{-}N(CH_3)_2$	126a, 568b, 967, 1148, 1217, 1373, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 2825, 3255, 3257, 3265, 3300, 5512, 5869a	568b, 3480, 3481, 3491, 3974b, 4249	
288.	624-80-6	Hydrazine, ethyl- $H_2N\text{-}NH\text{-}CH_2\text{-}CH_3$	2385, 4249		
289.	60-34-4	Hydrazine, methyl- $H_2N\text{-}NH\text{-}CH_3$	2385, 4249		
290.	7803-49-8	Hydroxylamine $HO\text{-}NH_2$		383a, 4249, 4520	
291.	105827-78-9	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl) methyl)-4,5-dihydro-*N*-nitro- {Admire®} 		2892a, 4249	
292.	51-45-6	1*H*-Imidazole-4-ethanamine 		568b, 4249, 4437	
293.	75614-87-8	1*H*-Imidazole-4-ethanamine, α-methyl- 		5603, 5777	
294.	60-27-5	4*H*-Imidazol-4-one, 2-amino-1,5-dihydro-3-methyl- {creatinine} 		568b, 751, 755, 756, 4249	
295.	105650-23-5	1*H*-Imidazo[4,5-*b*]pyridin-2-amine, 1-methyl-6-phenyl- {PhIP} 	1740, 1741, 1743, 1744,2095a, 2448, 2484a, 2601, 3265, 3300, 3714, 5002, 5512, 5811b		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

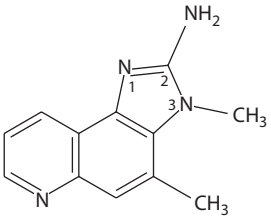
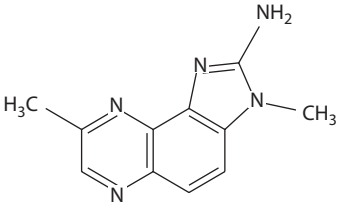
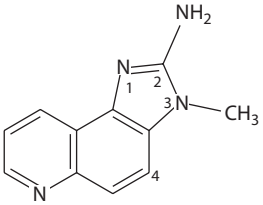
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
296.	77094-11-2	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3,4-dimethyl- {MeIQ} 	179a, 2095a, 2327c, 2354a, 2484a, 3255, 3257, 3265, 3300, 3714, 5002		
297.	77500-04-0	3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 3,8-dimethyl- 	5811a		
298.	76180-96-6	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3-methyl- {IQ} 	158a, 179a, 751, 755, 756, 1740, 1741, 1743, 1744, 2095a, 2327c, 2354a, 2484a, 2601, 3255, 3257, 3265, 3300, 3714, 3865c, 4367, 4368, 5002, 5512, 5811b, 5869a		
299.	95896-78-9	3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 3,4,8-trimethyl	5811a		
300.	5192-03-0	1*H*-Indole, 5-amino-	4407		
301.	61-54-1	1*H*-Indole-3-ethanamine		429b	
302.	50-67-9	1*H*-Indol-5-ol, 3-(2-aminoethyl)-	4249, 4848	4249, 4837	
303.	7004-09-3	Isoleucine $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(NH_2)\text{-}COOH$		3555, 3705, 3797, 3973, 4249, 4398c, 5079, 5413, 5699, 5785, 5827, 5831, 5905	
304.	1509-34-8	Isoleucine, allo-		3974b	
305.	73-32-5	*L*-Isoleucine $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(NH_2)\text{-}COOH$		120, 158, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 5699, 5785, 5811b, 5827, 5831, 5905	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

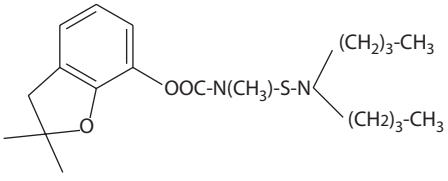
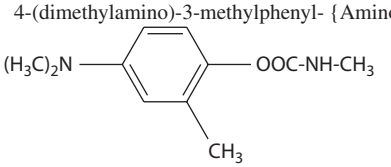
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
306.	139681-66-6	*L*-Isoleucine, *N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-valyl)-*L*-phenylalanyl]-*L*-leucyl]-		4249	
307.		Isoquinolinamine	1371		
308.	1532-84-9	1-Isoquinolinamine	568b, 1371, 2543, 2773, 4249		
309.	97281-47-5	Lecithins		120, 5079, 5126, 5374	
310.	7005-03-0	Leucine $(H_3C)_2$═CH-CH_2-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5699, 5785, 5827, 5831, 5881, 5905	
311.	61-90-5	*L*-Leucine	5811b	424a, 2338, 3973, 5811b	
312.	139681-65-5	*L*-Leucine, *N*-[*N*-[*N*-[*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-phenylalanyl)-*L*-seryl]-*L*-leucyl]-*L*-leucyl]-*L*-methionyl]-*L*-valyl]-*L*-valyl]-		4249	
313.	6899-06-5	Lysine H_2N-$(CH_2)_4$-CH(NH_2)-COOH		429b, 2911c, 3973, 4398c, 5079, 5623, 5785, 17B59	
314.	1190-94-9 28902-93-4	Lysine, hydroxy-		726, 749, 752–754, 4249	
315.	56-87-1	*L*-Lysine H_2N-$(CH_2)_4$-CH(NH_2)-COOH		120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 5623, 5785, 5811b	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
316.	14307-02-9	*D*-Mannose, 2-amino-2-deoxy- {mannosamine}		1063–1066, 1068–1074, 1370, 4249, 4422, 5811b	
317.	74-89-5	Methanamine {methylamine} CH_3-NH_2	126b, 172, 237, 239, 568b, 1099, 1137, 1140, 1263, 1437, 1445, 1674, 1744, 1842, 1902, 1911, 1971, 2001, 2079, 2133, 2170, 2224, 2270, 2455 (0), 2576, 2724, 2734, 2799a, 2858, 2882, 2883, 2889, 2939, 3255, 3300, 3308, 3398, 3491, 3797, 4052, 4056, 4249, 5079, 5512, 5811b	568b, 1877, 2001, 2746, 3491, 3797, 3973, 3974a, 4249, 5079, 5382, 5712, 5811b	4052, 4056
318.	75-50-3	Methanamine, *N,N*-dimethyl- {trimethylamine} $(H_3C)_3{\equiv}N$	568b, 1140, 1263, 1634, 1971, 2001, 2270, 2455, 2724, 2939, 3059, 3398, 3491, 3797, 4249, 5079, 5811b	120, 568b, 984, 1263, 2001, 2939, 3491, 3763, 3974a, 4249, 5079, 5390a, 5403, 5811b	
319.	124-40-3	Methanamine, *N*-methyl- {dimethylamine} $(H_3C)_2{=}NH$	126b, 158a, 237, 568b, 1099, 1137, 1140, 1263, 1445, 1674, 1971, 2001, 2133, 2270, 2455 (0), 2724, 2729, 2734, 2883, 2889, 2939, 3187, 3255, 3302, 3308, 3398, 3491, 3797, 4052, 4056, 4249, 5079, 5811b	558, 568b, 1877, 2001, 2746, 3491, 3974a, 3974b, 3984, 4249, 5079, 5390a, 5382, 5712, 5811b	4052, 4056
320.	62-75-9	Methanamine, *N*-methyl-*N*-nitroso- {NDMA} $(H_3C)_2{=}N$-NO	28, 30, 31, 50, 59, 126, 126a, 126b, 158a, 167, 172, 185, 191, 192, 203, 226, 237, 239, 241, 379, 380, 463, 466, 467, 471, 478, 480, 488, 489, 499, 514, 572, 573, 603, 649, 677b, 746c, 1057–1059, 1099, 1217, 1236, 1428, 1437, 1442, 1443, 1580, 1445, 1674, 1685, 1692, 1693, 1725, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1781, 1784, 1808, 1842, 1870, 1871, 1885, 1952, 1953, 2008, 2057a, 2118, 2129, 2133, 2135, 2134a, 2142, 2205, 2206, 2404, 2405, 2440–2443, 2472, 2516, 2537, 2561, 2635, 2686, 2724, 2750, 2751, 2825, 2884, 2990, 2991, 3123, 3124, 3190,	468, 478, 498, 499, 677b, 1685, 1712, 1727, 1870, 1871, 2313a, 2686, 2990, 3811a, 3943a, 3944–3948, 3973, 3974b, 4010, 4011, 4249, 5001, 5029, 5053. 5496, 5811b	45

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Methanamine, *N*-methyl-*N*-nitroso- {NDMA} $(H_3C)_2$═N-NO (cont.)	3255–3257, 3265, 3300, 3308, 3343, 3366, 3370, 3378, 3441a, 3491, 3493, 3595–3598, 3713, 3777, 3812, 3943a, 3944–3946, 3951, 3952, 3985, 3992, 3994, 4010, 4011, 4249, 5508, 5512, 5869a, 5811b		
321.	107-43-7	Methanaminium, 1-carboxy-*N,N,N*-trimethyl-, inner salt {betaine} $^-$OOC-CH_2-N^+≡$(CH_3)_3$		120, 1351, 2079, 2270, 2283, 2337, 2939, 3491, 3555, 3797, 3973, 3974a, 5079, 5390a, 5189. 5311, 5382, 5435, 5436, 5468	
322.	7005-18-7	Methionine		116, 120, 3705, 4249, 5907	
323.	63-68-3	*L*-Methionine H_3C-S-$(CH_2)_2$-CH(NH_2)-COOH		116, 120, 158, 172, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1128b, 1305a, 1329, 1330, 1332, 1351, 1493, 2049, 2270, 2337, 2359, 2532, 2597a, 2795, 2939, 3186, 3188, 3266, 3491, 3499, 3705, 3729, 3797, 3973, 3974a, 3978, 4226, 4249, 4398c, 5079, 5376, 5811b, 5907	
324.	55285-14-8	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl [(di-*N*-butylamino)thio] ester {Carbosulfan®} 		3633	
325.	2032-59-9	Methylcarbamic acid, 4-(dimethylamino)-3-methylphenyl- {Aminocarb®} 		2650a, 3633, 4271a	
326.	28258-64-2	Naphthalenamine, *N*-phenyl-	2724, 4249, 5811b		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

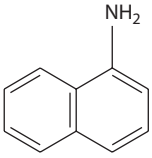
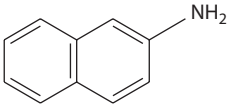
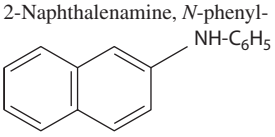
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
327.	134-32-7	1-Naphthalenamine {naphthalene, 1-amino-; α-naphthylamine} 	174b, 174c, 239, 329, 568b, 688, 1217, 1373, 1386, 1410, 1437, 1735, 1747, 1870, 1871, 2142, 2485, 2587, 2724, 2883, 2900, 3007, 3255, 3265, 3300, 3491, 3797, 4137, 4249, 4816, 5049, 5071, 5516, 5811b, 5869a		
328.	2246-44-8	1-Naphthalenamine, 2-methyl-	1735, 2142, 2900, 2957, 4249, 5811b		
329.	90-30-2	1-Naphthalenamine, *N*-phenyl-	568b, 4249		
330.	91-59-8	2-Naphthalenamine {naphthalene, 2-amino-; β-naphthylamine} 	126, 126a, 126b, 139, 174b, 174c, 239, 402, 688, 988a, 1026, 1099, 1217, 1373, 1386, 1410, 1437, 1442, 1445, 1674, 1727, 1740, 1741, 1743, 1744, 1747, 1773, 1781, 1808, 1842, 1870, 1871, 2489, 2553, 2587, 2724, 2825, 2900, 3007, 3255, 3257, 3260, 3265, 3300, 3441a, 3493, 3711, 3781, 4009, 4249, 4407, 4816, 5022, 5508, 5512, 5516, 5811b, 5836, 5869a		
331.	10546-24-4	2-Naphthalenamine, 3-methyl-	1735, 4249		
332.	135-88-6	2-Naphthalenamine, *N*-phenyl- 	568b, 1899, 2552, 2724, 3308, 3491, 4249, 5811b	5811b	
333.	327-57-1 5157-09-5	Norleucine {2-aminohexanoic acid} $H_3C\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		1351, 2337, 2597a, 3491, 3797, 3974a, 3978, 4249	
334.	97145-16-9	Octadecadienoic acid, 1-[[[(2-aminoethoxy) hydroxyphosphinyl]oxy]methyl]-1, 2-ethanediyl ester, (all-*Z*)-		4249	
335.	97190-11-9	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) hexadecanoate		4249	
336.	97190-13-1	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecanoate, (*Z*,*Z*)-		4249	
337.	554-62-1	1,3,4-Octadecanetriol, 2-amino-, [2S-(2R*,3R*,4S*)]-		4249, 4742	
338.	97190-08-4	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecadienoate, (all-*Z*)-		4249	
339.	111-86-4	1-Octanamine $H_3C\text{-}(CH_2)_6\text{-}CH_2\text{-}NH_2$	568b, 2889, 3491, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
340.	7006-33-9	Ornithine {2,3-diaminopentanoic acid} H_2N-$(CH_2)_3$-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 2858, 2939, 3302, 3491, 3797, 4249	555a, 622, 749, 752–754, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 2597a, 2795, 3491, 3705, 3797, 3973, 3974a, 3978, 4249, 5827, 17B34	
341.	70-26-8	*L*-Ornithine	429b, 5811b	429b, 5811b	
342.	20197-09-5	*L*-Ornithine, *N*2-(1-carboxyethyl)-, (R)-		3565, 4249	
343.	372-75-8	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline} H_2N-CO-NH-$(CH_2)_3$-CH(NH_2)-COOH		120, 622, 1305a, 1329, 1330, 1332, 1351, 2337, 2939, 3491, 3797, 3973, 3974a, 3978, 4249, 4398c, 5079	
344.	60918-97-0	1,3,4-Oxadiazol-2-amine, *N*-(4-bromophenyl)-5-(1-naphthalenylmethyl)-		4249	
345.	110-58-7	1-Pentanamine H_3C-$(CH_2)_4$-NH_2	568b, 1099, 1140, 2001, 2724, 2882, 2883, 2889, 3255, 3398, 3491, 3559, 3797, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	
346.	688-31-3	1-Pentanamine, 2-ethyl-*N,N*-dimethyl- H_3C-$(CH_2)_2$-CH(C_2H_5)-CH_2-N(CH_3)$_2$	2543, 2773, 4249		
347.	625-30-9	2-Pentanamine H_3C-$(CH_2)_2$-CH(NH_2)-CH_3	568b, 2724, 2883, 2889, 3491, 3797, 4249, 5811b	568b, 3491, 4249	
348.	616-24-0	3-Pentanamine (H_3C-CH_2)$_2$═CH-NH_2	568b, 2889, 4249	568b, 3491, 4249	
349.	25683-11-8	1,5-Pentanediamide, 2-amino- {glutamine amide} H_2N-OC-$(CH_2)_2$-CH(NH_2)-CO-NH_2		826a, 2914	
350.	462-94-2	1,5-Pentanediamine {cadaverine} H_2N-$(CH_2)_5$-NH_2		568b, 3973, 3974a, 4236, 4249, 4667, 5811b	
351.	6600-40-4	Pentanoic acid, 2-amino-		5777	
352.	63316-29-0	Pentanoic acid, 5-amino-2-hydroxy-, (R)-		5811, 5811b	
353.		Pentanoic acid, 2,5-di-(methylnitrosoamino)- R-$(CH_2)_3$-CH(R)-COOH where R═CH_3-N(NO)-	1008, 1009	1008, 1009, 1013, 3256, 3300	
354.	67920-51-8	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (±)- CH_3-CO-NH-$(CH_2)_3$-CHOH-COOH		2796, 4249, 4817a	
355.	63316-30-3	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (R)-		2796, 4249, 4817a, 5811b	
356.	63316-29-0	Pentanoic acid, 5-amino-2-hydroxy-, (R)-		5811, 5811b	
357.	16814-81-6	Pentanoic acid, 5-amino-2-hydroxy-, (S)- H_2N-$(CH_2)_3$-CHOH-COOH		2796, 4249	
358.	63316-28-9	Pentanoic acid, 5-amino-3-hydroxy- H_2N-$(CH_2)_2$-CHOH-CH_2-COOH		2796, 4249	
359.	106-60-5	Pentanoic acid, 5-amino-4-oxo- H_2N-CH_2-CO-$(CH_2)_2$-COOH		2024a, 4249, 4869	
360.	22537-07-1	4-Penten-1-amine H_2C═CH-$(CH_2)_3$-NH_2	2883, 3491, 4249		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

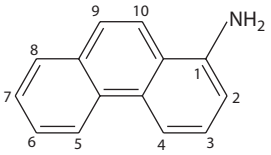
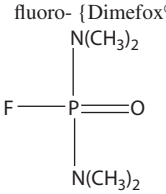
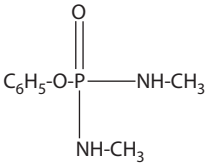
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
361.	1118-66-7	3-Penten-2-one, 4-amino- $H_3C\text{-}C(NH_2)\text{═}CH\text{-}CO\text{-}CH_3$	3559		
362.	64849-97-4	Phenanthrenamine	5811		
363.	4176-53-8	1-Phenanthrenamine 	1735, 4249		
364.	3366-65-2	2-Phenanthrenamine	1735, 4249		
365.	1892-54-2	3-Phenanthrenamine	1735, 4249		
366.	17423-48-2	4-Phenanthrenamine	1735, 4249		
367.	947-73-9	9-Phenanthrenamine	1735, 4249		
368.	3743-22-4	Phenol, 2-(dimethylamino)-	3674, 3712, 4249		
369.	591-27-5	Phenol, 3-amino-	1371, 2543, 2773, 2775, 3410, 3712, 4249		
370.	51-67-2	Phenol, 4-(2-aminoethyl)- {tyramine}	3491, 3674, 3712, 4249	1351, 2337, 3491, 3797, 3974a, 3978, 4249	
371.	63-91-2	*L*-Phenylalanine $C_6H_5\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3797, 4159, 4249, 5811b	120, 158, 622, 722, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1102, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 02359, 2394a, 2453, 2532, 2597a, 2795, 2903, 2905, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3829, 3973, 3974a, 3975, 3978, 4098a, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5811b, 5831, 5905, 5907	
372.	31105-03-0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
373.	51064-37-0	Phenylalanine, ar,ar-dihydroxy-		4249	
374.	115-26-4	Phosphine oxide, bis(dimethylamino) fluoro- {Dimefox®} 		2650b, 3633, 4271a	
375.	67255-31-6	Phosphonic acid, 2-chloroethyl-, hydrazine salt– {Hydrel®} $H_2PO_3\text{-}CH_2CH_2\text{-}Cl.\ H_2N\text{-}NH_2$		5811, 5811b	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

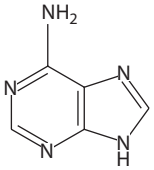
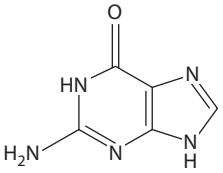
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
376.	1754-58-1	Phosphorodiamidic acid, *N,N′*-dimethyl-, phenyl ester {Diamidafos®} 	2527	2527	
377.	29232-93-7	Phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O*,*O*-dimethyl ester {Pirimiphos-methyl}		4249	
378.		Propanal, 3-(nitrosomethylamino) CH_3-N(NO)-$(CH_2)_2$-CHO		2791	
379.	7324-05-2	Propanamide, 2-amino-, (S)- H_3C-CH(NH_2)-CO-NH_2		4249, 4782	
380.	107-10-8	1-Propanamine $CH_3CH_2CH_2$-NH_2	172, 568b, 1140, 2001, 2724, 2734, 2889, 3219, 3255, 3308, 3398, 3491, 3797, 4052, 4056, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	4052, 4056
381.	5813-64-9	1-Propanamine, 2,2-dimethyl- $(CH_3)_3$≡C-CH_2-NH_2	4249, 4810		
382.	625-43-4	1-Propanamine, *N*,2-dimethyl- CH_3CH(CH3)CH_2-NH-CH_3	568b, 2724, 2734, 2889, 3219, 3308, 3491, 4249	568b, 1877, 3491, 3675, 4249	
383.	2504-18-9 34419-76-6	1-Propanamine, *N*,2-dimethyl-*N*-nitroso- CH_3CH(CH_3)CH_2-N(NO)-CH_3	568b, 2884, 2885, 3256, 3300, 4249	568b, 3561, 4249	
384.	20193-20-8	1-Propanamine, *N*-ethyl-	568b, 4249	568b, 4249	
385.	71607-99-3	1-Propanamine, *N*-ethyl-2-methyl-*N*-nitroso- CH_3CH(CH_3)CH_2-N(NO)-CH_2CH_3	2726, 2884, 2885, 3256, 3300, 4249	2726	
386.	25413-61-0	1-Propanamine, *N*-ethyl-*N*-nitroso- $CH_3CH_2CH_2$-N(NO)-CH_2CH_3	514, 568b, 2726, 3256, 3300, 4249, 5811b	514, 568b, 4249	
387.	627-35-0	1-Propanamine, *N*-methyl- $CH_3CH_2CH_2$-NH-CH_3	568b, 3491, 4249, 5811b	558, 568b, 2722, 2746, 3491, 4249, 5811b	
388.	78-81-9	1-Propanamine, 2-methyl- $(CH_3)_2$═CH-CH_2-NH_2	568b, 1140, 2724, 2734, 2882, 2883, 3255, 3308, 3398, 3491, 4052, 4056, 5811b	568b, 1877, 2746, 3491, 4249, 5811b	4052, 4056
389.		1-Propanamine, 2-methyl-, *N*-butyl- $(CH_3)_2$═CH-CH_2-NH-$(CH_2)_3$-CH_3	2724, 2882		
390.		1-Propanamine, 2-methyl-, *N*-(2-methylpropyl)-*N*-nitroso-	2726, 2884, 4249		
391.		1-Propanamine, *N*-(1-methylethyl)- $CH_3CH_2CH_2$-NH-CH═$(CH_3)_2$	1140, 2724, 2883, 3491, 3797, 4249	1877, 3491, 3675, 4249	
392.	22023-64-9	1-Propanamine, *N*-(1-methylethylidene)- $CH_3CH_2CH_2$-NH-C(CH_3)═CH_2	3559		
393.	924-46-9	1-Propanamine, *N*-methyl-*N*-nitroso- {NMPA} $CH_3CH_2CH_2$-N(NO)-CH_3	457, 470, 486, 1058, 1428, 3256, 3300, 3302, 4249, 5811b	466, 486	
394.	3405-42-3	1-Propanamine, *N*-methyl-*N*-propyl- $(CH_3CH_2CH_2)_2$═N-CH_3	2543, 4249		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
395.	621-64-7	1-Propanamine, *N*-nitroso-*N*-propyl- {NDPA} $(CH_3CH_2CH_2)_2$═N-NO	203, 239, 379, 457, 486, 572, 573, 746c, 1058, 1428, 1740, 1741, 1743, 1744, 1870–1872, 2442, 2443, 2516, 2825, 2884, 3255–3257, 3265, 3300, 3491, 3711, 3713, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	486, 498, 1870–1872	
396.	142-84-7	1-Propanamine, *N*-propyl- $(CH_3CH_2CH_2)_2$═NH	568b, 1140, 2724, 2883, 3797, 4249, 5811b	568b, 1877, 3476, 3675, 3803, 4249, 5811b	
397.	7239-24-9	1-Propanamine, *N,N*,2-trimethyl- $(CH_3)_2$═CH-CH_2-N═$(CH_3)_2$		3491, 4249, 4525	
398.	75-31-0	2-Propanamine $(CH_3)_2$═CH-NH_2	568b, 1099, 1140, 2722, 2724, 2883, 2889, 3255, 3308, 3398, 3491, 3797, 4052, 4056, 4249, 5811b	568b, 1877, 3491, 3974a, 4249	4052, 4056
399.	75-64-9	2-Propanamine, 2-methyl- $(CH_3)_3$≡C-NH_2	2000, 4249, 5811b	1877, 3491, 5811b	
400.	7515-80-2	2-Propanamine, 2-methyl-*N*-(1-methylethyl)- $(CH_3)_3$≡C-NH-$CH(CH_3)_2$	2889, 4249		
401.	3376-24-7	2-Propanamine, 2-methyl-*N*-(phenylmethylene)-, *N*-oxide	4249		
402.		2-Propanamine, *N*-(2,2-dimethylethyl)-	2889		
403.	4747-21-1	2-Propanamine, *N*-methyl- $(CH_3)_2$═CH-NH-CH_3	568b, 1140, 2889, 3491, 2889, 4249	568b, 1877, 3491, 3675, 4249	
404.	16339-04-1	2-Propanamine, *N*-methyl-*N*-nitroso-	568b, 4249		
405.	108-18-9	2-Propanamine, *N*-(1-methylethyl)- $(CH_3)_2$═CH-NH-CH═$(CH_3)_2$	568b, 2889, 3219, 4249		
406.	601-77-4	2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso $[(CH_3)_2$═$CH]_2$-N-NO	2884		
407.	3332-08-9	2-Propanamine, *N*-(1-methylethylidene)-	3559		
408.		2-Propanamine, *N*-(2-methylpropyl)-	2889		
409.	21968-17-2	2-Propanamine, *N*-propyl-═1-Propanamine, *N*-(1-methylethyl)- $CH_3CH_2CH_2$-NH-CH═$(CH_3)_2$	1140, 2724, 2883, 3491, 3797, 4249, 5811b	1877, 3491, 3675, 4249, 5811b	
410.	56-18-8	1,3-Propanediamine, *N*-(3-aminopropyl)- {norspermidine}		4236, 5811b	
411.	60153-49-3	Propanenitrile, 3-(methylnitrosamino)- {MNPN} CH_3-N(NO)-$(CH_2)_2$-CN	3256	2994, 3947, 3948	
412.	1738-25-6	Propanenitrile, 3-(dimethylamino)-	2506, 3559, 4249		
	10478-42-9	Propanoic acid, 3-(methylnitrosoamino)- {NMPA} CH_3-N(NO)-$(CH_2)_2$-COOH See β-alanine, *N*-methyl-*N*-nitroso- {NMPA}	3256, 3300, 3943a, 3944–3946	466, 485, 503, 982, 2852, 3943a, 3944–3946, 3971, 3973, 5001	
413.	298-08-8	2-Propanone, 1-amino- H_3C-CO-CH_2-NH_2	568b, 1371, 1587, 2543, 2773, 3410, 4249, 5811b		
414.	59001-33-1	2-Propenamide, 3-(3,4-dihydroxyphenyl)-*N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino] butyl]amino]propyl]- {dicaffeoylspermidine}		4249, 4567	
415.	29554-26-5	2-Propenamide, *N*-(4-aminobutyl)-3-(3,4-dihydroxyphenyl)-		4249, 4567, 5811b	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
416.	501-13-3	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxy-3-methoxyphenyl)-		4249, 5811b	
417.	34136-53-3	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxyphenyl)-		3491, 4249	
418.	107-11-9	2-Propen-1-amine {allyl amine; acrylamine} $H_2C{=}CH\text{-}CH_2\text{-}NH_2$	568b, 1140, 2724, 2883, 2889, 3491, 3797, 4249, 5811b		
419.	2878-14-0	2-Propen-1-amine, 2-methyl- $H_2C{=}C(CH_3)\text{-}CH_2\text{-}NH_2$	3559		
420.	58994-15-3	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, monoamide with *N*-(3-aminopropyl)-1, 4-butanediamine {caffeoylspermidine}		4249, 4567	
421.	73-24-5	1*H*-Purin-6-amine {adenine} 		120, 568b, 2270, 2539, 2939, 3491, 3797, 3973, 3974a, 4249, 5079, 5189, 5311, 5435, 5436, 5478	
422.	525-79-1	1*H*-Purin-6-amine, *N*-(2-furanylmethyl)-		3973, 4249, 4509	
423.	2365-40-4	1*H*-Purin-6-amine, *N*-(3-methyl-2-butenyl)-		4249, 4590	
424.	1214-39-7	1*H*-Purin-6-amine, *N*-(phenylmethyl)-		3973, 4249, 4557	
425.	56159-42-3	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-		4249, 4603	
426.	38477-23-5	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-		4249, 4603	
427.	54538-20-4	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-		4249, 4620	
428.	73-40-5	6*H*-Purin-6-one, 2-amino-1,7-dihydro- {guanine} 	3797	120, 2270, 2539, 2939, 3491, 3797, 3973, 3974a, 4249, 5079, 5189, 5311, 5435	
429.	33986-27-5	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methyl-2-butenyl)-		4249, 4665	
430.	33698-49-6	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methylbutyl)-		4249, 4665	
431.	34232-31-0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methyl-2-butenyl)-		4249, 4665	
432.	33986-28-6	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methylbutyl)-		4249, 4665	
433.	64990-23-4	Pyrenamine	2141, 4249, 5811b		
434.	64828-53-1	Pyrenamine, *N*-methyl-	2141, 4249, 5811b		
435.	1606-67-3	1-Pyreneamine	1410, 5811b		
436.	5716-15-4 21422-41-3	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt		3636, 4249	
437.	26445-05-6	Pyridinamine	3302		
438.	71607-77-7	Pyridinamine, *N*-methyl-	4249, 4866		
439.	504-29-0	2-Pyridinamine	568b, 1587, 3255, 3386, 4249, 5811b	568b, 3550, 4249	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

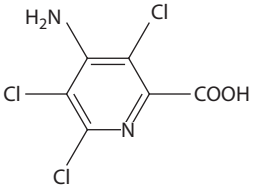
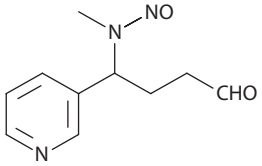
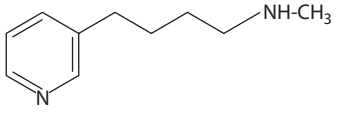
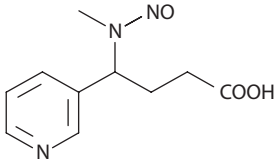
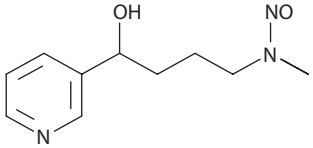
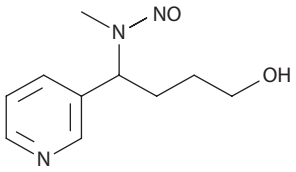
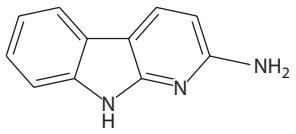
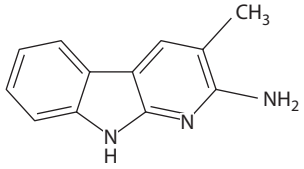
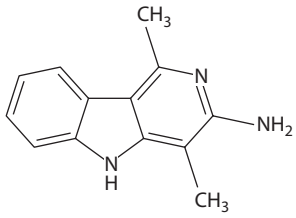
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
440.	1603-40-3	2-Pyridinamine, 3-methyl-	2378a		
441.	695-34-1	2-Pyridinamine, 4-methyl- {2-amino-4-picoline}	4249		
442.	1603-41-4	2-Pyridinamine, 5-methyl-	2378a		
443.	1824-81-3	2-Pyridinamine, 6-methyl-	568b, 2378a, 3410, 4249		
444.	30315-34-5	2-Pyridinamine, 5-(1-methyl-2-pyrrolidinyl)-, (S)-		4249, 4572	
445.	1202-34-2	2-Pyridinamine, *N*-2-pyridinyl-	441, 568b, 4249		
446.	462-08-8	3-Pyridinamine	568b, 3255, 3386, 3967, 4249		
447.	61771-67-3	3-Pyridinamine, 6-methoxy-*N*-methyl-	568b, 3553, 4249		
448.	3430-10-2	3-Pyridinamine, 2-methyl-	3797, 4249		
449.	3430-27-1	3-Pyridinamine, 4-methyl-	4249		
450.	18364-47-1	3-Pyridinamine, *N*-methyl-	1140, 2724, 2734, 3308, 3797, 4249		
451.	504-24-5	4-Pyridinamine	568b, 1587, 3559, 4249, 5811b		
452.	3731-52-0	Pyridine, 3-(aminomethyl)-	5811, 5811a, 5811b		
453.	1918-02-1	2-Pyridinecarboxylix acid, 4-amino-3,5,6-trichloro- {Picloram®} 		3973m 4249	
454.	70898-37-2	3-Pyridinebutanal, γ-(methylamino)-		553, 2226, 4249	
455.	64091-90-3	3-Pyridinebutanal, γ-(methylnitrosoamino)- {NNA}	772, 1568, 1584, 4249	554, 772, 1565, 1584, 3973, 3974b, 5577, 5811b	
456.	64142-45-6	3-Pyridinebutanal, γ-(methylnitrosoamino)-, (*Z*)- 	1012, 1563–1565, 1567a, 1569, 1702, 1751, 3256, 3491, 4249	466, 992, 1012, 1563–1565, 1567a, 1569, 1576, 1577, 1567a, 1702, 3491, 4249	
457.	6021-23-4	3-Pyridinebutanamine		5339, 5777, 5811	
458.	3000-74-6	3-Pyridinebutanamine, *N*-methyl- {dihydrometanicotine} 	568b, 761, 1078, 2228, 2724, 2730, 2734, 3054, 3302, 3308, 3505, 4249, 5811b	120, 568b, 2349, 2746, 2790, 3444, 4249, 5811b	
459.	17270-48-3	3-Pyridinebutanoic acid, γ-(methylamino)-, (±)-		4249, 4779	
460.	152720-16-6	3-Pyridinebutanoic acid, γ-(methylnitroamino)-		3444	
461.	123743-84-0 133201-36-2	3-Pyridinebutanoic acid, γ-(methylnitrosoamino)- {iso-NNAC} 	59, 486, 1008, 1009, 1012, 1013, 1584, 1702, 1751, 3256, 3300, 4249, 5811, 5811a, 5811b	465, 486, 992, 993, 995, 1008, 1009, 1012, 1013, 1584, 1702, 1750, 3973, 4236, 4249, 5811, 5811a, 5811b	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
462.	59578-66-4 76014-81-8	3-Pyridinebutanol, *d*-(methylnitrosoamino)- {NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-; 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-} 	24, 25, 59, 486, 991, 1565, 1571a, 1573a, 1584, 1702, 1751, 3184, 3256, 3300, 5565	469, 486, 507a, 728, 995, 1562a, 1565, 1571a, 1573a, 1584, 1702, 1771, 3943b, 3973, 4236, 4249, 5577, 5811b	
463.	133201-37-3	3-Pyridinebutanol, δ-(methylnitrosoamino)- {iso-NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-} 	59, 486, 508, 1584, 1702, 1751, 3256, 3943a, 3944–3946, 4249	486, 1562a, 1584, 1679, 1702, 3943a, 3944–3946, 3947, 3948, 3973, 4236, 5577	
464.	70898-36-1	3-Pyridinebutanol, δ-amino-		4249	
465.	38076-78-7	3-Pyridinecarbonitrile, 2-amino-5-methyl-	1587, 4249, 5811b		
466.		3-Pyridinemethanamine, ethyl-	1371		
467.	3000-75-7	3-Pyridinemethanamine, *N*-ethyl-	4249		
468.	85352-99-4	3-Pyridinemethanol, α-[3-(methylnitrosoamino) propyl]-, 1-oxide		4249	
469.	26148-68-5	1*H*-Pyrido[2,3-*b*]indol-2-amine {AαC} 	179a, 179b, 751, 755, 756, 933, 1740, 1741, 1743, 1744, 2354a, 2449, 2450, 2484a, 2492, 3265, 3300, 3714, 4249, 4367, 4368, 4388, 4389, 4390, 5002, 5512, 5869a		
470.	68006-83-7	1*H*-Pyrido[2,3-*b*]indol-2-amine, 3-methyl- {MeAαC} 	179a, 179b, 751, 755, 756, 933, 1740, 1741, 1743, 1744, 2354a, 2449, 2450, 2484a, 2492, 3265, 3300, 3714, 4249, 4367,4368, 4388, 4389, 4390, 5002, 5512,, 5811b, 5869a		
471.	62450-06-0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1,4-dimethyl- {Trp-P-1} 	751, 755, 756, 1373, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4249, 4367, 4368, 5002, 5512, 5869a		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

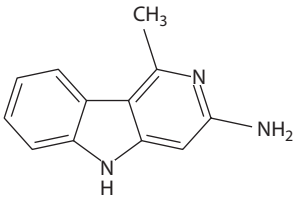
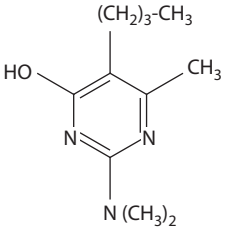
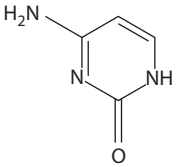
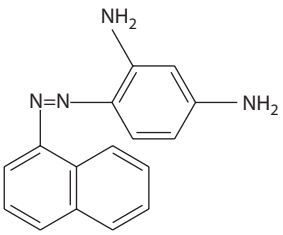
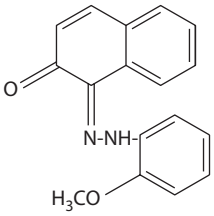
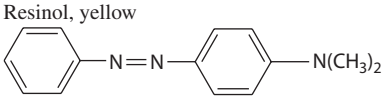
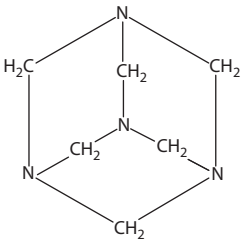
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
472.	62450-07-1	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1-methyl- {Trp-P-2} 	751, 755, 756, 1373, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4249, 4367, 4368, 5002, 5512, 5869a		
473.	5221-53-4	Pyrimidine, 5-butyl-2-dimethylamino-4-hydroxy-6-methyl- {Dimetherimol®} 		3633, 4249	
474.	71-30-7	2(1*H*)-Pyrimidinone, 4-amino- {cytosine} 	2539, 4249	120, 2270	
475.	487-90-1	1*H*-Pyrrole-3-propanoic acid, 5-(aminomethyl)-4-(carboxymethyl)-		4249, 4870	
476.	69730-92-3	Pyrrolidine, 1-[4-(dimethylamino)-1-oxobutyl]-2-(3-pyridinyl)-, (S)-		2497, 2498, 4236, 4249	
477.	31135-62-3	Quinolinamine	5811, 5811a, 5811b		
478.	580-22-3	2-Quinolinamine	722, 1121, 4249		
479.	611-34-7	Quinoline, 5-amino-	4407		
480.		Quinoline, 5-amino-6,8-dimethoxy-		2917a	
481.		Quinoline, 5-amino-2-hydroxymethyl-6-methoxy-		2917a	
482.	13207-66-4	8-Quinolinol, 5-amino-		2917a	
483.	6416-57-5	Resinol, brown 		5079, 5381	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	69772-40-3	Resinol, red 			
	60-11-7	Resinol, yellow 			
484.	6898-95-9	Serine $HO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 2858, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1063–1066, 1068–1074, 1223, 1305a, 1351, 1493, 1918, 1919, 2048, 2270, 2337, 2338, 2339b, 2445a, 2453, 2532, 2597a, 2795, 2911a, 2911c, 2939, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5699, 5827, 5831, 5881, 5896, 5905, 5907	
485.	35688-48-3	*D*-Serine, *N*-(carboxyacetyl)-		2048, 4249, 4728	
486.	56-45-1	*L*-Serine		3973, 5811b	
487.	5692-15-9	*L*-Serine, labeled with ^{14}C		4249, 4940	
488.	5147-00-2	*L*-Serine, acetate (ester) $CH_3\text{-}COO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$		429b, 4249, 4895	
489.	142785-07-7	*L*-Serine, *L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		4249	
490.	146440-48-4	*L*-Serine, *L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		4249	
491.	100-97-0	1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane {hexamethylenetetramine} 	172, 568b, 1321, 1371, 3255, 3411, 3559, 4249		

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

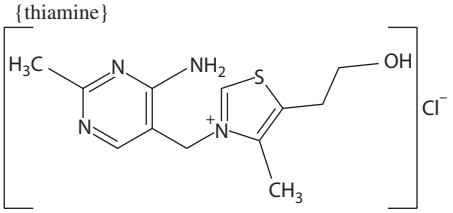
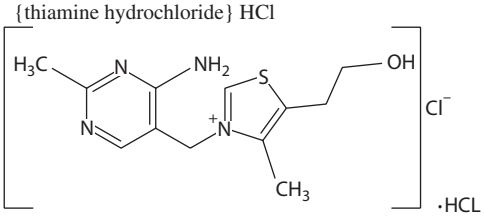
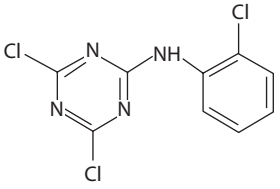
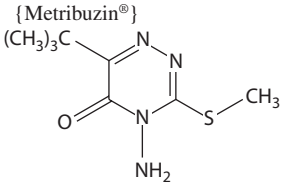
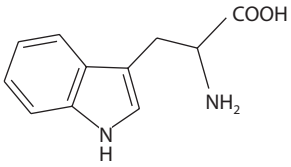
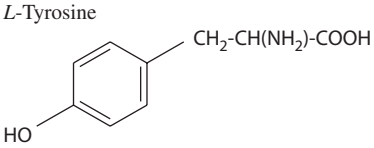
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
492.	154-87-0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-4-methyl-5-(4,6,6-trihydroxy-3,5-dioxa-4, 6-diphosphahex-1-yl)-, chloride, P,P′-dioxide		4051a, 4249, 4798	
493.	59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride {thiamine} 		120, 1941, 2270, 4249, 5079, 17B10	
494.	67-03-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-5-(2-hydroxyethyl)-4-methyl- chloride, monohydrochloride {thiamine hydrochloride} HCl 		1053, 3266, 4249	
495.	72-19-5	*L*-Threonine $H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3555, 3797, 4249, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1305a, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5811b, 5827, 5831, 5881	
496.	32190-57-1	*L*-Threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]- {tabtoxin}		3819a, 4249	
497.		*L*-Threonine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337	
498.	101-05-3	1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-(2-chlorophenyl)- {Anilazine®; Dyrene®} 		3633, 3661a, 3797, 4249, 4271a	

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
499.	21087-64-9	1,2,4-Triazin-5(4*H*)-one, 4-amino-6-tert-butyl-3-(methylthio)- {Metribuzin®} 		2913a, 4249	
500.	81901-03-3	3,5,9-Trioxa-4-phosphaheptacosadien-1-aminium, 4-hydroxy-*N,N,N*-trimethyl-10-oxo-7-[(1-oxooctadecadienyl)oxy]-, hydroxide, inner salt, 4-oxide		4249	
501.	70106-56-8	3,5,9-Trioxa-4-phosphaheptacosan-1-aminium, 4-hydroxy-*N,N,N*-trimethyl-10-oxo-7-[(1-oxooctadecatrienyl) oxy]-, hydroxide, inner salt, 4-oxide, hexadehydro derivative, (R)-		4249	
502.	6912-86-3	Tryptophan		3705	
503.	73-22-3	*L*-Tryptophan 		120, 480, 622, 722, 749, 751–756, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 2079, 2270, 2337, 2338, 2359, 2510, 2532, 2597a, 2795, 2902, 2903, 2911c, 2939, 3491, 3705, 3797, 3829, 3973, 3974a, 3978, 4103, 4224, 4244, 4249, 4286b, 4398c, 5079, 5603, 5785, 5811b, 5831, 5881, 5905	
504.	60738-11-6	*L*-Tryptophan, labeled with ^{14}C		2562a, 4249, 4876	
505.	55520-40-6	Tyrosine		3705	
506.	587-45-1	Tyrosine, 3-hydroxy-		429b	
507.	60-18-4	*L*-Tyrosine 		120, 158, 622, 749, 752-754, 826a, 927, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1965, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4398c, 5079, 5785, 5811b, 5827, 5905, 5907	

(*continued*)

TABLE 12.2 (continued)
Acyclic Amines Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
508.	34393-22-1	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-		1351, 2337, 4362	
509.	7004-03-7	Valine $(H_3C)_2$═CH-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4249, 4359, 4398c, 5079, 5493, 5785, 5827, 5831, 5881, 5905, 5907	
510.	72-18-4	*L*-Valine	5811b	424a, 429b, 2338, 5811b	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke.

13 Amides

In his 1954 compilation of smoke components, Kosak (2170) listed no amide identified to that date. In their 1959 review of tobacco and tobacco smoke components, Johnstone and Plimmer (1971) described the identification of asparagine and glutamine in tobacco and glutamine and nicotinamide in tobacco smoke. The latter two were identified in smoke by Buyske et al. (562). In its 1963 monograph on tobacco and smoke components, Philip Morris (2939) listed the amides, asparagine, glutamine, citrulline, and nicotinamide as tobacco components but only glutamine and nicotinamide as smoke components.

Stedman (3797) in his 1968 review of tobacco and smoke components listed asparagine, citrulline, and glutamine as amino-acid-related components not as amides [see Table XIV in (3797)]. Nicotinamide and *N*-methylnicotinamide were not listed specifically as amides but as alkaloid derivatives [see Table XI in (3797)]. Cotinine was also listed in the same table.

Ishiguro and Sugawara (1884) in their 1980 monograph on tobacco smoke components listed a total of 72 amides, imides, and lactams (49 amides, 7 imides, 16 lactams) [see Table I-15 in (1884)]. The reference for all but two of the listed compounds (formamide and urethane) was that of Schumacher et al. (3553). Several amides, imides, and lactams were listed by Ishiguro and Sugawara in other tables, e.g., asparagine and glutamine under amino acids [Table I-19 in (1884)], cotinine and norcotinine under alkaloids, and caffeine under *N*-polycyclics (excluding alkaloids).

Citing publications by Schmeltz and Hoffmann (3491), Schumacher et al. (3553), and Heckman and Best (1587), the International Agency for Research on Cancer (IARC) in its 1986 monograph on tobacco smoking stated [see p. 109 in (1870)] that there was a large spectrum of amides, imides, and lactams in tobacco smoke (including some 50 aliphatic amides). While the IARC commented on the Johnston et al. 1973 report on the per cigarette yields of formamide, acetamide, and propanamide, it did not mention that Johnston et al. in their 1973 report (1965) had noted that only three amides, glutamine, asparagine, and nicotinamide, had been identified in tobacco smoke at that time. The IARC expressed concern about the 24 secondary amides identified in smoke, particularly *N*-methylformamide, *N*-methylacetamide, *N*-methylpropanamide, and *N*-methylnicotinamide, because of their propensity to generate tumorigenic nitrosamides. Despite the fact that these secondary amides have been identified in tobacco smoke and are known to readily form *N*-nitrosamides, no such *N*-nitroso compound has been identified to date in tobacco smoke [Rodgman and Green (3300)].

IARC also mentioned the two lactams *N*-methyl-2-pyrrolidone and *N*-methyl-2-piperidone and the urethanes but made no textual comment about their biological effect. Of the 53 amides identified in tobacco smoke by Schumacher et al. (3553), 32 were new to tobacco smoke composition. Their contribution in this regard was the result of the use of an analytical technology that permitted the fractionation and identification of many components in the water-soluble portion of cigarette smoke condensate.

In his study of the composition of smoke from an all-burley tobacco cigarette, Heckman (1586) identified 16 amides, ranging in complexity from acetamide to *N′*-formylnornicotine.

Although 227 amides are cataloged in Table 13.1, it should be realized that the number of amides in tobacco far exceeds the number of amides listed in Table 13.1 for tobacco and tobacco smoke. Each of the many thousands of enzymes, proteins, and proteinaceous components in tobacco possesses many amido linkages. Nearly 500 of the well-characterized enzymes and proteins are cataloged in Table 22.2, but that number is only a small fraction of the great number of such components in tobacco.

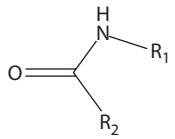
IARC had little to say about the possible ill effects of any of the amides in tobacco smoke. However, it did note in an appendix to its monograph [Appendix 2, pp. 389–394 in (1870)] that sufficient evidence existed for the initiating and cocarcinogenic activity in animals of urethane (ethyl carbamate) and the evidence was limited for acetamide. IARC listed the per cigarette yields of acetamide and urethane. In the first listing of tumorigens, carcinogens, and toxicants in tobacco smoke, by Hoffmann and Wynder in 1986 (1808), only urethane was included. Urethane was included in several subsequent lists, those by Hoffmann and Hecht (1727), Hoffmann et al. (1773), and Hoffmann and Hoffmann (1740). In their 1997 list (1740), Hoffmann and Hoffmann added acrylamide (2-propenamide) as present in cigarette smoke, but no per cigarette yield was included. In their next three lists of tumorigens, carcinogens, and toxicants in tobacco smoke issued between 1998 and 2001, Hoffmann and Hoffmann (1741, 1743, 1744) listed per cigarette yields of acetamide and urethane and the presence of acrylamide. Other listings of tumorigens, carcinogens, and toxicants in

tobacco and tobacco smoke by the Occupational Safety and Health Administration (OSHA) (2825) in 1994 and Fowles and Bates (1217) in 2001 included urethane but not acetamide or acrylamide. The various degrees of inclusion in the many lists issued between 1986 and 2001 were summarized by Rodgman (3265).

Acetamide, acrylamide, and urethane were not included in most of the requirements for "Hoffmann analyte" data as an indication of cigarette smoke hazard, e.g., the Department of Health (Canada) proposal in 2000 (25A06).

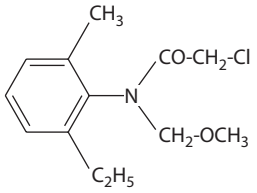
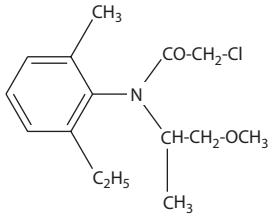
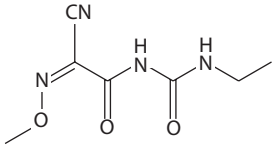
One other aspect of interest concerning amides is that several (asparagine, glutamine, urea) appear on the Doull et al. list of individual compounds used in cigarette manufacture by U.S. companies (1053). The Doull et al. list also includes the imide 3,7-dihydro-1,3,7-trimethyl-1*H*-purine-2,6-dione (caffeine).

Although they are on the borderline of the definition of an amide, urethane plus urea and several of its derivatives have been included in Table 13.1. Because each possesses structure I, each was included as an amide for the sake of completeness; e.g., urea is $H_2N\text{-}CO\text{-}NH_2$, and ethyl urethane is $H_2N\text{-}COO\text{-}C_2H_5$. Several of the urea derivatives are compounds used in tobacco agronomy.



The number of compounds in Table 13.1 totals 227 of which 191 are amides. The remaining components include urethane plus urea and several of its derivatives. Of the 227 compounds, 134 were identified in tobacco, 137 in tobacco smoke, and 44 were identified in both tobacco and smoke.

TABLE 13.1
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	60-35-5	Acetamide CH_3-CO-NH_2	167, 172, 568b, 1099, 1350, 1354, 1360, 1371, 1375, 1375a, 1375b, 1586, 1590, 1741, 1743, 1744, 1870, 1871, 1965, 1968, 2387, 2543, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 3190, 3255, 3265, 3300, 3386, 3397, 3410, 3491, 3553, 3557, 3559, 3714, 3992, 4228, 4249, 5512, 5811b, 5869a	568b, 2471, 4249	1354, 1360, 1375a, 2387
2.	1113-68-4	Acetamide, *N*-acetyl-*N*-methyl- CH_3-CO-N<(CH$_3$, CO-CH_3)	568b, 2543, 2767, 2773, 4249	568b, 2543, 4249	
3.	1119-49-9	Acetamide, *N*-butyl- CH_3-CO-NH-C_4H_9	568b, 3553, 4249, 5811b		
4.	15972-60-8	Acetamide, 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)- {Alachlor®} 		2650a, 2913a, 3633, 4271a	
5.	51218-45-2	Acetamide, 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)- {Metolachlor®} 		2650b, 4271a	
6.	107-91-5	Acetamide, 2-cyano- NC-CH_2-CO-NH_2	4249		
7.	57966-95-7	Acetamide, 2-cyano-2-methoxyimino-*N*-(ethylcarbamoyl)- {Cymoxanil®} 		3633	
8.	685-91-6	Acetamide, *N,N*-diethyl- CH_3-CO-N=(C_2H_5)$_2$	568b, 2141, 4249, 5811b		
9.	127-19-5	Acetamide, *N,N*-dimethyl- CH_3-CO-N=(CH_3)$_2$	568b, 3386, 3410, 3559, 4249	568b, 2389, 2544, 3491, 4249, 5811b	
10.	625-50-3	Acetamide, *N*-ethyl- CH_3-CO-NH-C_2H_5	568b, 3386, 3410, 3559, 4249		
11.	38806-26-7	Acetamide, *N*-ethyl-*N*-methyl- CH_3-CO-N<(CH_3, C_2H_5)	2141, 4249, 5811b		

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

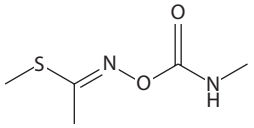
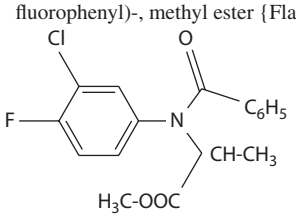
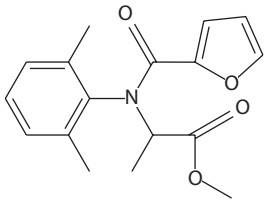
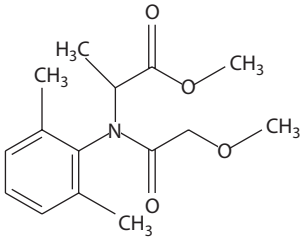
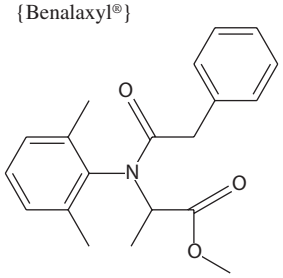
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
12.	5663-62-7	Acetamide, *N*-(2-furanylmethyl)-	568b, 1587, 4249, 5811b		
13.	621-42-1	Acetamide, 3-hydroxyphenyl-		2917a	
14.	4293-57-6	Acetamide *N*-(2-hydroxypropyl)- H_3C-CO-NH-CH_2-CHOH-CH_3	568b, 4249		
15.	79-16-3	Acetamide, *N*-methyl- CH_3-CO-NH-CH_3	568b, 1586, 2543, 2570, 2773, 2775, 3255, 3410, 3553, 3559, 4249, 5811b		
16.	54824-90-7	Acetamide, *N*-(2-methylbutyl)- CH_3-CO-NH-CH_2-CH(CH_3)-C_2H_5	568b, 1587, 4249, 5811b		
17.	13434-12-3	Acetamide, *N*-(3-methylbutyl)- CH_3-CO-NH-$(CH_2)_2$-CH═$(CH_3)_2$		568b, 937, 2389, 2544, 3491, 4249, 5811b	
18.	1189-05-5	Acetamide, *N*-(1-methylpropyl)- CH_3-CO-NH-CH(CH_3)-C_2H_5	568b, 1587, 4249, 5811b		
19.	1540-94-9	Acetamide, *N*-(2-methylpropyl)- CH_3-CO-NH-CH_2-CH═$(CH_3)_2$	568b, 3553, 4249	568b, 2389, 2544, 3491, 4249, 5811b	
20.	7737-16-8	Acetamide, *N*-(2-oxopropyl)- CH_3-CO-NH-CH_2-CO-CH_3	568b, 3553, 4249, 5811b		
21.	103-84-4	Acetamide, *N*-phenyl- CH_3-CO-NH-C_6H_5	3553, 4249		
22.	877-95-2	Acetamide, *N*-(2-phenylethyl)- CH_3-CO-NH-CH_2-CH_2-C_6H_5	568b, 1587, 4249, 5811b		
23.	692-33-1	Acetamide, *N*-2-propenyl- CH_3-CO-NH-CH_2-CH═CH_2	568b, 3553, 4249, 5811b		
24.	5331-48-6	Acetamide, *N*-propyl- CH_3-CO-NH-C_3H_7	568b, 3553, 4249, 5811b		
25.	354-38-1	Acetamide, 2,2,2-trifluoro- F_3C-CO-NH_2	2882, 4249		
26.	16752-77-5	Acetamidic acid, thio-, *N*-[(methylcarbamoyl) oxy]-, methyl ester {Methomyl®} 		1219, 1219b, 1219c, 1333, 2650b, 3633, 3977, 4271a	
27.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4708	
28.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	
29.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
30.	52756-25-9	*DL*-Alanine, *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-, methyl ester {Flamprop-methyl®} 		4271a	

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	57646-30-7	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(2-furanylcarbonyl)-, methyl ester {Furalaxyl®} 		3633	
32.	57837-19-1	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-, methyl ester {Ridomil®} 		2892a, 3633, 4271	
33.	71626-11-4	*DL*-Alanine, methyl-*N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)- {Benalaxyl®} 		3633	
34.	7006-34-0	Asparagine $H_2N\text{-}CO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 1965, 2724, 3266, 4159, 4249, 5811b	120, 480, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1223, 1305a, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2532, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4244, 4249, 4398c, 5048, 5079, 5126, 5189, 5437, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
35.	70-47-3	*L*-Asparagine		429b, 2338	

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

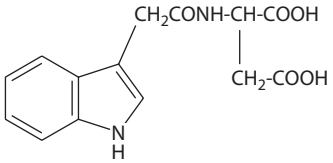
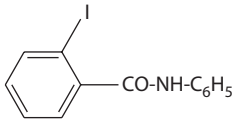
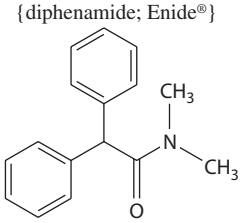
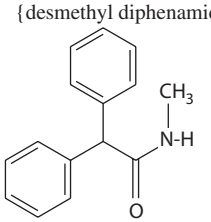
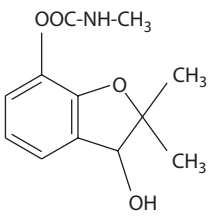
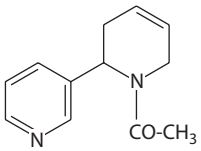
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
36.	5794-13-8	*L*-Asparagine monohydrate		3973	
37.	2456-73-7	*L*-Aspartic acid, *N*-(1*H*-indol-3-ylacetyl)- 		4249, 4659	
38.	55-21-0	Benzamide C_6H_5-CO-NH_2	1365, 2543, 2767, 2773, 3553, 3557, 4249, 5811b	3550	
39.	15310-01-7	Benzamide, 2-iodo-*N*-phenyl- {Benodanil®} 		774a, 4271a, 4249, 4552	
40.	103-81-1	Benzeneacetamide {phenylacetamide}	568b, 1063–1066, 1068–1074, 1371, 3410, 3553, 5811b	568b, 3550, 4249	
41.	4695-13-0	Benzeneacetamide, α-phenyl-		4249, 5811b	
42.	957-51-7	Benzeneacetamide, *N,N*-dimethyl-α-phenyl- {diphenamide; Enide®} 	346, 1333, 4249	1219b, 1219c, 1333, 2650a, 3633, 3767a, 3973, 3977, 4249, 4271a, 5811b	
43.	954-21-2	Benzeneacetamide, *N*-methyl-α-phenyl- {desmethyl diphenamid} 	346	3491, 5811b	
44.	102-93-2	Benzenepropanamide	568b, 1063–1066, 1068–1074, 1365, 1371, 2543, 2773, 2775, 3410, 3553, 4249, 5811b	568b, 3869, 4249	
45.	121850-61-1	Benzenepropanamide, *N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]-3,4-dihydroxy-		4249, 5811b	
46.	19044-88-3	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro- {Oryzalin®}		4271a	
47.	16655-82-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate) {3-Hydroxycarbofuran®} 	1553, 4249, 21A19	1280, 1553, 3481, 5811b, 21A19	

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
48.	3619-22-5	Benzoic acid, 4-methyl-, hydrazide C_6H_5-CO-NH-NH_2	3327a, 5811b		
49.	61892-64-6	2,3′-Bipyridine, 1-acetyl-1,2,3,6-tetrahydro-, (S)- {*N*′-acetylanatabine} 	3553, 3739, 3740, 4249, 5811b	64, 1248, 2566, 3973, 4236, 4249, 5811b	
50.	96552-71-5	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxohexyl)-, (S)- {*N*′-hexanoylanatabine}	3739, 3740, 4249, 5811b		
51.	96552-72-6	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxooctyl)-, (S)-{*N*′-octanoylanatabine}	3739, 3740, 4249, 5811b		
52.	61892-65-7	[2,3′-Bipyridine]-1(2*H*)-carboxaldehyde, 3,6-dihydro-, (S)- {*N*′-formylanatabine}	568b, 3553, 3739, 3740, 4249, 5811b	64, 568b, 3550, 3973, 4236, 4249, 5811b	
53.	541-35-5	Butanamide H_3C-$(CH_2)_2$-CO-NH_2	568b, 1371, 1375, 1375b, 1586, 2767, 3255, 3386, 3410, 3553, 3557, 3559, 4249, 5811b		
54.	66309-91-9	Butanamide, 2,3-dimethyl- $(H_3C)_2$═CH-$CH(CH_3)$-CO-NH_2	568b, 2570, 2769, 3553, 4249		
55.	1113-57-1	Butanamide, 2-methyl- H_3C-CH_2-$CH(CH_3)$-CO-NH_2	568b, 2387, 2775, 3553, 3557, 3559, 4249, 4570a, 5811b		2387
56.	61892-66-8	Butanamide, 3-cyano-3-methyl- $(H_3C)_2$═C(CN)-CH_2-CO-NH_2	568b, 3553, 4249, 5811b		
57.	541-46-8	Butanamide, 3-methyl- $(H_3C)_2$═CH-CH_2-CO-NH_2	568b, 1063–1066, 1068–1074, 1365, 1586, 2543, 2570, 2760, 2761, 2762, 2765–2767, 2773,2775, 2777, 3386, 3410, 3553, 3557, 3559, 4249, 4570a, 5811b		
58.	53897-27-1	Butanamide, 4-cyano- NC-$(CH_2)_3$-CO-NH_2	568b, 3553, 4249, 5811b		
59.	110-14-5	Butanediamide {succinamide} H_2N-CO-$(CH_2)_2$-CO-NH_2	568b, 4249, 4573		
60.	16748-73-5	Butanediamide, 2-amino-, (S)- {asparagine amide} H_2N-CO-CH_2-$CH(NH_2)$-CO-NH_2		826a, 2914	
61.	70185-59-0	1,4-Butanediamine, *N*-[3-(amino)-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy- {*p*-coumaroylspermidine}		5811, 5811b	
62.	625-37-6 23350-58-5	2-Butenamide, (*E*)- {*trans*-crotonamide}	568b, 2570, 3553, 4249, 5811b		
63.	31110-30-2	2-Butenamide, (*Z*)-	3410, 3553, 4249, 5811b		
64.	1187-41-3 72693-06-2	2-Butenamide, *N*,2-dimethyl-	568b, 3226, 3553, 4249		
65.	23350-60-9	2-Butenamide, *N*-ethyl-	568b, 4249		
66.	6923-22-4	2-Butenamide, 3-hydroxy-*N*-methyl-, dimethylphosphate, (*Z*)- {Monocrotophos®}		5811, 5811b	
67.	32793-37-6	2-Butenamide, 2-methyl-	568b, 3553, 4249, 5811b		
68.	28446-58-4	3-Butenamide	568b, 3553, 3559, 4249, 5811b		
69.	18938-03-9	3-Butenamide, 3-methyl-	568b, 3553, 4249, 5811b		

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

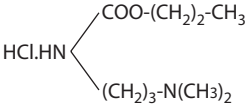
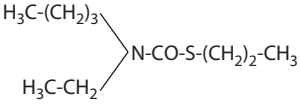
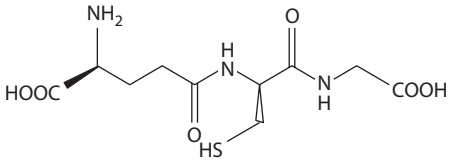
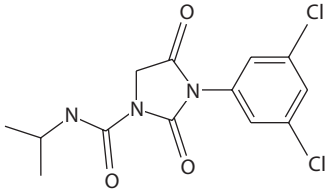
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
70.	32040-41-8	2-Butenoic acid, 4-(formylamino)-4-oxo-, (Z)- O═CH-NH-CO-CH═CH-COOH		4249, 4918	
71.	23103-98-2	Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester {Pirimicarb®}		3633, 4271a	
72.	25606-41-1	Carbamic acid, 3-(dimethylamino)propyl-, propyl ester, hydrochloride {Propamocarb hydrochloride®}  		3633	
73.	51-79-6	Carbamic acid, ethyl ester {urethane} H_2N-COO-C_2H_5	126a, 239, 757, 1148, 1217, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1870, 1871, 2825, 3255, 3257, 3265, 3300, 3483, 3714, 4005–4007, 4010, 4011, 4249, 5512, 5811b, 5869a	757, 3483, 3973, 3974b, 4249, 5524	
74.	598-55-0	Carbamic acid, methyl ester H_2N-COO-CH_3		3483, 4249	
75.	137-42-8	Carbamic acid, *N*-methyldithio-, monosodium salt {Metham-sodium®} H_3C-NH-CS-SNa		3633, 3646a, 4271a	
76.	1114-71-2	Carbamothioic acid, butylethyl-, *S*-propyl ester {Pebulate®}  		1219b, 1219c, 2913a, 3633, 4271a	
77.	759-94-4	Carbamothioic acid, dipropyl-, *S*-ethyl ester {EPTC®}		3633	
78.	1929-77-7	Carbamothioic acid, dipropyl-, *S*-propyl ester {Vernolate®}		2650a	
79.	2303-17-5	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester amothioic acid, dipropyl-, *S*-propyl ester {Triallate®}		2650a	
80.	14995-49-4	Dodecanamide, *N*-(1-methylethyl)-	568b, 4249		
81.	75-12-7	Formamide H-CO-NH_2	568b, 1965, 1968, 3255, 3491, 3553, 3559, 4249		
82.	871-71-6	Formamide, *N*-butyl- H-CO-NH-$(CH_2)_3$-CH_3	1587, 3553, 4249		
83.	68-12-2	Formamide, *N,N*-dimethyl- H-CO-N═$(CH_3)_2$	568b, 3410, 3559, 4249, 5869a	568b, 2917a, 4249	
84.	72693-10-8	Formamide, *N*-(2-furanylmethyl)-	568b, 1587, 4249, 5811b		
85.	123-39-7	Formamide, *N*-methyl- H-CO-NH-CH_3	568b, 3553, 3559, 4249, 5811b		
86.	10285-87-7	Formamide, *N*-(3-methylbutyl)-	568b, 3553, 3557, 3559, 4249	568b, 937, 3491, 4249	
87.		Formamide, *N*-(3-methylpyrrolyl-2-ethyl)-	568b, 4249		
88.	2591-79-9	Formamide, *N*-pentyl- H-CO-NH-$(CH_2)_4$-CH_3	568b, 1587, 4249, 5811b		
89.	103-70-8	Formamide, *N*-phenyl-	2543, 2773, 4249		
90.	6343-54-0	Formamide, *N*-(phenylmethyl)-	568b, 1587, 4249, 5811b		
91.	56625-04-8	Formamide, *N*-(3-pyridinylmethyl)-	568b, 1587, 4249, 5811b		

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
92.	29988-76-9	Furancarboxamide	2767, 3557	2337a	
93.	609-38-1	2-Furancarboxamide	568b, 1586, 2787, 3553, 3557, 3559, 4249, 5811b	568b, 2336, 4249	
94.		2-Furancarboxamide, *N*-ethyl-	568b, 4249	568b, 4249	
95.	61190-74-7	2-Furancarboxamide, *N*-(2-furanylmethyl)-	568b, 4249	568b, 4249	
96.	3736-81-0	2-Furancarboxylic acid, 4-[(2,2-dichloroacetyl)-methylamino]phenyl ester	5811, 5811a, 5811b		
97.	1398-61-4	*D*-Glucose, β-(1,4)-2-acetamido-2-deoxy-		1102	
98.	6899-04-3	Glutamine $H_2N\text{-}CO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	562, 1910, 1914, 2939	1971, 2939, 3705	
99.	56-85-9	*L*-Glutamine $H_2N\text{-}CO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	480, 562, 563, 1351, 1668, 1910, 1914, 1965, 2079, 2724, 2858, 2939, 3059, 3266, 3302, 3491, 3797, 4159, 4249	120, 480, 563, 622, 749, 751–756, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2529, 2532, 2939, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 5079, 5189, 5434, 5437, 5699, 5785, 5811b, 5827, 5831, 5881, 5905, 5907	
100.	88476-94-2	Glycine, *N*-(1-nitroso-*L*-prolyl)-		3951, 4249	
101.	70-18-8	Glycine, *N*-(*N*-*L*-γ-glutamyl-*L*-cysteinyl)- {glutathione} 		120, 1351, 1668, 2337, 2939, 3491, 3797, 3974a, 4249, 5079, 5220, 5572, 5811b	
102.	628-02-4	Hexanamide $H_3C\text{-}(CH_2)_4\text{-}CO\text{-}NH_2$	568b, 1364, 1371, 1586, 2570, 2762, 2767, 3410, 3553, 3557, 4249, 4570a, 5811b		
103.	36734-19-7	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®} 		3585c, 3633, 3661a	

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

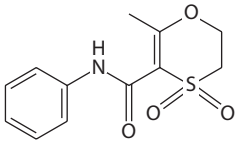
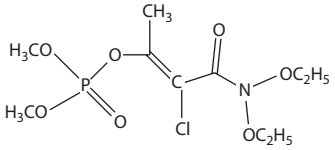
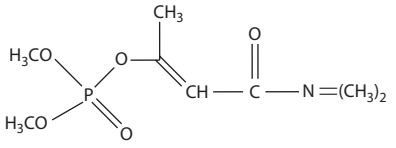
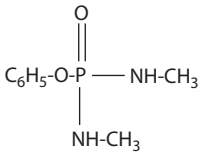
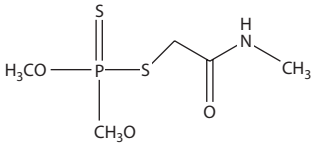
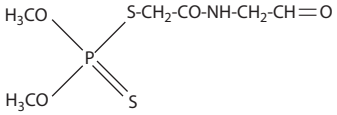
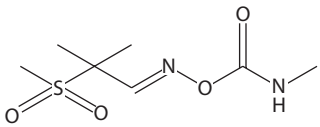
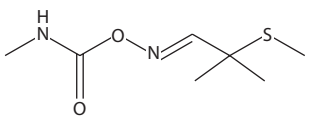
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
104.	31212-21-2	1*H*-Indoleacetamide		4249	
105.	70699-77-3	3-Morpholinepropanamide, 2-oxo-6-(1,2,3,4-tetrahydroxybutyl)-, [3S-[3α,6α(1R*,2S*,3S*)]]-		1863a	
106.	372-75-8	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline} $H_2N\text{-}CO\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$		120, 622, 1305a, 1329, 1330, 1332, 1351, 2337, 2939, 3491, 3797, 3973, 3974a, 3978, 4249, 4398c, 5079	
107.	5259-88-1	1,4-Oxathiin-3-carboxamide4,4-dioxide,5,6-dihydro-2-methyl-*N*-phenyl- {Oxycarboxin®} 		2650b	
108.	626-97-1	Pentanamide {valeramide} $H_3C\text{-}(CH_2)_3\text{-}CO\text{-}NH_2$	568b, 1360, 1364, 1365, 1586, 2387, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3410, 3553, 3557, 3559, 4249, 5811b		1360, 1375a, 2387
109.	61892-69-1	Pentanamide, 3-methyl-	568b, 1375, 1375b, 2543, 2767, 2773, 2775, 3553, 3557, 3559, 4249, 5811b		
110.	1119-29-5	Pentanamide, 4-methyl-	568b, 1063–1066, 1068–1074, 1375, 1375b, 1586, 2543, 2570, 2767, 2773, 2775, 3553, 3557, 3559, 4249, 4570a, 5811b		
111.	54007-33-9	Pentanamide, *N*-ethyl- $H_3C\text{-}(CH_2)_3\text{-}CO\text{-}NH\text{-}C_2H_5$	568b, 1587, 4249, 5811b		
112.	25683-11-8	1,5-Pentanediamide, 2-amino- {glutamine amide} $H_2N\text{-}OC\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$		826a, 2914	
113.	15856-96-9	2-Pentenamide	568b, 3553, 4249, 5811b		
114.	61892-67-9	2-Pentenamide, *N*-methyl-	568b, 3553, 4249, 5811b		
115.		3-Pentenamide, *N*-methyl-	568b, 4249		
116.	70265-05-3	3-Pentenamide, 4-methyl-	568b, 3553, 4249		
117.	13171-21-6	Phosphoric acid, 2-chloro-3-(diethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Phosphamidon®} 		3380, 3633, 4271a	
118.	141-66-2	Phosphoric acid, 3-(dimethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Dicrotophos®} 		3380	

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
119.	1754-58-1	Phosphorodiamidic acid, *N,N′*-dimethyl-, phenyl ester {Diamidafos®} 	2527	2527	
120.	60-51-5	Phosphorodithioic acid, *O,O*-dimethyl-*S*-[2-(methylamino)-2-oxoethyl] ester {Dimethoate®} 	5553b, 5811b	3380, 3633, 3797, 3973, 4271a, 5811b	
121.	2540-82-1	Phosphorodithioic acid, *S*-[2-(formylmethylamino)-2-oxoethyl] *O,O*-dimethyl ester {Formothion®} 	4858	2058a, 2650b, 3380, 3633, 4271a	
122.	20300-00-9	Phosphorothioic acid, *O,O*-dimethyl-*S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfinyl]ethyl] ester		3992a, 4249	
123.	2275-23-2	Phosphorothioic acid, *O,O*-dimethyl-*S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester {Vamidothion®}		822a, 2650a, 3633, 4249	
124.	70898-34-9	Phosphorothioic acid, *O,O*-dimethyl-*S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfonyl]ethyl] ester		4249, 4917	
125.	1646-87-3	Propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb Sulfoxide®}		1280, 2650a, 4249, 4271a	
126.	1646-88-4	Propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino)carbonyl]oxime {Aldoxycarb®} 		1280, 3585d, 4249, 5811b	
127.	116-06-3	Propanal, 2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb®} 		11280, 1451, 2650a, 3585d, 3633, 3634, 3646a, 3973, 4249, 4271a, 5811b	

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

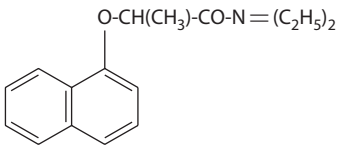
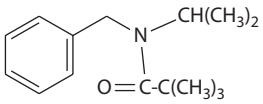
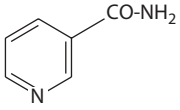
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
128.	79-05-0	Propanamide $H_3C\text{-}CH_2\text{-}CO\text{-}NH_2$	167, 568b, 1371, 1375, 1375b, 1586, 1590, 1965, 1968, 2543, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3386, 3410, 3491, 3553, 3557, 3559, 5811b		
129.	7324-05-2	Propanamide, 2-amino-, (S)- $H_3C\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$		4249, 4782	
130.	563-83-7	Propanamide, 2-methyl- $(H_3C)_2{=}CH\text{-}CO\text{-}NH_2$	568b, 2570, 2762, 2767, 3386, 3410, 3553, 3557, 3559, 5811b		
131.	631-66-3	Propanamide, 2-oxo- {pyruvamide} $H_3C\text{-}CO\text{-}CO\text{-}NH_2$	568b, 1586, 2543, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3553, 3557, 5811b		
132.	61892-68-0	Propanamide, 3-cyano- $NC\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}NH_2$	568b, 3553, 4249, 5811b		
133.	15299-99-7	Propanamide, diethyl-2-(1-naphthyloxy)- {Devrinol®; Napropamide®} 		1219b, 1219c, 2913a, 3633, 3973, 4271a	
134.	2675-88-9	Propanamide, *N*,2-dimethyl- $CH_3\text{-}CH(CH_3)\text{-}CO\text{-}NH\text{-}CH_3$	568b, 3553, 4249		
135.	35256-85-0	Propanamide, dimethyl-*N*-(1-methylethyl)-*N*-(phenylmethyl) {Butam®} 		4271a	
136.	5129-72-6	Propanamide, *N*-ethyl- $CH_3\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH_3$	568b, 2767, 3553, 4249, 5811b		
137.	1187-58-2	Propanamide, *N*-methyl- $CH_3\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH_3$	568b, 1360, 1375a, 3553, 3559, 5811, 5811a, 5811b		1360, 1375a
138.	25457-49-2	Propanamide, *N*-methyl-*N*-(1-oxopropyl)-	2543, 2773		
139.		Propanamide, *N*-(2-methylpyridyl)-	568b, 4249		
140.	79-06-1	2-Propenamide {acrylamide} $H_2C{=}CH\text{-}CONH_2$	568b, 1360, 1371, 1375, 1375a, 1375b, 1586, 1740, 1741, 1743, 1744, 2570, 2767, 3051, 3190, 3265, 3300, 3410, 3441a, 3553, 3557, 3713, 3992, 4228, 4249, 5032, 5070, 5512, 5811b, 5869a	568b, 4249, 5032, 5493	1360, 1375a
141.	79-39-0	2-Propenamide, 2-methyl- {methacrylamide}	568b, 3255, 3553, 3559, 4249, 5811b		
142.	1202-41-1	2-Propenamide, 3-(3,4-dihydroxyphenyl)-		4249	
143.	59001-33-1	2-Propenamide, 3-(3,4-dihydroxyphenyl)-*N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]- {dicaffeoylspermidine}		4249, 4567	
144.	59576-98-6	2-Propenamide, 3-(4-hydroxyphenyl)-		3973, 5811b	
145.	621-79-4	2-Propenamide, 3-phenyl-	568b, 1360, 1375a, 1587, 4249, 5811b		1360, 1375a
146.	61892-63-5	2-Propenamide, *N*-(1-oxopropyl)-	3553, 5811b		

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

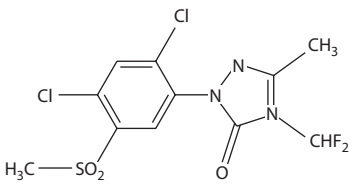
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
147.	29554-26-5	2-Propenamide, *N*-(4-aminobutyl)-3-(3,4-dihydroxyphenyl)- {caffeoylputrescine}		4249, 4567, 5811b	
148.	501-13-3	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxy-3-methoxyphenyl)-		4249, 5811b	
149.	34136-53-3	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxyphenyl)-		3491, 4249	
150.	42369-86-8	2-Propenamide, *N*,*N*′-1,4-butanediylbis[3-(4-hydroxy-3-methoxyphenyl)]-		4249, 4769, 5811b	
151.	58994-15-3	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, monoamide with *N*-(3-aminopropyl)-1,4-butanediamine {caffeoylspermidine}		4249, 4567	
152.	1452-77-3	2-Pyridinecarboxamide	568b, 1586, 2543, 3553, 3557, 4249, 5811b		
153.	72693-02-8	2-Pyridinecarboxamide, 4,6-dimethyl-	568b, 1587, 4249, 5811b		
154.	32743-35-4	2-Pyridinecarboxamide, 4-ethyl-	568b, 1587, 4249, 5811b		
155.	13509-17-6	2-Pyridinecarboxamide, 5-ethyl-	568b, 1587, 4249, 5811b		
156.	78210-61-4	2-Pyridinecarboxamide, 6-ethyl-	568b, 1587, 4249, 5811b		
157.	20970-77-8	2-Pyridinecarboxamide, 5-methyl-	568b, 1587, 2767, 3557, 4249, 5811b		
158.	63668-37-1	2-Pyridinecarboxamide, 6-methyl-	568b, 3553, 3557, 4249		
159.		3-Pyridinebutanamide, *N*-methyl-	1371, 2775, 4249		
160.	98-92-0	3-Pyridinecarboxamide {nicotinamide} 	442, 515, 562, 563, 568b, 1224, 1360, 1371, 1375a, 1586, 1668, 1890, 1891, 1966, 2079, 2224, 2228, 2724, 2761, 2762, 2765, 2766, 2939, 3059, 3302, 3308, 3309, 3386, 3410, 3444, 3491, 3505, 3553, 3559, 3967, 4080, 4249, 5811b	120, 563, 568b, 1224–1226, 2724, 2939, 3444, 3491, 3797, 3973, 3974a, 3983a, 4249, 5079	1360, 1375a
161.	72692-96-7	3-Pyridinecarboxamide, 2,4-dimethyl-	568b, 1587, 4249, 5811b		
162.	10131-48-3	3-Pyridinecarboxamide, 2,6-dimethyl-	568b, 1587, 4249, 5811b		
163.	58539-65-4	3-Pyridinecarboxamide, 2-methyl-	568b, 1587, 2761, 2762, 2765, 3410, 3553, 4249, 5811b	568b, 3549, 4249	
164.	78210-59-0	3-Pyridinecarboxamide, 4-ethyl-	568b, 1587, 4249, 5811b		
165.	78210-60-3	3-Pyridinecarboxamide, 6-ethyl-	568b, 1587, 4249, 5811b		
166.	6960-22-1	3-Pyridinecarboxamide, 6-methyl-	568b, 1586, 2761, 2762, 2767, 4249		
167.	4314-66-3	3-Pyridinecarboxamide, *N*-ethyl-	3559		
168.	114-33-0	3-Pyridinecarboxamide, *N*-methyl-	568b, 1371, 1568, 1586, 2776, 2775, 3054, 3056, 3255, 3302, 3386, 3410, 3444, 3553, 3559, 3742, 4249, 5811b	120, 404, 568b, 927, 1226, 1568, 2939, 3056, 3444, 3491, 3550, 3797, 3973, 3974a, 4093, 4249, 5811b	
169.	1453-82-3	4-Pyridinecarboxamide {isonicotinamide}		3973	
170.	78538-74-6	9*H*-Pyrido[3,4-*b*]indole-3-carboxamide, *N*-methyl-	2447a		
171.	609-41-6	1*H*-Pyrrole, 1-acetyl-	4249		
172.	23105-58-0	1*H*-Pyrrole, 1-acetyl-2,3-dihydro-	568b, 1587, 4249, 5811b		
173.	38207-11-3	1*H*-Pyrrole, 1-acetyl-2-methyl-	4249, 4633	2386, 3491, 4249	
174.		1*H*-Pyrrole, 1-acetyl-3-methyl-	4249	937, 3491, 4249	
175.	4551-72-8	1*H*-Pyrrole-2-carboxamide	568b, 2767, 2775, 3553, 3557, 4249, 5811b		

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

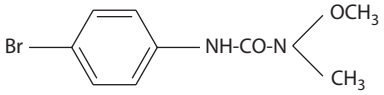
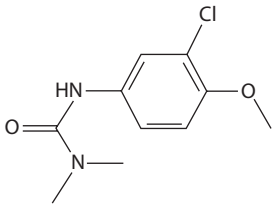
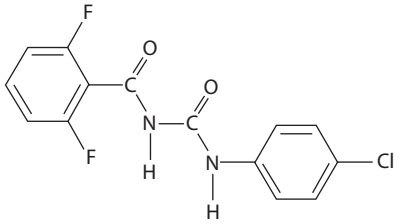
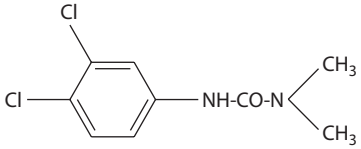
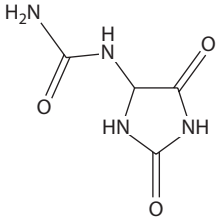
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
176.	4030-18-6	Pyrrolidine, 1-acetyl-	568b, 1371, 2543, 2570, 2773, 2775, 3553, 4249, 5811b	568b, 2336, 2386, 2389, 2544, 3491, 4249, 5811b	
177.	5979-94-2	Pyrrolidine, 1-acetyl-2-(3-pyridinyl)-, (S)- (*N*′-acetylnornicotine)	568b, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 2761, 2762, 2765–2767, 2777, 3410, 3553, 3739–3741, 4249, 5811b	64, 568b, 993, 2359, 3550, 3260a, 3973, 4133, 4236, 4249, 5811b	1360, 1375a
178.	117642-93-0	Pyrrolidine, 1-(10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		4249	
179.	120376-92-3	Pyrrolidine, 1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		4249	
180.	117642-94-1	Pyrrolidine, 1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-, (S)-		4249	
181.	120042-36-6	Pyrrolidine, 1-(11-methyl-1-oxododecyl)-2-(3-pyridinyl)-, (S)-		4249	
182.	120376-93-4	Pyrrolidine, 1-(12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
183.	33527-93-4	Pyrrolidine, 1-(1-oxobutyl)-	568b, 4249		
184.	69730-91-2	Pyrrolidine, 1-(1-oxobutyl)-2-(3-pyridinyl)-, (S)-	568b, 1587, 2775, 3410, 3742, 4249, 5811b	64, 568b, 994, 1248, 2497, 2498, 3742, 4236, 4249, 5811b	
185.	115849-75-7	Pyrrolidine, 1-(1-oxododecyl)-2-(3-pyridinyl)-, (S)-		4249	
186.	74173-71-0	Pyrrolidine, 1-(1-oxoheptyl)-2-(3-pyridinyl)-, (S)-	3742, 4249, 5811b		
187.	38854-09-0	Pyrrolidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-	1587, 3742, 4249, 5811b	64, 389, 994, 3491, 3742, 4236, 4249, 5811b	
188.		Pyrrolidine, 1-(1-oxo-?-octenyl)-2-(3-pyridinyl)-, (S)-	3742		
189.		Pyrrolidine, 1-(1-oxo-5-octenyl)-2-(3-pyridinyl)-	3742, 4249		
190.		Pyrrolidine, 1-(1-oxo-6-octenyl)-2-(3-pyridinyl)-	3742, 4249		
191.		Pyrrolidine, 1-(1-oxo-7-octenyl)-2-(3-pyridinyl)-	3742, 4249		
192.	38854-10-3	Pyrrolidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-	568b, 1587, 2865a, 3742, 4249, 5811b	64, 389, 404, 568b, 994, 2389, 2544, 2865a, 3491, 3742, 4236, 4249, 5811b	
193.	120042-35-5	Pyrrolidine, 1-(1-oxotridecyl)-2-(3-pyridinyl)-, (S)-		4249	
194.	115849-82-6	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		4249	
195.	115849-79-1	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		4249	
196.	116353-95-8	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotetradecyl)-2-(3-pyridinyl)-		4249	
197.	115849-84-8	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
198.	120042-33-3	Pyrrolidine, 1-(3-hydroxy-14-methyl-1-oxopentadecyl)-2-(3-pyridinyl)-		4249	
199.	115849-80-4	Pyrrolidine, 1-(3-hydroxy-1-oxododecyl)-2-(3-pyridinyl)-		4249	
200.	120042-32-2	Pyrrolidine, 1-(3-hydroxy-1-oxohexadecyl)-2-(3-pyridinyl)-		4249	
201.	120042-34-4	Pyrrolidine, 1-(3-hydroxy-1-oxopentadecyl)-2-(3-pyridinyl)-		4249	

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
202.	115849-85-9	Pyrrolidine, 1-(3-hydroxy-1-oxotetradecyl)-2-(3-pyridinyl)-		4249	
203.	115849-83-7	Pyrrolidine, 1-(3-hydroxy-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
204.	60026-17-7	Pyrrolidine, 1-(3-methyl-1-oxobutyl)-		568b, 2389, 2544, 4249	
205.	96552-73-7	Pyrrolidine, 1-(4-methyl-1-oxohexyl)-2-(3-pyridinyl)-	3742, 4249, 5811b		
206.	77829-17-5	Pyrrolidine, 1-(6-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		994, 2566, 2567, 3973, 4236, 4249, 5811b	
207.	96574-02-6	Pyrrolidine, 1-(6-methyl-1-oxoheptyl)-2-(3-pyridinyl)-, (S)-	3742, 4249, 5811b		
208.	77829-18-6	Pyrrolidine, 1-(7-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		994, 2566, 2567, 3973, 4236, 4249, 5811b	
209.	69730-92-3	Pyrrolidine, 1-[4-(dimethylamino)-1-oxobutyl]-2-(3-pyridinyl)-, (S)-		2497, 2498, 4236, 4249	
210.	3760-54-1	1-Pyrrolidinecarboxaldehyde	568b, 1371, 2543, 2773, 2775, 3410, 3553, 4249, 5811b	404, 568b, 2389, 2544, 3491, 4249, 5811b	
211.	78914-62-2	1-Pyrrolidinecarboxaldehyde, 2-methyl-, (R)-	568b, 3553, 4249	568b, 2554, 4249	
212.	38840-03-8 3000-81-5	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)- (*N*′-formylnornicotine)	568b, 830a, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 1586, 2601a, 2761, 2762, 2765–2767, 2777, 3255, 3410, 3553, 3739–3742, 4249, 4407, 5811b	64, 568b, 689, 994, 2359, 2952, 3491, 3549, 3550, 3742, 3973, 4133, 4249, 5811b	1360, 1375a
213.	61892-80-6	2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-3-ethyl-4-methyl-	568b, 3553, 4249		
214.		2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-4-ethyl-3-methyl-	568b, 4249		
215.	142785-07-7	*L*-Serine, *L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		4249	
216.	146440-48-4	*L*-Serine, *L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		4249	
217.	137-26-8	Thioformamide, 1,1′-dithiobis(*N,N*-dimethyl-) {Thiram®}		3633, 5811b	
218.	122836-35-5	1*H*-1,2,4-Triazol-1-yl)phenyl) methane-sulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-Oxo-1*H*-1,2,4-triazol-1-yl) phenyl)-; Sulfentrazone®} 		2913a	

(*continued*)

TABLE 13.1 (continued)
Amides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
219.	57-13-6	Urea $H_2N\text{-}CO\text{-}NH_2$	568b, 3266, 4249	172a, 174b, 568b, 622, 1053, 1073, 3266, 3370, 3973, 5079, 5811b	
220.	3060-89-7	Urea, *N′*-(4-bromophenyl)-*N′*-methoxy-*N′*-methyl- {Patoran®} 	822, 21A19	822, 3633, 4271a, 21A19	
221.	19937-59-8	Urea, *N′*-(3-chloro-4-methoxyphenyl)-*N,N*-dimethyl- {Metoxuron®} 		622, 3633, 4249, 4271a	
222.	1746-81-2	Urea, *N′*-(4-chlorophenyl)-*N*-methoxy-*N*-methyl- {Linuron®, 30% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
223.	35367-38-5	Urea, 1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)- {Diflubenzuron®} 	21A19	4911, 21A19	
224.	330-55-2	Urea, *N′*-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methyl- {Monolinuron®, 20% of Molipan®}	822, 21A19	822, 3633, 4271a, 21A19	
225.	150-68-5	Urea, 1,1-dimethyl-3-(4-chlorophenyl) {Monuron®}		3633, 4271a	
226.	330-54-1	Urea, 1,1-dimethyl-3-(3,4-dichlorophenyl) {Diuron®} 		3973	
227.	97-59-6	Urea, (2,5-dioxo-4-imidazolidinyl)- {allantoin} 		120, 2270, 3973, 5079, 5188, 5189, 5436, 5435	

14 Imides

In his 1954 compilation of tobacco smoke components, Kosak (2170) listed no imide identified in tobacco smoke to that date.

Ishiguro and Sugawara in their 1980 monograph on tobacco smoke components listed a total of 72 amides, imides, and lactams, including 7 imides [see Table I-15 in (1884)]. Their reference for all the imides listed was that of Schumacher et al. (3553). Ishiguro and Sugawara did not list caffeine as an imide but listed it under *N*-polycyclics (excluding alkaloids) [see Table I-14 in (1884)].

In its 1986 monograph on tobacco smoking, the International Agency for Research on Cancer (IARC) stated that there was a large spectrum of amides, imides, and lactams in tobacco smoke (including some 50 aliphatic amides) [see p. 109 in (1870)]. The basis for the IARC comments was the 1977 review of *N*-containing components in tobacco and tobacco smoke by Schmeltz and Hoffmann (3491) and the smoke composition publication in 1977 of Schumacher et al. (3553) and in 1981 by Heckman and Best (1587).

Of the 24 imides identified in tobacco smoke by Schumacher et al. (3553), 6 were new to tobacco smoke composition. Many of the previously identified imides were derivatives of 1*H*-pyrrole-2,5-dione (maleimide), 2,5-pyrrolidinedione (succinimide), and 1*H*-isoindole-1,3(2*H*)-dione (phthalimide). The use of a recently developed analytical technology that permitted the fractionation and identification of components in the water-soluble portion of cigarette smoke condensate (CSC) was a key factor in their mid-1977 study. In a detailed study of the ether-soluble portion from the same CSC studied by Schumacher et al., Newell et al. (2769) identified five imides. In his earlier study of the composition of smoke from an all-burley tobacco cigarette, Heckman (1586) identified 15 imides.

Examination of the structures of several of the CSC components indicates that the decision of their categorization is somewhat difficult. In Figure 14.1, representative structures for an amide, an imide, and a lactam are presented. To which of these categories—amide, imide, or lactam—should the smoke component 1-acetyl-3-ethyl-1,5-dihydro-4-methyl-2*H*-pyrrol-2-one {I} be assigned? Its structure is depicted in Figure 14.2. In Structure {II} of Figure 14.2, the amide configuration is shown. Structures {III} and {IV} show the imide and lactam configurations, respectively. This same situation is present with several other smoke components. While there may be some disagreement of the preciseness of our selection, for completeness sake, such components are listed in each chapter in its major catalog table. As a result, the total number of components in each of the major catalog tables may be slightly inflated.

In addition to several amides (asparagine, glutamine, urea) on the Doull et al. list of individual compounds used in cigarette manufacture by U.S. companies (1053) is the imide 3,7-dihydro-1,3,7-trimethyl-1*H*-purine-2,6-dione (caffeine).

Over 100 imides identified in tobacco and tobacco smoke are cataloged in Table 14.1. Of the reported 103 imides, 45 have been identified in tobacco, 82 in tobacco smoke, and 24 in both tobacco and tobacco smoke.

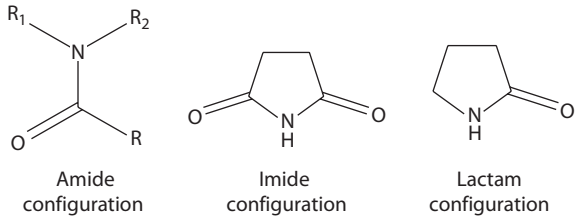
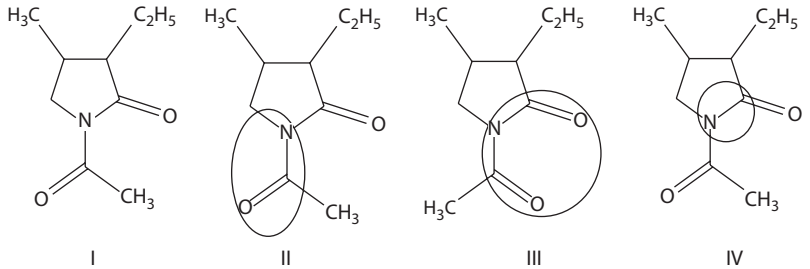


FIGURE 14.1 The amide, imide, and lactam configurations.



2*H*-Pyrrol-2-one, 1-acetyl-3-ethyl-1,5-dihydro-4-methyl- (CAS No. 61892-80-6)

FIGURE 14.2 The amide {II}, imide {III}, and lactam {IV} configurations in 1-acetyl-3-ethyl-1,5-dihydro-4-methyl-2*H*-pyrrol-2-one {I}.

TABLE 14.1
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

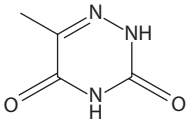
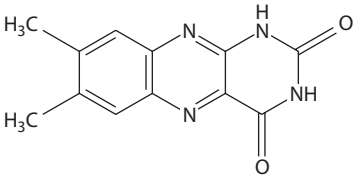
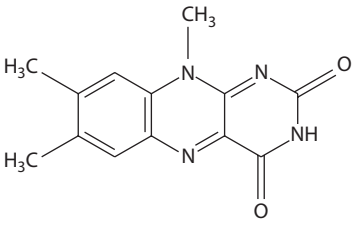
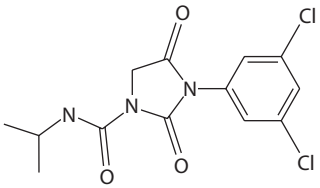
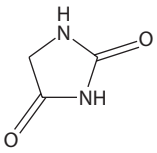
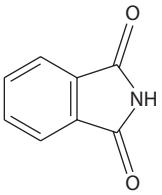
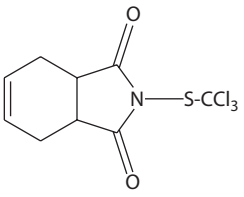
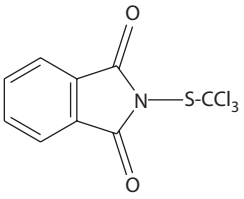
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	932-53-6	Azathymine 		3973	
2.	4250-90-2	Benzo[*g*]pteridine-10(2*H*)-acetaldehyde, 3, 4-dihydro-7,8-dimethyl-2,4-dioxo-		4249	
3.	1086-80-2	Benzo[*g*]pteridine-2,4(1*H*,3*H*)-dione, 7,8-dimethyl- 		4249	
4.	1088-56-8	Benzo[*g*]pteridine-2,4(3*H*,10*H*)-dione, 7,8,10-trimethyl- 		4249	
5.	36734-19-7	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®} 		3585c, 3633, 3661a	
6.	461-72-3	2,4-Imidazolidinedione {hydantoin} 	568b, 3553, 4249, 5811b		
7.	61893-10-5	2,4-Imidazolidinedione, 1-(1-methylethyl)-	3553, 4249, 5811b		
8.	17374-27-5	2,4-Imidazolidinedione, 1,5-dimethyl-	568b, 3553, 4249, 5811b		
9.	61893-09-2	2,4-Imidazolidinedione, 1-ethyl-	568b, 3553, 4249, 5811b		
10.	63637-90-1	2,4-Imidazolidinedione, 3-(1-methylethyl)-	568b, 4249		
11.	16935-34-5	2,4-Imidazolidinedione, 5-(1-methylethyl)-	568b, 2767, 3553, 4249, 5811b		
12.	15414-82-1	2,4-Imidazolidinedione, 5-ethyl-	568b, 2601a, 3553, 4249, 5811b		

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
13.	616-04-6	2,4-Imidazolidinedione, 1-methyl-	568b, 4249		
14.		2,4-Imidazolidinedione, 3-methyl-	568b, 4249		
15.	616-03-5	2,4-Imidazolidinedione, 5-methyl-	568b, 2767, 3255, 3553, 3557, 4249, 5811b	568b, 3561, 4249	
16.	85-41-6	1*H*-Isoindole-1,3(2*H*)-dione {phthalimide} 	568b, 1375, 1375b, 2769, 3553; 3557, 3733–3735, 3750, 3752, 4249		
17.	66309-86-2	1*H*-Isoindole-1,3(2*H*)-dione, 4,5-dimethyl-	2769, 3553, 3557, 3733–3735, 3750, 3752, 4249		
18.	17100-62-8	1*H*-Isoindole-1,3(2*H*)-dione, 4,6-dimethyl-	568b, 4249		
19.	15540-88-2	1*H*-Isoindole-1,3(2*H*)-dione, 4,7-dimethyl-	568b, 4249		
20.		1*H*-Isoindole-1,3(2*H*)-dione, methyl-	3553		
21.	7251-82-3	1*H*-Isoindole-1,3(2*H*)-dione, 4-methyl-	568b, 1586, 2570, 2769, 3557, 3733–3735, 3750, 3752, 4249		
22.	40314-06-5	1*H*-Isoindole-1,3(2*H*)-dione, 5-methyl-	568b, 2769, 3557, 3733–3735, 3750, 3752, 4249		
23.	550-44-7	1*H*-Isoindole-1,3(2*H*)-dione, *N*-methyl-	568b, 4249		
24.	133-06-2	1*H*-Isoindole-1,3(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]- {Captan®} 	1884, 3302, 4249, 21A19	1219c, 1884, 3633, 21A19	
25.	133-07-3	1*H*-Isoindole-1,3(2*H*)-dione, 2-[(trichloromethyl)thio]- {Folpan®} 		3633	
26.	480-91-1	1*H*-Isoindol-1-one, 2,3-dihydro- {phthalimidine}	568b, 4249, 5811b		
27.	6091-76-5	1*H*-Isoindol-1-one, 2,3-dihydro-3-methyl-	568b, 1587, 4249, 5811b		

(*continued*)

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

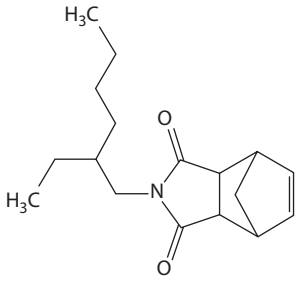
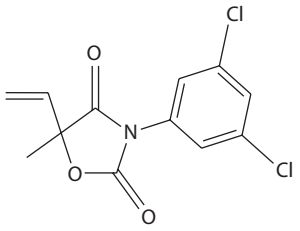
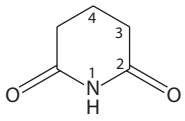
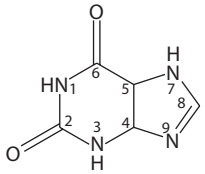
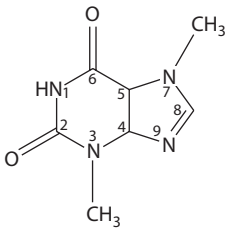
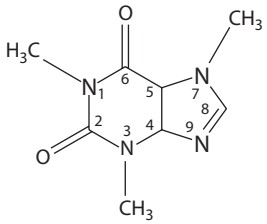
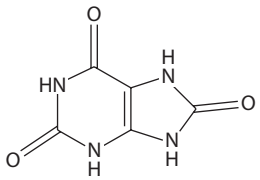
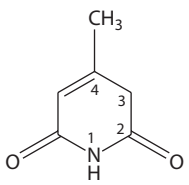
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
28.	113-48-4	4,7-Methano-1*H*-isoindole-1,3(2*H*)-dione, 2-(2-ethylhexyl)-3a,4,7,7a-tetrahydro-		3633	
					
29.	2346-26-1	2,4-Oxazolidinedione	568b, 1884, 3224, 3553, 3557, 4249, 5811b		
30.	50471-44-8	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- {Vinclozolin®}		2650a	
					
31.		2,4-Oxazolidinedione, 5-ethyl-1-methyl-	3224, 3553, 3557, 4249		
32.	27770-23-6	2,4-Oxazolidinedione, 5-methyl-	568b, 1884, 3224, 3553, 3557, 4249, 5811b		
33.	58628-98-1	2-Oxazolidinone, 4.5-dimethyl-	568b, 4249		
34.	1121-89-7	2,6-Piperidinedione {glutarimide}	568b, 1360, 1371, 1375, 1375a, 1375b, 1586, 2543, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3553, 3557, 4249, 4407, 5811b		1360, 1375a
					
35.		2,6-Piperidinedione, methoxy-	1371, 1586, 4249		
36.		2,6-Piperidinedione, 3-methoxy-	568b, 4249		
37.	61892-70-4	2,6-Piperidinedione, 4-methoxy-	1365, 2773, 2775, 3553, 4249, 5811b		
38.	72692-70-7	2,6-Piperidinedione, methyl-	1586, 2767, 3557, 4249		

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
39.	29553-51-3	2,6-Piperidinedione, 3-methyl-	568b, 2767, 3553, 3557, 4249, 5811b		
40.	25077-26-3	2,6-Piperidinedione, 4-methyl-	568b, 3553, 3557, 3559, 4249, 5811b		
41.	69-89-6	6*H*-Purin-2,6-dione, 3,7-dihydro- {xanthine} 	5811b	429b, 2539, 2939, 4249, 5727	
42.	58-55-9	1*H*-Purine-2,6-dione, 3,7-dihydro-1,7-dimethyl-		568b, 4249	
43.	83-67-0	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- {theobromine} 	568b, 1375, 1375b, 2601a, 3255, 3257, 3265, 3553, 4249, 5811b	568b, 1204, 2313, 4249	
44.	33073-01-7	1*H*-Purine-2,6-dione, 3,9-dihydro-1,9-dimethyl-	1587, 4249, 5811b		
45.	58-08-2	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine} 	568b, 1365, 1842, 3255, 3257, 3265, 3266, 3553, 4249, 5811b	568b, 1053, 3266, 4249	
46.		6*H*-Purin-2,6-dione, 3,7-dihydro-, C_3-alkyl-	1587, 4249		
47.	69-93-2	1*H*-Purine-2,6,8-trione, 7,9-dihydro- {uric acid} 	2170, 5079, 5456		
48.	70898-25-8	2,6(1*H*,3*H*)-Pyridinedione, 3,5-dimethyl-	2767, 3553, 4249	2389, 4249	
49.	72692-95-6	2,6(1*H*,3*H*)-Pyridinedione, 4-methyl- 	2767, 3553, 3557, 4249		

(*continued*)

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

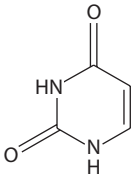
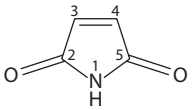
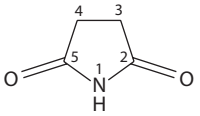
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
50.	72692-94-5	2,6(1*H*,3*H*)-Pyridinedione, 5-methyl-	2767, 3553, 4249		
51.	66-22-8	2,4(1*H*,3*H*)-Pyrimidinedione {uracil} 		568b, 3973, 4249	
52.	4160-77-4	2,4(1*H*,3*H*)-Pyrimidinedione, 3,5-dimethyl-	568b, 3553, 4249, 5811b		
53.	61893-13-8	2,4(1*H*,3*H*)-Pyrimidinedione, 3-ethyldihydro-5-methyl-	568b, 3553, 4249		
54.	608-34-4	2,4(1*H*,3*H*)-Pyrimidinedione, 3-methyl-	568b, 4249		
55.	65-71-4	2,4(1*H*,3*H*)-Pyrimidinedione, 5-methyl- {thymine}	1580, 4249	1580, 3491, 3797, 3974a, 4249	
56.	50-06-6	2,4,6(1*H*,3*H*, 5*H*)-Pyrimidinetrione, 5-ethyl-5-phenyl- {phenobarbital}		5003, 5021	
57.		4(1*H*)-Pyrimidinone, 2,3-dimethyl-6-phenyl-3,4,5,6-tetrahydro-	568b, 4249		
58.	541-59-3	1*H*-Pyrrole-2,5-dione {maleimide} 	568b, 1580, 2775, 3553, 3557, 4249	568b, 1580, 2336, 2389, 2544, 3186, 3188, 3491, 3974a, 4249, 5811b	
59.		1*H*-Pyrrole-2,5-dione, 1,3-dimethyl-4-ethyl-	568b, 4249		
60.	29720-92-1	1*H*-Pyrrole-2,5-dione, ethylmethyl-	1586, 4249	937, 3491, 3560, 3561, 4249	
61.	128-53-0	1*H*-Pyrrole-2,5-dione, 1-ethyl-	568b, 1586, 2767, 4249		
62.	5997-61-5	1*H*-Pyrrole-2,5-dione, 3-ethyl-	568b, 1586, 4249		
63.	15542-97-9	1*H*-Pyrrole-2,5-dione, 3-ethyl-1-methyl-	568b, 4249		
64.	61892-73-7	1*H*-Pyrrole-2,5-dione, 3-(hydroxymethyl)-	3553, 4249		
65.	61892-71-5	1*H*-Pyrrole-2,5-dione, 3,4-bis(hydroxymethyl)-1-methyl-	568b, 3553, 4249	568b, 2544, 3186, 4249	
66.	17825-86-4	1*H*-Pyrrole-2,5-dione, 3,4-dimethyl-	568b, 1075, 1364, 1586, 2545, 2570, 2767, 3553, 3557, 4407, 4249, 5811b	404, 568b, 2389, 2544, 3215, 3491, 4249, 5811b	
67.	61892-72-6	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-(hydroxymethyl)-	3553, 4249	2544, 3186, 4249	
68.	20189-42-8	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	568b, 1063–1066, 1068–1075, 1364, 2382, 2387, 2545, 2570, 2767, 3553, 3557, 4249, 4407, 5811b	404, 568b, 937, 1256, 1590a, 2339a, 2386, 2389, 2544, 3215, 3491, 3543, 3547, 3549, 3550, 3560, 3561, 3905, 4249, 5811b	2387

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
69.	1072-87-3	1*H*-Pyrrole-2,5-dione, 3-methyl-	1375, 1375b, 1586, 2543, 2767, 2773, 3553, 3557, 4249, 4407, 5811b		
70.	60026-19-9	1*H*-Pyrrole-2,5-dione, 3-propyl-		2389, 2544, 3491, 4249	
71.	123-56-8	2,5-Pyrrolidinedione {succinimide} 	568b, 1360, 1371, 1375, 1375a, 1375b, 1580, 1586, 2387, 2543, 2545, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3410, 3553, 3557, 4249, 4407, 5811b	568b, 1580, 2389, 2544, 3215, 3491, 3550, 3974a, 4249, 5811b	1360, 1375a, 2387
72.	15542-96-8	2,5-Pyrrolidinedione, 1,3-dimethyl-	568b, 1360, 1375, 1375a, 1375b, 1586, 2570, 2767, 3553, 3557, 4249, 5811b		1360, 1375a
73.	33425-47-7	2,5-Pyrrolidinedione, 3,4-dimethyl-	1375, 1375b, 1586, 2761, 2762, 2773, 2775, 3553, 4249, 5811b		
74.		2,5-Pyrrolidinedione, ethylmethyl-	1586, 2767, 4249		
75.	5835-19-8 58467-27-9	2,5-Pyrrolidinedione, 3-ethyl-	568b, 1364, 1375, 1375b, 1586, 2767, 3553, 3557, 4249, 5811b		
76.	15542-97-9	2,5-Pyrrolidinedione, 3-ethyl-1-methyl-	568b, 3255, 3553, 4249, 5811b	568b, 2389, 2544, 3491, 4249, 5811b	
77.	77-67-8	2,5-Pyrrolidinedione, 3-ethyl-3-methyl-	568b, 3553, 4249	404, 568b, 4249	
78.	58501-92-1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-	568b, 1375, 1375b, 3553, 3557, 4249, 5811, 5811a, 5811b	568b, 937, 2339a, 2389, 2544, 3215, 3491, 3550, 3767a, 4249, 5811, 5811a, 5811b	
79.	16824-61-6	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*Z*)-	1586, 2767, 3553, 3557, 4249	937, 1256, 2544, 3561, 4249	
80.	15510-11-9	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*E*)-		5811b	

(*continued*)

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

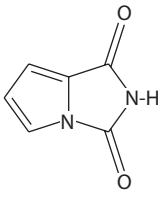
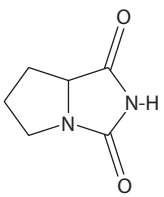
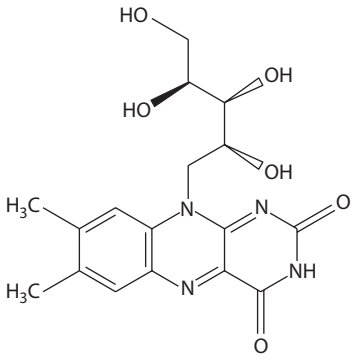
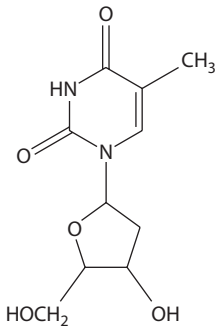
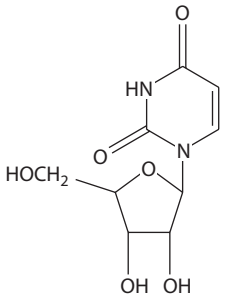
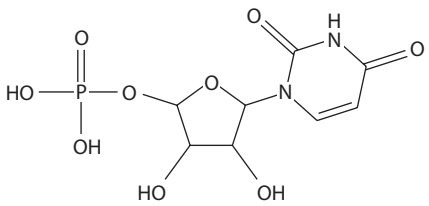
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
81.		2,5-Pyrrolidinedione, 3-ethylene-4-methyl-	568b, 1375, 4249		
82.	14156-12-8	2,5-Pyrrolidinedione, 3-ethylidene-	568b, 3553, 3557, 4249, 5811b		
83.	61892-74-8	2,5-Pyrrolidinedione, 3-ethylidene-1-methyl-	568b, 1375, 1375b, 3553, 4249		
84.	16395-79-2	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-	568b, 1375, 1375b, 2570, 3553, 3557, 4249	568b, 2389, 2544,, 3491, 3550, 4249, 5811b	
85.	28098-82-0	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-, (*E*)-		5811b	
86.	18366-19-3	2,5-Pyrrolidinedione, 3-hydroxy- (*S*)	2767, 3553, 4249		
87.	1121-07-9	2,5-Pyrrolidinedione, 1-methyl-	568b, 1360, 1371, 1375, 1375a, 1375b, 1586, 2570, 2767, 3553, 3557, 4249, 5811b	404, 568b, 2386, 2389, 2544, 3491, 3550, 4249, 5811b	1360, 1375a
88.	5615-90-7	2,5-Pyrrolidinedione, 3-methyl-	568b, 1063–1066, 1068–1074, 1371, 1375, 1375b, 2545, 2570, 2767, 2773, 2775, 3553, 3557, 4249, 5512, 5811b	568b, 2389, 2544, 3491, 3550, 4249, 5811b	
89.	72693-03-9	2,5-Pyrrolidinedione, 3-(1-methylethyl)-	568b, 2767, 4249	568b, 3550, 4249	
90.	15542-99-1	2,5-Pyrrolidinedione, 1-methyl-3-(1-methylethyl)-	568b, 3553, 4249		
91.	71099-03-1	2,5-Pyrrolidinedione, 1,3,4-trimethyl-	568b, 1586, 2767, 4249	568b, 2336, 4249	
92.	13939-91-8	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione 	3553, 4249		
93.	5768-79-6	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione, tetrahydro- 	568b, 3553, 4249, 5811b		
94.	61892-80-6	2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-3-ethyl-4-methyl-	568b, 3553, 4249		
95.		2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-4-ethyl-3-methyl-	568b, 4249		

TABLE 14.1 (continued)
Imides Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
96.	83-88-5	Riboflavin 		120, 1941, 2270, 3973, 4249, 5079	
97.	146-17-8	Riboflavin 5′-(dihydrogen phosphate)		4249, 4956	
98.	50-89-5	Thymidine 		3973, 4249	
99.	58-96-8	Uridine 		3973, 4249	
100.	133-89-1	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-glucopyranosyl ester		4249, 4489, 4580	
101.	3616-06-6	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester		429b, 4249	
102.	19253-25-9	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester		4249, 4458	
103.	58-97-9	5′-Uridylic acid 		429b, 4249, 4474	

15 *N*-Nitrosamines

The introduction to this chapter on *N*-nitrosamines (NNAs) in tobacco and/or tobacco smoke is a considerably abbreviated but updated version of the lengthy unpublished 1993 memorandum by Rodgman (3256). Omitted from this outline are several sections covered in detail in (3256). These include much of the discussion on the early studies of the biological properties of NNAs [see pp. 117–178 in (3256)] and studies on alternate sources of exposure to NNAs [see pp. 107–116 in (3257)].

The numerous publications during the past two decades on the identification, quantitation, and bioassay of NNAs, particularly those found in tobacco-related entities (tobacco, mainstream smoke [MSS], sidestream cigarette smoke [SSS], and environmental tobacco smoke [ETS]), raise the question as to why this class of tobacco/tobacco smoke components has received such emphasis. Since the early 1950s, several classes of compounds in tobacco smoke have been proposed as prime contributors to cancer of the respiratory tract in smokers. The events that triggered detailed examination of the composition of cigarette MSS included:

1. The results of retrospective studies which were interpreted as indicating an association between cigarette smoking and carcinoma of the lung in smokers [Levin et al. (2355), Mills and Porter (2556), Schrek et al. (3529), Wynder and Graham (4306b), Doll and Hill (1027), McConnell et al. (2525), Sadowky et al. (3375a)]. Subsequently, the results from additional retrospective studies and several prospective studies on smoking and respiratory tract cancer bolstered the evidence for this association.
2. Bioassay results from studies (4306a, 4306c) in which carcinomas were produced in susceptible mouse strains at the site of repeated skin painting with massive doses of cigarette smoke condensate (CSC) prepared in a manner supposedly simulating the human smoking process (the puff frequency used was a 2 s puff each 20 s *vs*. the usually accepted routine was a 2 s puff each 60 s). Between 1953 and late 1966, the major skin-painting studies involving CSC administered to various laboratory animal species numbered about 60 (4332).

Despite numerous statements to the contrary—that the data from mouse-skin-painting experiments with CSC were not extrapolable from mouse skin to the human lung—some authorities continued to imply that such data were meaningful in terms of respiratory tract cancer in smokers. For example, Wynder (4292) wrote:

> The mouse skin test cannot give definitive proof for a human carcinogen, although it has long been used as a reliable tool for testing of carcinogenic materials…The animal data must be considered, not as a proof for the human experience, but as a tool with which to work toward the isolation and identification of carcinogenic agent(s). At this time we can only assume, on the basis of the combined human and animal data, that these carcinogens are the same for man and for mice.

In 1956, Wynder (4295) stated:

> We believe that no animal data can be used to establish a causative role in cancer in man. Such proof can come only from human epidemiologic data… animal evidence by itself can never establish a human carcinogen nor can it ever disprove it… For example, if we suspect tobacco as a carcinogen to man, animal experimentation can determine the specific parts of tobacco which are carcinogenic to animals. Once identified, we can only assume that the specific carcinogens are the same to which man also responds and introduce preventive measures accordingly.

Despite comments such as these and additional ones in later publications, animal experimentation, particularly mouse-skin-painting studies, constituted a substantial part of the bioassays on tobacco smoke. Such bioassays are not only expensive but also extremely time consuming (18–24 months). Because of the absence of a positive response in studies of tobacco smoke inhalation by laboratory animals, mouse-skin painting with CSC was selected as the bioassay of choice in the massive decade-long (1970–1980) study conducted by the National Cancer Institute (NCI) on "less hazardous" cigarettes, a study that involved nearly 100 test cigarettes and 30 standard or reference cigarettes (1329, 1330, 1332, 1333, 2683).

Successively after the late 1950s, various classes of smoke components were proposed as either the cause of (as tumor initiators) or contributors to (as promoters, cocarcinogens, ciliastats) the lung cancer in smokers:

1. Polycyclic aromatic hydrocarbons (PAHs).
2. Their polycyclic nitrogen analogs, the aza-arenes, reported to be carcinogenic to mouse skin.
3. Low-molecular-weight phenols reported to be promoters of tumorigenic PAHs.
4. Aldehydes and ketones reported to be ciliastatic in *in vitro* ciliated systems.
5. Aromatic amines.
6. Metallic items (^{210}Po, Ni).
7. Other miscellaneous compounds, e.g., ethyl urethan.

One by one, the claims for involvement of each of these classes of compounds were either discounted or seriously questioned [Rodgman (3255, 3257), Rodgman et al. (3307)].

PAHs were described as the only major tumor initiators in mouse-skin carcinogenesis [Wynder and Hoffmann (4332)]:

> The many detailed data obtained in studies of tobacco carcinogenesis on mouse skin exclude with some certainty the major tumor initiators other than the PAH type play a role in this assay system.

Benzo[*a*]pyrene (B[*a*]P), because of its potency in skin-tumor carcinogenesis and per cigarette MSS yield, was considered the major PAH of concern in tobacco smoke. In 1981, the Surgeon General commented as follows on PAHs [see p. 36 in (4009)]:

> BaP appears to be the most important single member of this class of compounds, taking into consideration both its concentration and its relative carcinogenic potency.

It was obvious that additional mechanisms were needed to explain the observed biological effect since (1) B[*a*]P in CSC acting alone accounted for less than 2% of the observed biological response in mouse-skin-painting studies, (2) the total PAH fraction accounted for less than 3% of the observed biological response in mouse-skin-painting studies, (3) no "supercarcinogenic" PAH was found in CSC (3756–3758, 4282), and (4) inclusion of tumorigenic aza-arenes in CSC explained very little more of the unexplained tumorigenicity.

The first additional explanation of the observed effect in skin-painting studies with CSC involved the mechanisms of promotion and cocarcinogenesis of tobacco smoke components. The smoke components first classified as promoters were the low-molecular-weight phenols because of their known promotion of such potent tumorigenic PAHs as B[*a*]P and dibenz[*a,h*]anthracene (DB[*a,h*]A) (414).

However, the significance of the promoting/cocarcinogenic effect of tobacco smoke phenols on PAH tumorigenicity [Wynder and Hoffmann (4309, 4317, 4344)] was offset by the following observations:

1. Removal of a substantial amount (70%–85%) of the low-molecular-weight phenols from CSC by selective filtration of the MSS did "not change significantly the biological activity of the resulting condensate" [Wynder and Hoffmann [see p. 626 in (4332)], Hecht et al. [see p. 2 in presentation manuscript (1582, 1583)]].
2. Low-molecular-weight phenols inhibited the tumorigenicity of B[*a*]P [Van Duuren et al. (4029, 4035)].
3. Inclusion of known initiators, promoters, and cocarcinogens in tobacco smoke in the calculation of its tumorigenicity explained less than 5% of the observed biological effect in skin-painting studies.

The failure of several groups of investigators [Candeli et al. (587), Kaburaki et al. (2006), Schmeltz et al. (3499, 3512), Snook (3733), Snook et al. (3750), Grimmer et al. (1409), Kamati et al. (2021), Sasaki and Moldoveanu (3414), Rustemeier et al. (3370)] to reproduce the findings of Van Duuren et al. (4027) on the presence and/or levels of the aza-arenes dibenz[a,h] acridine, dibenz[a,j]acridine, and 7*H*-dibenzo[c,g]carbazole in tobacco smoke was discussed by Rodgman [3255, 3260; see Table 4 in (3265)] and Baker (172).

The failure to explain the observed tumorigenicity of CSC in the mouse-skin bioassay by consideration of the following tobacco smoke systems led to the inclusion of ciliastasis by various water-soluble vapor-phase (VP) tobacco smoke components in an attempt to explain the causation of respiratory tract cancer in smokers:

1. The levels in CSC of mouse-skin tumorigenic PAHs, acting individually or in concert, could not account for the response in CSC-painted animals.
2. The CSC levels of mouse-skin tumorigenic PAHs plus the promoting/cocarcinogenic phenols, acting individually or in concert, could not account for the observed response in CSC-painted animals.
3. The CSC levels of mouse-skin tumorigenic PAHs plus promoting/cocarcinogenic phenols and non-tumorigenic PAHs, acting individually or in concert, could not account for the observed response in CSC-painted animals.
4. Inclusion of tumorigenic aza-arenes in the calculation could not account for the observed biological response.

In fact, when the levels of the known tumorigenic, promoting, and cocarcinogenic components of tobacco smoke and their activity toward mouse skin are included in the assessment, less than 5% of the observed biological response in the CSC-painted animals can be explained!

To circumvent this failure to explain the observations with CSC-treated laboratory animals and attempt to explain the epidemiological findings in human smokers, ciliastasis was introduced as an additional mechanism involved in the causation of smokers' lung cancer. In a variety of *in vitro* systems, ciliastasis was produced by cigarette MSS VP and by individual MSS VP components (hydrogen cyanide, formaldehyde, acetaldehyde, acetone, phenol). It was proposed that ciliastasis occurred in the smokers' respiratory tract and significantly diminished the lung clearance mechanism of the cilia, thus permitting tobacco smoke particulate-phase particles (and their included "tumorigens") to remain on the lung surface and initiate the cellular changes required for tumor development. However, this proposal was seriously compromised by the demonstration in intact animals as well as in human smokers that a large proportion (60%–75%) of the *in vitro* ciliastats (all water-soluble) in the inhaled smoke failed to reach the ciliated tissue in the respiratory tract because of solution in the aqueous secretions coating the oral cavity tissues [Rodgman et al. (3306), Dalhamn et al. (892, 893)].

Prior to the emphasis on NNAs, the class of tobacco smoke components subjected to the most study was the PAHs, with

particular emphasis on the CSC compound considered the most potent, B[*a*]P. Although the NNAs identified in tobacco and/or tobacco smoke number fewer than 60, the number of PAHs either identified or partially identified* exceeds 500 [Severson et al. (3619), Snook et al. (3756–3758), Rodgman and Perfetti (3306a)].

The role played by the PAHs, particularly B[*a*]P, in induction of skin carcinoma in skin-painted laboratory animals was seriously questioned because of the demonstrations by Roe (3310, 3311) that a 10-fold increase and by Lazar et al. (2320) that a 30-fold increase in the B[*a*]P level of CSC failed to produce an increase in its tumorigenicity to mouse skin. This lack of correlation between levels of PAHs [B[*a*]P, benz[*a*]anthracene (B[*a*]A)] in CSC and % tumor-bearing animals (TBAs) was demonstrated in the NCI "less hazardous" cigarette study [Gori (3329, 3230, 3232, 3233), NCI (2683)]. The results were acknowledged in the U.S. Surgeon General's 1981 report [see p. 36 in (4009)]:

> The contribution of BaP or PAH in general to mouse skin carcinogenesis by cigarette smoke condensate cannot be fully measured at this time. Wynder and Hoffmann (4332) found a correlation between BaP levels and carcinogenic activity of smoke condensates from several types of cigarettes. A much larger series of experimental cigarettes was studied in the smoking and health program of the National Cancer Institute. No significant dependence of carcinogenic potency on BaP was observed. [Gori (3329, 3230, 3232, 3233), NCI (2683)]

It should be noted that in the NCI "less hazardous" cigarette study, neither the tobaccos used in the nearly 100 experimental cigarettes and 30 standard and reference cigarettes nor the MSSs generated from them were analyzed for NNAs.

Despite observations that NNAs in CSC or NNAs individually induce few, if any, tumors at the application site in mouse-skin-painting studies with CSC, they are one of the two classes of tobacco product components to which the pro-health forces continue to devote their major efforts. In 1990, Hoffmann and Hecht (1727) noted:

> Mouse skin is particularly responsive to PAH tumorigenesis. It is not equally responsive to other important classes of carcinogens such as *N*-nitrosamines…

As noted in 1984 by Hoffmann et al. (1696), three types of NNAs are formed in tobacco processing and during the tobacco smoking process: volatile *N*-nitrosamines (VNAs), tobacco-specific *N*-nitrosamines (TSNAs), and nonvolatile NNAs. The latter include *N*-nitrosodiethanolamine (NDELA) and *N*-nitrosoproline (NPRO). Recently, several *N*-nitrosamino acids were identified in tobacco. The major NNAs identified in tobacco and/or tobacco smoke are listed in Table 15.1.

In the mid-1960s, Fredrickson (1236), using a laboratory procedure which precluded artifactual formation of NNAs, identified several volatile NNAs in cigarette MSS. He also reported that volatile NNAs, like the low-molecular-weight phenols, are selectively removed from MSS by plasticized (triacetin) cellulose acetate filters. Per cigarette MSS, volatile NNA yields are reduced by 75%–80% in this manner, a value similar to that observed with the selective filtration of low-molecular-weight phenols. This diminution of volatile NNA yields was confirmed several years later by Morie and Sloan (2635) and Brunnemann et al. (514).

TSNAs, because of their low volatility, occur predominantly in the MSS particulate phase and behave similarly to other particulate-phase components such as the PAHs; i.e., they are not selectively reduced by filtration with plasticized cellulose acetate. However, Hoffmann et al. (1685) noted that MSS TSNA yields are reduced by any technology designed to reduce the MSS particulate phase such as increased filtration efficiency, increased air dilution (filter-tip perforation, paper porosity), and tobacco expansion.

The precursors in tobacco of the NNAs in tobacco smoke have been studied extensively. Tobacco protein is reported by Brunnemann et al. (511) to be the major precursor of the volatile NNAs and NPRO. Based on these findings, Hoffmann et al. (1696) wrote:

> The protein fraction of tobacco appears to represent the major precursor group of the carcinogenic volatile nitrosamines in smoke. In addition, Tso et al. (3985) had previously reported that the volatile NNAs in smoke are proportional to the nitrate content of the tobacco filler, an observation also made by Morie and Sloan (2635).

Precursors of TSNAs in tobacco and smoke are nicotine, nornicotine, anabasine, and anatabine [Hecht et al. (1564), Adams et al. (29)]. Both nicotine and nornicotine are considered precursors of *N′*-nitrosonornicotine (NNN). Direct transfer of TSNAs from tobacco to the smoke accounts for about 40% of NNN and 30% of 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK) in MSS. The remainder of these two TSNAs in the MSS is formed during the smoking process [Hoffmann et al. (1734), Hecht et al. (1564)]. Like the levels of the volatile NNAs in MSS, the yields of the TSNAs in MSS are proportional to the nitrate content of the tobacco filler (3985).

PAHs are ubiquitous: They are present in the atmosphere as components of a variety of dusts, soots, tars, oils, engine exhaust gases; in water; in many commonly consumed foodstuffs, particularly those that are heated, roasted, or broiled [Rodgman (15A48), Grasso (1345), Maga (2438)]; and in ETS. Similarly, exposure to NNAs is widespread. Volatile NNAs are not only components of MSS, SSS, and ETS, but they are also present in a variety of foodstuffs and beverages. Sen et al. (15A52) noted:

> Nitrosopyrrolidine,† which is a potent liver carcinogen [in laboratory animals], has been shown to be formed during the frying of bacon, and to be present in sausage, corned beef, luncheon meat, fried pig liver, cooked and uncooked cod fish and finned herring.

* The partial identification of a PAH refers to the instances where the positions of alkyl substituents and/or their precise identity are uncertain, e.g., a trimethyl *vs.* an ethylmethyl derivative.

† As noted previously, NPYR is a tobacco smoke component.

TABLE 15.1
Major NNAs in Tobacco and/or Tobacco Smoke

Chemical Name	Abbreviation	Common Name
VNAs		
1-Butanamine, *N*-butyl-*N*-nitroso-	NDBA	*N*-nitrosodibutylamine
1-Butanamine, *N*-methyl-*N*-nitroso-	NBMA	*N*-nitrosobutylmethylamine
Ethanamine, *N*,1-dimethyl-*N*-nitroso-		*N*-nitrosoisopropylmethylamine
Ethanamine, *N*-ethyl-*N*-nitroso-	NDEA	*N*-nitrosodiethylamine
Ethanamine, *N*-methyl-*N*-nitroso-	NEMA	*N*-nitrosoethylmethylamine
Methanamine, *N*-methyl-*N*-nitroso-	NDMA	*N*-nitrosodimethylamine
Morpholine, 4-nitroso-	NMOR	*N*-nitrosomorpholine
Piperidine, 1-nitroso-	NPIP	*N*-nitrosopiperidine
Propanal, 3-(methylnitrosamino)-		3-(methylnitrosamino)propionaldehyde
1-Propanamine, *N*,2-dimethyl-*N*-nitroso-		*N*-nitrosoisobutylmethylamine; *N*-nitrosomethyl(2-methylpropyl)amine
1-Propanamine, *N*-ethyl-2-methyl-*N*-nitroso-		*N*-nitrosoethylisobutylamine; *N*-nitrosoethyl(2-methylpropyl)amine
1-Propanamine, *N*-ethyl-*N*-nitroso-		*N*-nitrosoethylpropylamine
1-Propanamine, *N*-methyl-*N*-nitroso		*N*-nitrosomethylpropylamine
1-Propanamine, *N*-nitroso-*N*-propyl-	NDPA	*N*-nitrosodipropylamine
Propionitrile, 3-(methylnitrosamino)-		3-(methylnitrosamino)propionitrile
Pyrrolidine, 1-nitroso-	NPYR	*N*-nitrosopyrrolidine
Nonvolatile NNAs		
Diethanolamine, *N*-nitroso-	NDELA	*N*-nitrosodiethanolamine
2-Pyrrolidinecarboxylic acid, 1-nitroso-	NPRO	*N*-nitrosoproline; 2-pyrrolidinecarboxylic acid, 1-nitroso-
TSNAs		
2,3′-Bipyridine, 1-nitroso-1,2,3,6-tetrahydro-	NAT	*N*′-nitrosoanatabine
Butanal, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-		4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-butanal
Butanoic acid, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-	*iso*-NNAC	4-(*N*-methylnitrosamino)-4-(3-pyridinyl)- butanoic acid
1-Butanol, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-	NNAL	4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-butanol
1-Butanol, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-	*iso*-NNAL	4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-butanol
1-Butanone, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-	NNK	4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-butanone
1		2
Pyridine, 3-(1-nitroso-2-piperidinyl)-	NAB	*N*′-nitrosoanabasine
Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-	NNN	*N*′-nitrosonornicotine
N-Nitrosamino acids, esters, nitriles		
Acetic acid, 2-(methylnitrosamino)-	NSAR	*N*-nitrosarcosine; *N*-methyl-*N*-nitrosoglycine
Acetic acid, 2-(methylnitrosamino)-, methyl ester		
Butanoic acid, 4-(methylnitrosamino)-	NMBA	4-(methylnitrosamino)butanoic acid
Butanoic acid, 4-(methylnitrosamino)-, methyl ester		4-(methylnitrosamino)butanoic acid, methyl ester
Hexanoic acid, 2,6-di-(methylnitrosamino)-		2,6-di-(methylnitrosamino)hexanoic acid
Pentanoic acid, 2,5-di-(methylnitrosamino)-		2,5-di-(methylnitrosamino)pentanoic acid
2-Piperidinecarboxylic acid, 1-nitroso-		1-nitroso-2-piperidinecarboxylic acid
Propanoic acid, 3-(methylnitrosamino)-	NMPA	3-(methylnitrosamino)propanoic acid; *N*-methyl-*N*-nitroso-β-alanine
Propanoic acid, 3-(methylnitrosamino)-, methyl ester		3-(methylnitrosamino)propanoic acid, methyl ester
Propanoic acid, 2-(methylnitrosamino)-3-phenyl-		2-(methylnitrosamino)-3-phenylpropanoic acid
2-Pyrrolidinecarboxylic acid, 1-nitroso-, methyl ester		1-nitroso-2-pyrrolidinecarboxylic acid, methyl ester; *N*-nitrosoproline, methyl ester

The magnitude of the occurrence of NDMA in beer was studied by Spiegelhalder (15A54) in a survey of many German beers: 70% of the sample showed NDMA at a mean concentration of 2.7 ppb with a maximum of 68 ppb. Barley malt was considered the NNA source. In 1988, Maga (2438) reviewed some 40 publications on NNAs in common foodstuffs, beverages, and spices.

The generation of NNAs by the reaction of ingested nitrates with body chemical components was discussed in a survey by the Office of Technology Assessment (15A38):

> Nitrate and nitrate salts naturally occur in vegetable, fish and meats, are in food for their preservative properties and are present in pesticide and drug residues in food. They react with other chemicals in the body to produce NNAs and *N*-nitrosamides.

In their 1990 list of 43 "tumorigenic agents in tobacco and tobacco smoke," a list cited frequently in reports issued by various governmental agencies (EPA, USPHS), Hoffmann and Hecht (1727) included five volatile NNAs (NDMA, NDEA, NEMA, NPYR, and NMOR), one nonvolatile NNA (NDELA), and three TSNAs (NNN, NNK, and NAB). Repetitively since the mid-1980s, Hoffmann et al. have published detailed reviews on NNAs, particularly TSNAs, their levels in tobacco, MSS, SSS, and ETS, and their supposed involvement in cancer induction in tobacco users plus many reports on other aspects of NNAs [Hecht et al. (15A18), Hoffmann et al. (1688, 1698, 1731, 1745, 1746, 1750, 1770–1772, 1774–1776), Hecht and Hoffmann (1571, 1571a, 15A19, 15A20), Hoffmann and Hecht (1725, 1727), Brunnemann et al. (459, 477), Brunnemann and Hoffmann (483, 484, 486, 487), Djordjevic et al. (977, 1013, 1015–1017), Andersen et al. (76), Rivenson et al. (3182), Prokopczyk et al. (2994, 2997)].

In addition to the studies by Hoffmann et al., a great number of conference presentations and journal publications on NNAs, particularly TSNAs, have been provided by other investigators. A representative sample includes the contributions by Brown et al. (437), Bush et al. (557), d'Andres et al. (895), de Roton et al. (951), Katsuya et al. (2050–2052), Moldoveanu et al. (2599), Nestor et al. (2700), Peele et al. (2917), Risner et al. (3176a), Risner and Wendelboe (3177), Tricker (3953), and Tricker et al. (3944–3948).

Finally, with regard to NNAs, it should be noted that CSCs from tobaccos grown under high-nitrate-fertilization regimes produce fewer TBAs than do the CSCs from tobaccos grown under low-nitrate-fertilization regimes even though high-nitrate tobaccos usually show higher levels of both volatile NNAs and TSNAs, and their smokes contain higher levels of these compounds than do low-nitrate tobaccos. The responses observed in mutagenicity testing (Ames test with *Salmonella typhimurium*) are opposite from those observed in mouse-skin-painting studies. Nitrate addition, use of high-nitrate tobacco, and/or use of tobacco stems which are generally much higher in nitrate than laminae result in reduced levels of MSS total particulate matter (and "tar") and in mainstream CSCs with reduced levels of phenols and PAHs, including B[*a*]P, plus increased levels of NNAs [Wynder and Hoffmann (4312, 4317), Hoffmann and Wynder (1797, 1798, 1801, 1802), Rathkamp and Hoffmann (3081, 3082), Hoffmann et al. (1783), Brunnemann and Hoffmann (480), Adams et al. (28)].

15.1 VOLATILE NNAs

The volatile NNAs in tobacco smoke usually reported as tobacco smoke components that contribute to the smoking health problem, particularly the cigarette smoke respiratory tract cancer problem, are the first seven listed in Table 15.2.

Table 15.3 summarizes much of the early research on the VNAs.

Almost a decade after the proposal by Boyland et al. (422, 423, 15A00) that the TSNAs, NNN, and NAB might be present in tobacco and tobacco smoke, NNN was identified in cigarette MSS by Klus and Kuhn (2136). This and subsequent identification of other TSNAs in tobacco and smoke resulted in a gradual decrease in the research effort on volatile NNAs and a significant increase in the research effort on TSNAs.

15.2 NONVOLATILE NNAs

As noted in Table 15.1, NDELA and NPRO are classified as nonvolatile NNAs in tobacco and tobacco smoke. In bioassays in laboratory animals, NPRO is the only tobacco/tobacco smoke NNA to give negative responses.

The one considered the more controversial of the two is NDELA. Prior to its identification in tobacco in 1977 and smoke in 1981, its biological properties in laboratory animals and other test systems had been studied for over a decade. Druckrey et al. (1058) reported that NDELA was a hepatic carcinogen in rats. In its review of biological data generated in NNA studies, the IARC (1866) reported that this compound induced tracheal carcinomas in the hamster. Lijinsky et al. (15A35) reported that NDELA induced carcinoma of the liver and kidney in rats. McMahon et al. (2521) reported that NDELA was mutagenic when tested in modifications of the Ames test with *S. typhimurium*.

In 1977, Schmeltz et al. (3480) isolated NDELA from tobacco and identified it. In 1981, Brunnemann and Hoffmann (479) reported that cigarettes fabricated from tobaccos treated with the diethanolamine salt of maleic hydrazide delivered 10–40 ng/cig of NDELA in the MSS. These two studies were conducted when it was permissible to treat tobacco with the diethanolamine salt of maleic hydrazide, a sucker growth inhibitor. Previously reported findings on the tumorigenicity in laboratory animals of NDELA and its level in cigarette MSS eventually led to the banning by the Environmental Protection Agency (EPA) (1147) of the use on tobacco of maleic hydrazide diethanolamine salt in the United States and acceptance of the maleic hydrazide potassium salt as replacement for the maleic hydrazide diethanolamine salt.

TABLE 15.2
Summary of Lists of Tumorigenic *N*-Nitrosamines in Tobacco and Tobacco Smoke

	MSS Delivery/Cigarette Reported by								
NNA	**1986 IARC (1870)**	**1986 Hoffmann and Wynder (1808)**	**1990, 1993 Hoffmann and Hecht (1727), Hoffmann et al. (1773)**	**1994 OSHA (2825)**	**1997 Hoffmann and Hoffmann (1740)**	**1998 Hoffmann and Hoffmann (1741)[a]**	**2001 Hoffmann and Hoffmann (1743)**	**2001 Hoffmann et al. (1744)**	**2001 Fowles and Bates (1217)**
NDMA	1–200 ng	1–180 ng	0.1–180 ng	10–40 ng	0.1–180 ng	2–180 ng	2–180 ng	2–1000 ng	24.4 ng
NEMA	0.1–10 ng	1–40 ng	3–13 ng	NL	3–13 ng	3–13 ng	3–13 ng	3–13 ng	6.0 ng
N-Nitrosodiethylamine	ND–10 ng	0.1–28 ng	ND–25 ng	ND–25 ng	ND–2.8 ng	ND–2.8 ng	ND–2.8 ng	ND–2.8 ng	8.3 n
N-Nitrosodi-*n*-propylamine	ND–1 ng	NL	NL	P, NYL	NL	ND–1.0 ng	ND–1.0 ng	ND–1.0 ng	NL
N-Nitrosodi-*n*-butylamine	ND–3 ng	NL	NL	P, NYL	NL	ND–30 ng	ND–30 ng	ND–30 ng	12 ng
NPYR	2–42 ng	2–110 ng	**1.5–110 ng**	6–30 ng	**3–60 ng**	**3–110 ng**	**3–110 ng**	**3–110 ng**	113 ng
NPIP	ND–9 ng	ND–9 ng	NL	P, NYL	NL	ND–9 ng	ND–9 ng	ND–9 ng	NL
NDELA[a]	ND–90 ng	ND–40 ng	ND–36 ng	20–70 ng	ND–68 ng	ND–68 ng	ND–68 ng	ND–68 ng	30 ng
***N*-Nitrososarcosine**	NL	NL	NL	NL	ND	ND	NL	NL	NL
NNN	0.13–2.5 μg	**0.12–3.7 μg[b]**	**0.12–3.7 μg**	0.2–3.0 μg	**0.12–3.7 μg**	**120–3.7 μg**	**0.12–3.7 μg**	**0.12–3.7 μg**	1.90 μg
4-(*N*-Methylnitrosamino)-1-(3-pyridyl)-1-butanone	0.08–0.77 μg	0.12–0.95 μg	0.08–0.77 μg	0.1–1.0 μg	0.08–0.77 μg	0.08–0.77 μg	0.08–0.77 μg	0.08–0.77 μg	300 μg
N′-Nitrosoanabasine	ND–200 ng	**40–400 ng**	**0.14–4.6 μg**	NL	**0.14–-4.6 μg**	**ND–150 ng**	NL	NL	19 ng
N′-Nitrosoanatabine	ND–3.7 μg	NL	NL	NL	NL	NL	NL	NL	**72.2 μg**
NMOR	NL	NL	ND in MSS	NL	ND in MSS	ND in MSS	NL	NL	NYL

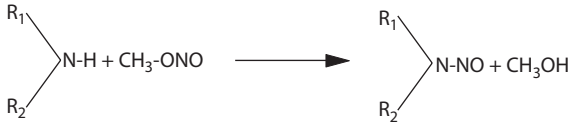
ND, not detected; P, present; NYL, no yield level listed for cigarette MSS; NL, not listed as a tumorigenic or carcinogenic component of cigarette MSS.

[a] A component listed in bold is no longer relevant (3300).

[b] A range listed in bold type contains a numerical error and/or a unit error (ng *vs*. μg).

TABLE 15.3
A Brief Chronology of the Research on VNAs from 1937 to 1990

Year	Investigation
1937	Freund (15A13) reported the acute toxicity of NDMA in humans accidentally exposed to the reagent
1954	Barnes and Magee (192) reported the hepatotoxicity of *N*-nitrosodialkylamines in several laboratory animal species
1956	Magee and Barnes (2441a) reported that almost all rats fed a diet containing 50 ppm of NDMA developed malignant liver tumors within less than a year
1960	Zak et al. (15A59) reported that feeding and daily oral dosing of rats with NDMA resulted in induction of lung tumors which adenomas, not the lung tumor type—squamous cell carcinoma—reported in various epidemiological studies to be associated with cigarette smoking
1960	Rodgman (15A49) proposed that NNAs were likely cigarette MSS components
1960	Tindall (15A55) patented the preparation of NNAs from methyl nitrite and secondary amines



The demonstration of the presence of methyl nitrite in tobacco smoke [Laurene (2293), Philippe and Hackney (2841), Laurene et al. (2310)] led to the suggestion by Rodgman (15A49) that this was their mode of formation in tobacco smoke. This mechanism of formation of volatile NNAs was also proposed by Wynder and Hoffmann [see p. 437 in (4332)]: "An opportunity for the formation of nitrosamines is the interaction of methyl nitrite and secondary amines. It could be demonstrated in these laboratories, that at least in the presence of water, methyl nitrite and diethylamine form DENA."

This proposal was subsequently negated when Vilcins and Lephardt (4058) demonstrated that methyl nitrite does not exist in the smoke within the cigarette or in the smoke at the instant it issues from the mouth end of the cigarette but begins to form artifactually immediately after the smoke exits the mouth end of the cigarette. As the level of the methyl nitrite in the aging smoke increases, its methanol level decreases. This artifactual formation of methyl nitrite was recognized by Brunnemann and Hoffmann (480): "Being aware of the artifactual formation of nitrogen dioxide and methyl nitrite by aging of smoke we prefer to report nitrogen oxides in cigarette smoke as NO [nitric oxide]."

1961	Druckrey et al. (1059) reported the results of their study on the formation, chemical structure, and tumorigenicity of NNAs. This publication did not deal with the possible presence in tobacco smoke of the NNAs, but their findings probably led to the1962 publication by Druckrey and Preussmann (1057)
1962	Druckrey and Preussmann (1057) theorized that the conditions in a burning cigarette were appropriate for the generation of NNAs; i.e., present in the reaction mixture were secondary amines, water, and nitrogen oxides
1962	Data reported by Dontenwill and Mohr (15A09) indicated that NDEA had an organ-specific effect in the tracheobronchial tree of hamsters
1962	Pasternak (15A40) and Rapoport (15A45) reported the mutagenicity of NNAs in pre-Ames (*S. typhimurium*) test systems. Numerous reports describing the mutagenicity of NNAs were issued over the next few years. The test systems used included *Drosophila melanogaster*, *Escherichia coli*, *Neurospora crassa*, *Saccharomyces cerevisiae*, among others [see review by Magee and Barnes (2442)]
1963–1964	Herrold (15A24) studied the tumorigenicity of NDEA. Herrold and Dunham (15A25) studied the tumorigenicity of subcutaneously injected NDMA and reported that intratracheal or intragastric administration of NDEA to laboratory animals resulted in a large number of respiratory tract tumors
1963	Boyland et al. (15A01) discussed the possibility of the presence of NNAs in tobacco smoke, particularly "in the acidic environment of the cigarette smoke" ($pH \leq 6.7$) as opposed to the alkaline environment ($pH \geq 7.0$) of cigar and pipe smoke
1964	Boyland et al. (422, 423) suggested that it was possible, because of the formation of NNAs by the reaction of NO_x with secondary amines, that cigarette MSS could contain NAB and NNN because of the presence in tobacco MSS of nornicotine and anabasine. They reported that NAB, when administered orally to rats, produced numerous esophageal tumors in the treated animals
1964	Neurath et al. (2751) reported the isolation and identification of *N*-nitroso-*n*-butylmethylamine and the isolation of two unidentified NNAs in cigarette MSS
1964	Boyland et al. (422, 423) suggested that it was possible, because of the formation of NNAs by the reaction of NO_x with secondary amines, that cigarette MSS could contain NAB and NNN because of the presence in tobacco MSS of nornicotine and anabasine. They reported that NAB, when administered orally to rats, produced numerous esophageal tumors in the treated animals
1964	Serfontein and Hurter (3595) reported the identification of NNAs in the MSS from South African cigarettes. Serfontein (15A53) reported the identification of NPIP. Robertson (15A47), president of the National Cancer Association of South Africa, commented on Serfontein and Hurter's report of the identification of NNAs in cigarette MSS: "The significance of this discovery lies in the fact that although the nitrosamine compound is known as a carcinogen, this is the first time that it has been established beyond doubt that various nitrosamines occur in cigarette smoke."
1964–1966	Serfontein and Hurter (3596–3598) developed a thin-layer chromatographic method for separation and analysis of extremely small amounts of NNAs and noted that "the method has been successfully applied to the analysis of nitrosamines in cigarette smoke." In a detailed account of the identification of NNAs in CSC, they reported: "In the course of initial scanning experiments, strong evidence was obtained by means of gas chromatographic analysis of the neutral fraction of cigarette smoke condensate…that various nitrosamines [*N*-nitrosodimethylamine (NDMA), *N*-nitrosodiethylamine (NDEA), and *N*-nitrosopiperidine (NPIP)] were present in cigarette smoke in measurable quantities."

They estimated the level of NPIP to range from 1 to 5 μg/cig

(*continued*)

TABLE 15.3 (continued)
A Brief Chronology of the Research on VNAs from 1937 to 1990

Year	Investigation
1965	Neurath et al. (2750) discounted their reported 1964 findings (2751) on the identification of MSS NNAs because of their artifactual formation during their collection and analytical procedure. However, with a modified analytical and collection procedure, NDMA (4 ng/cig) and NPYR (4 ng/cig) were identified in MSS. The previously reported *N*-nitroso-*n*-butylmethylamine (NBMA) was found in the part of the collection system where artifactual formation was possible. Artifactual formation of NNAs during smoke generation, separation, and analysis was a recognized problem since the first NNA identification in MSS (573, 2750, 2751, 15A10, 15A33) and resulted in much debate. Krull et al. (15A33) discussed the artifactual generation of NNAs during their determination. Subsequent research eventually resolved the question concerning the presence or absence of NNAs in tobacco and/or tobacco smoke. However, some artifactual formation did occur, resulting in inflated values for NNAs in MSS and SSS [Caldwell and Conner (572–574)]
1965	Eisenstark et al. (15A11), nearly a decade before Ames' 1973 presentation on the use of *S. typhimurium* to test for mutagenicity, described the high mutagenicity obtained with NNAs in tests with *S. typhimurium*. Several potent NNAs became positive standards, e.g., *N*-methyl-*N′*-nitro-*N*-nitrosoguanidine in the Ames test with *S. typhimurium*
1965–1967	Besides identifying several volatile NNAs in burley tobacco MSS with a procedure that precluded artifactual formation, Fredrickson (1236) demonstrated that MSS volatile NNA yields were significantly reduced (60%–85%) by a plasticized cellulose acetate filter, a finding later confirmed (514, 1761, 2635). This reduction of volatile NNA yields by selective filtration paralleled that observed for phenols (2312, 4312). Concern over phenols and their promotion effect diminished after reports of removal of significant amounts of them from MSS by selective filtration. While concern about volatile NNAs did diminish, a new NNA concern arose: one involving TSNAs, a class of NNAs newly identified in tobacco and tobacco smoke, namely, NNN, and NAB
1967	In their NNA review, Magee and Barnes (2442) [cf. Barnes and Magee (192)] noted: "It is too early to be able to suggest with any confidence the part nitrosamines might play in the etiology of human cancer. In a whole range of experimental animals tumors can be produced in a number of different sites which bear in some cases a striking pathological resemblance to cancers seen in man. However, the species, the nature of the nitroso compound, and the dose and route by which it is administered can all play a part in determining the nature of the malignant lesion produced."
1967	Brune and Henning (15A02) reported the induction of eyelid carcinoma in mice treated with methylbutyl-*N*-nitrosamine
1967	Wynder and Hoffmann noted [see p. 436 and p. 628 in (4332)]: "To date, we lack a method of quantitative determination of nitrosamines in tobacco smoke although a few good quantitative techniques have emerged. Since the presence of nitrosamines in cigarette smoke bears considerable implications in tobacco carcinogenesis, it is hoped that further and more detailed studies will also be initiated by other groups to clarify fully this important factor… A most important question, however, is whether nitrosamines are indeed formed during smoking of tobacco and whether the induction of papillary tumors in the respiratory tree of hamsters bears any relation to the induction of human bronchiogenic cancer." They concluded [p. 639 in (4332)]: "At this time one cannot deny the potential of tobacco smoke to form nitrosamines; however, we are not convinced that these agents actually exist in the cigarette smoke inhaled by man."
1967	Hoffmann and Wynder (1797) and Rathkamp and Hoffmann (3081, 3082) demonstrated that addition of nitrates to tobacco decreased the per cigarette yields of TPM, promoting/cocarcinogenic phenols, and tumorigenic PAHs (including B[*a*]P) in MSS and the tumorigenicity of the mainstream CSC to mouse skin. Later, Brunnemann et al. (471, 499) reported that increased levels of tobacco nitrate increased MSS yields of both volatile NNAs and TSNAs, resulting in recommendations to reduce the nitrate levels in tobacco stems and ribs
1968	Montesano and Saffiotti (15A37) studied the carcinogenic response of the respiratory tract of Syrian golden hamsters to different doses of NDEA. They also summarized over two dozen previous studies with NDEA
1968	In their review of the identification and quantitation of NNAs in MSS, Johnson et al. (1952) wrote: "It is possible…that little or no nitrosamines are present in cigarette smoke under normal conditions of smoking. Because of the importance of these compounds and the known high incidence of lung cancer, the establishment of their presence in smoke is of importance in the health of man… Even if the nitrosamines are identified and unequivocally established as being present in cigarette smoke at a certain level then it must be investigated whether they contribute to the total toxic activity of tobacco smoke."
1970	Volatile NNA tumorigenicity in laboratory animals was repeatedly cited with the implication that this property was extrapolable to man because of cigarette smoke NNAs. In laboratory animals, NNAs are organ-specific tumorigens and seldom have been shown to induce carcinoma at the painting site in mouse-skin-painting experiments. Hoffmann and Wynder (15A29) noted: "We…need to consider that nitrosamines have so far not been reported to be carcinogenic to man."
1971	Hoffmann and Vais (1784) reported NDMA and NEMA in unaged MSS from an 85 mm nonfiltered U.S. blend cigarette: NDMA and NEMA yields were 80 and 30 ng/cig, respectively. NDEA and NDBA were not detected. The properties of an NNA thought to be NPIP did not match those of an authentic sample
1972	The chapter in the 1972 Surgeon General's report (4003) dealing with the harmful components of tobacco smoke noted that the reports describing the presence of various NNAs in cigarette smoke were published after the June 1970 conference on which the chapter was based
1973	Morie and Sloan (2636) reported the substantial reduction of the volatile NNA (NDMA) by plasticized cellulose acetate filters *vs*. the negligible reduction obtained with paper filters. Substantial selective filtration of NDMA was demonstrated by the 85% reduction in its delivery *vs*. the 36% reduction observed in the delivery of total particulate matter with the plasticized cellulose acetate filter. Minimal selective filtration was obtained with the paper filter: 66% reduction in NDMA *vs*. 55% reduction in total particulate matter, cf. Fredrickson (1236)

TABLE 15.3 (continued)
A Brief Chronology of the Research on VNAs from 1937 to 1990

Year	Investigation
1974	Hoffmann et al. (1761) confirmed the findings of Hoffmann and Vais (1784) on NNAs in cigarette MSS. They reported 84 ng/cig of NDMA, 30 ng/cig of NEMA, and less than 5 ng/cig of NDEA in the MSS of a nonfiltered U.S. blend cigarette. They also reported that selective filtration produced a 60%–85% reduction of volatile NNAs by use of a plasticized cellulose acetate filter, cf. Fredrickson (1236), Morie and Sloan (2636)
1974	Barnes (191) [the codiscoverer with Magee of the tumorigenicity of NNAs (Magee and Barnes (2441a)] stated: "Preoccupation with the occurrence and behavior of minute amounts of nitrosamines in the human environment will probably divert skills from more profitable studies of the behavior of nitrosamines in experimental systems… If [this essay] leaves the reader with the impression that nitrosamines have a much greater potential as research tools than they have as health hazards, it will have served its purpose."
1976	Magee et al. (2443) wrote: "That a wide range of species is susceptible to the carcinogenic action of nitrosamines suggests that man is probably not resistant…Many *N*-nitroso compounds are powerfully carcinogenic in experimental animals, and, although there is no proof, it is highly probable that they are also carcinogenic in man."
1977	Brunnemann et al. (514) reported that the volatile NNA levels in MSS and SSS were lower than previously reported, attributing the lower levels to the avoidance of artifactual formation of NNAs during smoke collection and analysis. They wrote: "In fact, several of the cigarettes which were machine smoked earlier and analyzed without precautions, when smoked by us under the same conditions but with precautions, yielded 25 to 100% lower values for DMN [*N*-nitrosodimethylamine] and NPY [*N*-nitrosopyrrolidine] for the mainstream smoke…The nitrate content of the tobacco appears to be a determining factor for the concentration of volatile nitrosamines in the smoke. Selective removal of these nitrosamines does occur with cellulose acetate filter tips but not with charcoal filter tips."
	They determined the levels of volatile NNA for unaged MSS and SSS from 17 commercial and experimental cigarettes (Table 15.3)

	Level Found, ng/cig	
Volatile NNA	**MSS**	**SSS**
NDMA	1.7–97	680–1770
NEMA	0.1–9.1	9–75
NDEA	0–4.8	8–73
NPYR	0–4.8	8–73

1977	The Royal College of Physicians (3364) reported that *N*-nitroso compounds were, along with the PAHs, the chief initiators of cancer in tobacco smoke. The College noted: "The NNAs in food and drink are regarded as a potential health hazards at concentrations as low as one part per billion. *N*′-Nitrosonornicotine has been identified in both tobacco smoke and unburnt tobacco, the concentration in the latter being 2,000 to 9,000 parts per billion…concentrations much higher than those of other nitroso compounds found in meat, fish, or beverages. Its presence may be of great biological importance and could explain the correlation between tobacco chewing and the development of cancer of the mouth."
1978	The problem of the artifactual formation of volatile NNAs during smoke collection and analysis was discussed previously by Neurath (2750, 2751) and by Fredrickson (1236). It was once again revisited. Krull et al. (15A33) described the problem of artifactual formation of NNAs during the collection, fractionation, and analysis of cigarette smoke and proposed methodology to reduce the problem. This problem resurfaced several times in the next decade in the determination of both volatile NNAs [Eisenbrand et al. (15A10); Caldwell and Conner (572, 573)] and TSNAs in tobacco smoke (572, 573); preventative measures were described
1978	Brunnemann and Hoffmann (477) described the results of their measurements of volatile NNAs in indoor air containing ETS
1979	In the 1979 U.S. Surgeon General report [see p. 107 in (4005)], it was noted: "The *N*-nitrosamine formation in tobacco smoke is determined by the nitrate content of the tobacco… More importantly…selective removal (70 to 80 percent) of volatile nitrosamines from the smoke can be achieved by cellulose filters [sic][a]… At present, it has not been demonstrated that a significant reduction of volatile *N*-nitrosamines will lead to a significant reduction of the tumorigenic potential of cigarette smoke."
	It was also stated that NNAs are animal carcinogens with the ability to induce pulmonary tumors (adenomas)
1979	Rinkus and Legator (3157) listed numerous tobacco and cigarette smoke components as mutagenic in the *S. typhimurium* system. Among these were the following volatile NNAs [excluding (NMOR)] known to occur in tobacco smoke: NDMA, NDEA, NPYR, NDBA, NDPA, NMOR, NPIP
1980	In discussing "The Less Harmful Cigarette," Hoffmann et al. (1783) included a table which showed that nitrate fertilization of tobacco (which leads to increased NNAs formation) has led to significant reductions in MSS levels of "tar," nicotine, and B[*a*]P, as well as in the specific tumorigenicity of the "tar" administered via skin painting to laboratory animals. They wrote that "the reduction of the tar content of cigarettes [*sic*] was an important step in reducing the hazards of cigarette smoking."
1980	Hoffmann et al. (1711) noted: "In the mainstream smoke of a cigarette, these carcinogens [the volatile *N*-nitrosamines] can be reduced significantly by utilization of tobacco low in nitrate content and acetate filter tips that selectively retain volatile *N*-nitrosamines."
	They also stated that "most present-day commercial filter cigarettes are effectively reducing volatile NNAs." This effective reduction in volatile NNAs in cigarette MSS has not lessened during the intervening years from 1980 to date
1980	Brunnemann et al. (467) presented additional data on the levels of NNAs in MSS and SSS, cf. Brunnemann et al. (457). The SSS levels exceeded those in the MSS. Much of the MSS and sidestream data for NNAs were summarized by Hoffmann et al. (1685)

(*continued*)

TABLE 15.3 (continued)
A Brief Chronology of the Research on VNAs from 1937 to 1990

Year	Investigation
1980	Bartsch et al. (203) listed numerous NNAs as mutagenic in the Ames *S. typhimurium* test system. The following volatile NNAs reported as tobacco and/or smoke components were included: NDMA, NDEA, NMPA, NDPA, NDBA, NPYR, NMOR, and NPIP. NNN was also tested
1980	Rühl et al. (3366) reported the levels of volatile NNAs and TSNAs in the MSSs and SSSs from American, German, and French cigarettes
1981	In the 1981 Surgeon General's report (4009) on smoking *vs*. health, volatile NNAs were discussed as "organ-specific carcinogens." The Surgeon General, citing Brunnemann et al. (514), noted that "The volatile nitrosamines…can be selectively reduced by filtration…" [cf. Fredrickson (1236), Morie and Sloan (2636)]
1982	In the Third Annual Report on Carcinogens by the National Technical Information Service (2686), it was noted that "there is sufficient evidence for the carcinogenicity of *N*-nitrosodimethylamine (NDMA) in experimental animals." Similar comments were made about NPYR (MSS yield estimated as being as much as 113 ng/cig) and NDEA (MSS, 8 ng/cig; SSS yield, about 10 times that in MSS)
1982	Hoffmann and Wynder (1807a) included a table which indicated that nitrate fertilization (known to increase the levels of NNAs in the tobacco and the smoke from it) significantly reduced the biological activity (carcinogenicity) of CSC to mouse skin. The PAH levels in the CSC were also reported to be reduced
1982	In contrast to suggestions made in the late 1950s/early 1960s to control the pyrogenesis of PAHs by reduction of the tobacco wax components, e.g., long-chained saturated hydrocarbons such as *n*-hentriacontane, and/or the use of high-nitrate tobacco, Brunnemann and Hoffmann (480) recommended the following approaches—the direct opposite of the earlier suggestions from the Wynder and Hoffmann laboratory—to control both the PAHs and the NNAs in tobacco smoke: "Selective filtration is highly effective in removing volatile *N*-nitrosamines from the smoke stream, but is ineffective for the selective reduction of tobacco-specific nitrosamines. Selective reduction of nitrate in tobacco stems offers one possible approach, but additional means of reducing nitrogen oxides and *N*-nitrosamines without diminishing PAH reduction need to be found. Selection of tobacco with high levels of long chain hydrocarbons (e.g. hentriacontane $C_{31}H_{64}$) may be helpful." These 1982 suggestions for the design of a "less hazardous" cigarette were in direct contradiction to those offered two decades previously when the main emphasis was not on NNAs (their presence in tobacco smoke was, at best, theoretical in the early 1960s) but on the tetracyclic and higher PAHs, particularly B[*a*]P, because of the known effect of it and other PAHs on the skin of laboratory animals
1982	The 1982 report of the Surgeon General (4010), citing the studies of Magee et al. (2443) and the IARC (1866), concluded: "More than 50 of the approximately 100 NNAs which have been tested have various degrees of carcinogenic potency in laboratory animals… There is a lack of direct evidence that these compounds are also human carcinogens. Nonetheless, many scientists concur with the [IARC] that, for practical purposes, these nitrosamines should be regarded as carcinogenic in humans." It was noted that NDMA and NPYR were the most plentiful NNAs in cigarette smoke. NDMA is listed in this report as a "toxic and tumorigenic agent" in the vapor phase of cigarette smoke. Both NEMA (MSS delivery, 1–40 ng/cig) and NDEA (MSS delivery, 0.1–28 ng/cig) were reported as "among the most potent environmental carcinogens" of the NNAs
1982	Stehlik et al. (3812) determined the levels of NDMA in the air of cigarette smoke-filled rooms
1983	In his concluding remarks at the 1983 NNA conference (published in 1984), Magee (2441) stated: "A major component of this evidence [that N-nitroso compounds probably can cause human cancer] is the large number of species known to be susceptible to cancer induction by nitrosamines… The question of whether any human cancer has been caused by nitrosamines remains open, but several relevant and interesting presentations were given during the meeting… Following up the well-established relationship between cigarette smoking and the incidence of human lung cancer, these workers [Hoffmann, Hecht, Castonguay, and their colleagues] presented persuasive evidence for a relationship between the use of chewing tobacco and snuff and human cancer…A role for nitrosamines in the causation of human cancer has not been established, but it should not be excluded and merits further study."
1984	Although their data showed that an increase in the nitrate content of cigarette tobacco reduced the levels of FTC "tar," nicotine, carbon monoxide, catechol, and B[*a*]P, Adams et al. (28) emphasized that significantly higher yields of volatile NNAs and TSNAs were found in the MSS of an 85 mm nonfiltered cigarette. They concluded: "The findings of this study support the recommendation that the nitrate content of tobacco products should be reduced." [Cf. 1967/1970 studies and comments by Hoffmann and Wynder (1797, 1798) and Rathkamp and Hoffmann (3081, 3082) that use of high-nitrate tobacco was beneficial in that it reduced the levels of CSC, PAHs, and CSC tumorigenicity to mouse skin. Also, the findings of Brunnemann et al. (481, 482) that addition of stems, high in nitrate, did not reduce "tar," nicotine, or carbon monoxide yields]
1984	Despite three decades of a variety of claims against the PAHs and their role in carcinoma induction in laboratory animals skin painted with CSC and their alleged role in carcinoma induction in cigarette smokers, it is interesting to note that in the *American Chemical Society Monograph* (2nd edn.) edited by Searle (3568), the only class of compounds in tobacco or cigarette smoke discussed with regard to their tumorigenicity in laboratory animals was the NNAs. Even though several chapters were written by experts in the fields of PAH, their nitrogen analogs, and aromatic amines; no mention was made throughout this two-volume 1400-page monograph of the numerous PAHs in tobacco or cigarette smoke, their levels, or their role in respiratory tract cancer attributed by some to the PAHs in cigarette smoke. The only class of tumorigens discussed was the NNAs and TSNAs. Most of the data cited were those of Hoffmann et al.
1984	The Preussmann and Eisenbrand summary (2990) of research on NNAs in tobacco and tobacco smoke was, according to their article, taken largely from a 1982 review by Hoffmann et al. Preussmann and Eisenbrand commented: "Although Hoffmann et al. have clearly demonstrated the effectiveness of cellulose acetate filters in model experiments, the values for U.S. commercial cigarettes are about the same for filter as for nonfilter cigarettes; the reductive effect of filters in practice may be counteracted by variations in tobacco composition between the two types of cigarettes… In conclusion, tobacco and tobacco smoke represent the largest nonoccupational source of exposure for preformed nitrosamines."

TABLE 15.3 (continued)
A Brief Chronology of the Research on VNAs from 1937 to 1990

Year	Investigation
1984	Matsushita and Mori (2495) determined the levels of nitrogen dioxide and volatile NNAs in indoor air and cigarette SSS
1984	Preussmann (15A43) tabulated the ranges of the reported levels of a variety of NNAs in tobacco and in cigarette MSS and SSS
1986	The IARC (170) concluded that NDMA, NDEA, NPYR, and NEMA were tumorigenic to laboratory animals and that NDMA was one of the two most abundant volatile NNAs in cigarette MSS
1987	Klus et al. (15A32) reported the levels of several volatile NNAs in ETS in several real-life situations
1987	The RTECS (Registry of Toxic Effects of Chemical Substances) (3095) reviewed the studies in which lung tumors were observed in laboratory animals treated with an NNA by a variety of administration routes. The RTECS categorized the positive inhalation findings involving NNAs as "equivocal." For example, the dose level used (200,000 ng/m^3) for NDMA in the inhalation experiments was significantly greater than the NDMA level observed (10–240 ng/m^3) in ETS exposure
1989–1990	Caldwell and Conner (573) reported: "The methodology previously reported [by others] leads to significant overestimation of *N*-nitrosamine concentrations in cigarette smoke."
	The overestimations were true for both volatile and tobacco-specific NNAs in MSS and SSS for the Kentucky Reference Cigarette 1R4F: MSS data indicated that the levels were 380% high for NPYR and 83%, 38%, 27%, and 19% for NAB, NAT, NNK, and NNN, respectively. Thus, it is probable that many of the previously reported levels of NNAs in MSS and SSS, tabulated in various articles [cf. Adams et al. (31), Hoffmann and Hecht (1727)] and cited by EPA (1148) and the U.S. Surgeon General (4005, 4009, 4010, 15A57) are incorrect.
	Hoffmann and Hecht (1727) did not acknowledge that the MSS levels listed for volatile NNAs and the TSNAs were likely to be incorrect (and high) because of the artifactual formation of both types during MSS (and SSS) collection for analysis as reported by Caldwell and Conner (572–574). EPA (1148) accepted without question the MSS volatile NNA and TSNA yields listed by Hoffmann and Hecht (1727) whose data were cited by the U.S. Surgeon General (4012). The levels of various NNAs reported in foodstuffs and beverages are also possibly in error because of artifactual formation of NNAs during the isolation procedure and subsequent quantitation
1990	In their list of 43 "tumorigenic agents" in tobacco and/or smoke, Hoffmann and Hecht (1727) included the following volatile NNAs: NDMA, NDEA, NEMA, and NPYR. Little comment was made about these four volatile NNAs and their supposed tumorigenicity to smokers. However, they did note that IARC (1870) had evaluated the bioassay data from laboratory animals exposed to these NNAs and considered the data sufficient to classify all four as tumorigenic to animals. IARC did not express an opinion as to whether these four were tumorigenic to humans
	Brunnemann et al. (1459, 460, 462) summarized data from several publications on the levels of various volatile NNAs (NDMA and NPYR) in indoor air at various sites (trains, offices, coffee shops, dance halls)

[a] This should read "cellulose acetate."

In his response to the Environmental Protection Agency's draft document (1148) on ETS, Rodgman (3255) criticized the inclusion by EPA of NDELA as a tumorigenic agent in tobacco and/or smoke. EPA had based its assessment of this compound on the Hoffmann–Hecht list of 43 "tumorigenic agents in tobacco and tobacco smoke" (1727). Rodgman's reasoning was as follows: since the diethanolamine salt had not been used in the United States for nearly a decade, the level of this nitrosamine should now be substantially reduced in tobacco as well as in MSS and SSS from cigarettes containing such tobacco.

The chronological pattern of decrease in levels of NDELA might parallel those reported for the decrease in levels of arsenic and DDT in tobacco (and its smoke) when arsenicals and DDT were no longer used on tobacco in the United States. For example, in 1952, arsenicals were removed from the list of recommended and permissible insecticides for tobacco. By 1968, the arsenic content of U.S.-grown tobacco had decreased to 0.5–1.0 μg/g from the 1951 level of about 50 μg/g of tobacco (1870, 4005); arsenic levels reported in 1975 by GRIFFIN et al. (1391) were 0.5–0.9 μg/g of tobacco. Similarly, discontinuance of the use of chlorinated insecticides such as DDT in U.S. tobacco culture in the late 1960s resulted in a gradual and substantial reduction of DDT residues in leaf tobacco. Between 1968 and 1974, the residual DDT level in American flue-cured tobacco decreased rapidly and substantially (1870, 4005) from 52 μg/g in 1968 to 6 μg/g in 1970, and to 0.23 μg/g in 1974.

Hoffmann et al. (1696) had predicted that the NDELA level in tobacco would decrease:

> At present, NDELA [*N*-nitrosodiethanolamine] levels are relatively high in US brands (290–300 mg/kg) but they are expected to decrease, since the herbicide was banned from use on tobacco as of October 1981 (1147).

In 1982, the U.S. Surgeon General concluded (4010) that NDELA was a carcinogen, noting not only did NDELA induce carcinomas in treated laboratory animals (carcinoma of the liver and kidneys in rats, carcinoma of the trachea in hamsters), but also it was present in tobaccos treated with the diethanolamine salt of maleic hydrazide.

In the National Technical Information Service Third Annual Report on Carcinogens (2686), it was concluded that there was sufficient evidence to classify NDELA as a carcinogen in laboratory animals.

In its review of tumorigenic components of tobacco and tobacco smoke, the IARC (1870) noted for NDELA:

> Its presence in tobacco products has been related to the use of the sucker growth inhibitor, maleic hydrazide when formulated with the diethanolamine salt ('MH-30' or 'MH-40')…; in the USA, that formulation has been replaced by the potassium salt… Tobaccos grown in a pesticide-free environment and smoke generated from such tobaccos are devoid of N-nitroso-diethanolamine. [(NDELA)]

Hoffmann and Hecht (1727) included five volatile NNAs [NDMA, NDEA, NEMA, NPYR, and NMOR] and the nonvolatile NDELA in their list of 43 "tumorigenic agents in tobacco and tobacco smoke." They noted that NMOR had not been reported as a tobacco smoke component. Possible relationships between diethanolamine {I}, NDELA {II}, morpholine {III}, and NMOR {IV} are illustrated in Figure 15.1. It is possible that as the NDELA level in tobacco has declined, the levels of morpholine and NMOR also have declined. More recent major efforts in the NNA-tobacco area have been devoted to the study of TSNAs and *N*-nitrosamino acids rather than to the NDELA/NMOR question.

Tobacco products and smoke, however, are not the only source of exposure to NDELA. As noted previously, it is highly likely that the current levels of NDELA in tobacco products are approaching zero because of the discontinued use of the diethanolamine salt of maleic hydrazide in U.S. tobacco agronomy. However, consumer exposure to NDELA from nontobacco sources is possible. Studies of NDELA-contaminated cosmetics indicated substantial levels of NDELA have been identified in cosmetics; e.g., Fan et al. (15A12) detected NDELA in 27 of 29 products tested at levels ranging from 1 to 48,000 ppb; Klein et al. (15A31) detected it in 5 of 10 cosmetic products (range from 20 to 4113 ppb). Hecht (15A15) found no NDELA in the products but did find *N*-nitrosomethyldodecylamine in six of seven cosmetics containing laurylamine (dodecylamine). NDELA is readily absorbed through the skin after application of NDELA-contaminated cosmetics and is detected in cosmetic users' urine, cf. Preussmann and Eisenbrand (2990).

The other nonvolatile NNA is NPRO (see Table 15.1). It was not included by Hoffmann and Hecht (1727) in their list of 43 "tumorigenic agents in tobacco and tobacco smoke" or any of the subsequent lists tabulated in Table 15.2.

Scott et al. (3566) and Brunnemann et al. (511) reported that cigarette and chewing tobaccos differed in their NPRO levels: Cigarette tobacco contained ≈2 ppm (less than 1% of free proline was nitrosated); chewing tobacco contained about 35 ppm (up to 40% of free proline was nitrosated). They reported that the NPRO level is dependent on proline level, nitrate level, and curing method.

Brunnemann et al. (509) reported the measurement of the endogenous formation of NPRO in smokers and nonsmokers on a controlled diet, relatively low in proline and ascorbic acid. The NPRO in urine was determined in 24-h urine samples on days 3, 6, 9, and 12. Different groups in the study were administered proline and/or ascorbic acid at appropriate times during the experiment. Ascorbic acid intake reduced urinary levels of NPRO. Differences in NPRO excretion by smokers and nonsmokers on the controlled diet, ascorbic acid supplement, no proline supplement were not statistically significant.

The results of numerous studies on the *in vivo* formation of NNAs were presented at the 1983 IARC conference [O'Neill et al. (15A39)]. Many dealt with the *in vivo* generation of NPRO in nitrite- and proline-treated mammalian species, including humans. Numerous investigations have been conducted on NPRO because of its presence not only in tobacco and tobacco smoke but also in a variety of consumer products (meat, bacon, ham, chicken, fish, toast, biscuits, cornflakes, beer) [Brunnemann et al. (509), Hansen et al. (15A14), Pensabene et al. (15A41), Pollock (15A42), Sen and Seaman (15A50), Sen et al. (15A51)].

In the IARC monograph (1870), it was noted that NPRO was detected in cigarette smoke at extremely low levels (<1 ng/cig) by Brunnemann et al. (511) despite the fact it is readily detected in tobaccos. Hoffmann et al. (1696) listed the levels of NPRO in various tobacco products (cigarette tobaccos, little cigars, cigars, chewing tobaccos, snuff). The reported values ranged from a low of 450 to a high of 22,000 ng/g of tobacco (dry weight).

15.3 TOBACCO-SPECIFIC NNAs

A year after the proposal by Druckrey and Preussmann (1057) that the conditions in a smoked cigarette were appropriate for the generation of NNAs, Boyland et al. (422, 423, 15A01) speculated that it was possible, because of the formation of NNAs by the reaction of nitrogen oxides with secondary

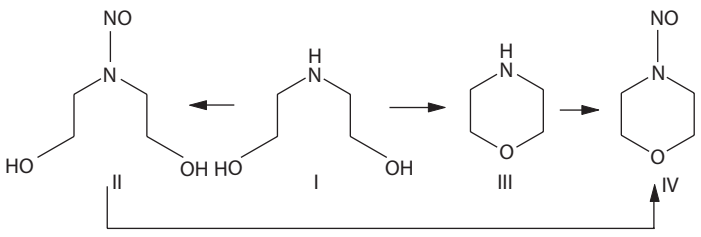


FIGURE 15.1 NDELA and *N*-nitrosomorpholine (NMOR).

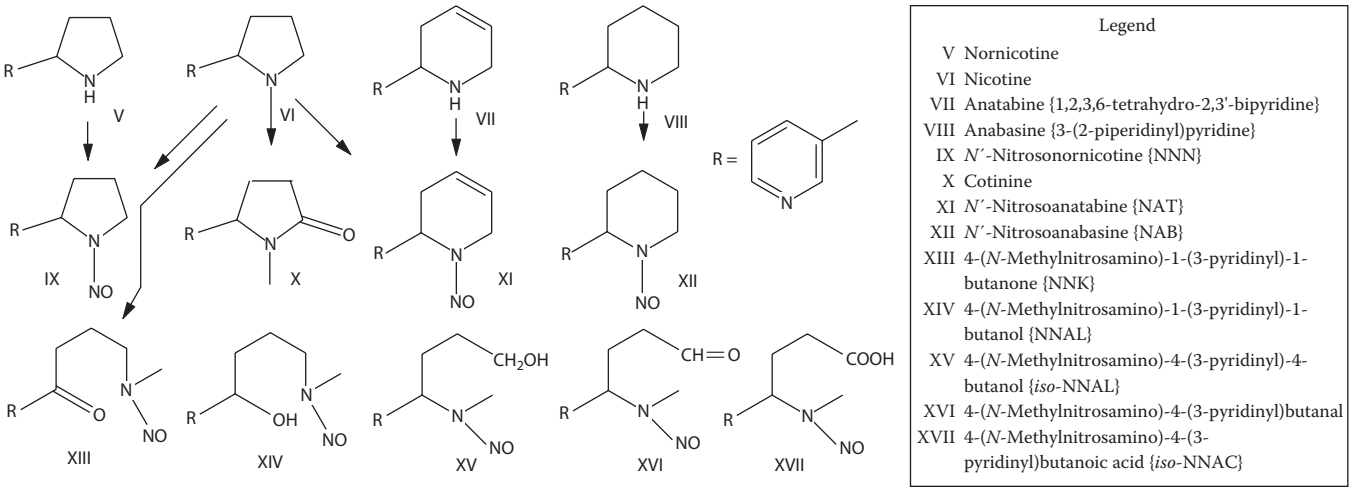


FIGURE 15.2 Tobacco-specific *N*-nitrosamines.

amines, that cigarette MSS could contain NNN and NAB because of the presence of the secondary amines nornicotine and anabasine in tobacco and smoke. They also reported that oral administration of NAB to rats induced esophageal tumors. After nearly a decade of investigation on the volatile NNAs in tobacco smoke, attention was turned to the higher molecular weight NNAs.

In Figure 15.2 are shown the relationships among the nicotine-related alkaloids—nornicotine {V}, nicotine {VI}, anatabine {VII}, anabasine {VIII}—and the NNAs {IX, XI–XVII} and cotinine {X}. Table 15.4 summarizes some of the early research on the TSNAs.

Between the early 1980s and 2004, a substantial number of studies were devoted to some aspect of the TSNAs in tobacco and/or its smoke. Included were conference presentations and journal publications in which analytical technology, artifactual TSNA generation during collection and analysis, quantitation, adverse biological effects and their inhibition, effect on various biological systems, and tobacco users. Figure 15.3 is a plot of the chronology from 1983 through 2004 of TSNA-related references listed in our Bibliography section. It is obvious from the graphical depiction that the decade from the late 1980s to the late 1990s was a highly productive period for such studies. It is also obvious from the references in bold print that the American Health Foundation was a major contributor to our knowledge on TSNAs.

15.4 *N*-NITROSAMINO ACIDS

The results of several epidemiological studies suggested an association between the use of chewing tobacco or snuff and oral cancer. These products differ from smoking products (cigarettes, cigars, pipe tobaccos) in that they are not subjected to the high temperatures encountered in the smoking process. Thus, smokeless products contain little, if any, of the combustion products alleged to be significant tumorigens, e.g., the PAHs and their *N*-containing analogs, in tobacco smoke. As a result, snuff and chewing tobacco NNAs became suspect because they were the only components known to be laboratory animal tumorigens. Preformed NNAs in these tobacco products and NNAs endogenously formed in the product users were considered by many to be the causal factor for oral cancer in snuff dippers [Hoffmann and Adams (1677), Brunnemann et al. (507a, 510, 15A04), Hoffmann et al. (1684, 1697, 1707, 1713, 1722), Hecht et al. (15A23), Adams et al. (33), Prokopczyk et al. (15A44), Carmella et al. (15A06), Tsuda and Kurashima (15A56), Djordjevic et al. (1008)] and in tobacco chewers [Brunnemann et al. (468, 498), Wenke et al. (15A58), Hoffmann et al. (1730, 1731), IARC (1869), Prokopczyk et al. (2995), Tsuda and Kurashima (15A56)].

In studies to elucidate the possible tumorigens in chewing tobacco and snuff, the only known components tumorigenic in laboratory animals identified were various NNAs, particularly the TSNAs, NNN, and NNK plus a group of *N*-nitrosamino acids, including NPRO. Whereas discussions and investigations on volatile NNAs [Druckrey and Preussmann (1057), Serfontein and Hurter (3595–3599)] and several TSNAs, NNN, and NAB [Boyland et al. (422, 423)] have appeared in the literature for over four decades, reports on identifications of *N*-nitrosamino acids are much more recent.

Ohshima et al. (2852) identified several *N*-nitrosamino acids, 3-(methylnitrosamino)propanoic acid (also known as *N*-methyl-*N*-nitroso-β-alanine) (NMPA), 4-(methylnitrosamino)butanoic acid (NMBA), and 1-nitroso-2-piperidinecarboxylic acid (also known as *N*-nitrosopipecolic acid), in various types of tobacco (cigarette, chewing, pipe, cigar, and snuff tobaccos). Decarboxylation of these *N*-nitrosamino acids would yield NEMA, *N*-nitrosomethylpropylamine, and NPIP. IARC (1986) did note the 1985 Ohshima et al. findings on these *N*-nitrosamino acids in tobacco.

Following their identification of several *N*-nitrosamino acids in snuff, Djordjevic et al. (992) investigated these acids in 1R1 and 1R4F reference tobaccos from the University of Kentucky. In addition to detecting 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-1-butanol (*iso*-NNAL), 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-1-butanal,

TABLE 15.4
A Brief Chronology of the Research on TSNAs

Year	Investigation
1964	Boyland et al. (422, 423) suggested that, because of the possibility of the formation of NNAs by the reaction of NO_x with secondary amines, cigarette MSS could contain NAB and NNN generated from nornicotine and anabasine in tobacco MSS. NAB, when administered orally to rats, induced esophageal tumors in the treated animals
1973	At the Austria Tabakwerke A.G., Klus and Kuhn (2136) detected 40 ng/cig of NNN in the MSS from cigarettes made with nornicotine-rich tobacco (1.95% nornicotine). However, they failed to detect NNN in the MSS from a blended commercial cigarette. They concluded: "From the biological and toxicological points of view, the expected quantity of nornicotine nitrosamine developed from a commercial cigarette containing an average of 0.04% nornicotine is almost meaningless."
1973	Rathkamp et al. (3080) reported that MSS from an 85 mm U.S. blend nonfiltered cigarette contained NAT at less than 20 ng/cig
1974	Hoffmann et al. (1761) confirmed the report by Klus and Kuhn (2136) of the presence of NNN in cigarette MSS. They suggested that nicotine and nornicotine were NNN precursors with nicotine actually being the more important precursor because of its preponderance in tobacco. Their results differed, however, from those of Klus and Kuhn on the level of NNN in MSS from a commercial blended cigarette; Hoffmann et al. (1761) reported that the MSS from a nonfiltered U.S. blended cigarette contained 137 ng of NNN
1974	Hecht et al. (1576) reported the level of NNN in tobacco paralleled the nitrate level. They also suggested the TSNA levels in tobacco may be controllable by appropriate selection of the curing process. Flue-cured tobaccos usually show the lowest NNN level *vs*. the levels in tobaccos cured by other methods, e.g., air curing
1974	Hoffmann et al. (1733) reported that various types of commercial tobacco contained substantial levels of NNN at levels ranging from 2 to 90 mg/g (2–90 ppm). Two commercial cigarette samples showed NNN levels of 2.2 and 6.6 mg/g. They noted: "This is to our knowledge the highest concentration of a positively identified NNA yet reported in an environmental source. NNAs in meat, fish, beverages, and related materials rarely exceed 0.1 ppm."
1976–1977	Hecht et al. (1563, 1565) suggested that nicotine was the precursor of NNK and 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-1-butanal in tobacco via opening of the pyrrolidine ring of nicotine
1977	The Royal College of Physicians (3364) noted: "*N*′-Nitrosonornicotine has been identified in both tobacco smoke and unburnt tobacco, the concentration in the latter being 2,000 to 9,000 parts per billion—concentrations much higher than those of other nitroso compounds found in meat, fish, or beverages. Its presence may be of great biological importance and could explain the correlation between tobacco chewing and the development of cancer of the mouth."
1979	For tobaccos, Hoffmann et al. (1679) reported levels of 0.2–45 ppm of NNN and 0.1–35 ppm of NNK. For cigarettes, they reported MSS levels of 0.2–3.7 µg/cig for NNN and 0.12–0.44 µg/cig for NNK
1979	After reviewing earlier data that indicated NNN was moderately carcinogenic in the Syrian golden hamster, Hoffmann et al. (15A28) concluded: "Since NNN is present in ppm levels in tobacco and in microgram amounts in the smoke of a cigarette, it may contribute to the carcinogenicity of tobacco smoke."
1979	The U.S. Surgeon General (4005) reported the identification of NNN and NAT in MSS. MSS levels listed for NNN were those reported by Hoffmann et al. (1679) (0.2–3.7 µg/cig). No quantitative data were listed for NAT
1980	Hecht et al. (15A18) reported high rates of benign and malignant tumors in two groups of F344 rats treated with TSNAs. One group of rats was treated with NNN; the other group was treated with NNK. For each group, the TSNA (3.4 mmol total dosage) was administered in 60 subdoses over a period of 20 weeks
1981	Adams et al. (23) reported the results of their study on the transfer of 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK) from tobacco to MSS and its formation from tobacco components during the tobacco smoking process
1981	McCoy et al. (15A36) studied the influence of ethanol in the diet on the tumorigenicity of NNN administered to Syrian golden hamsters at two dose levels. In the group of test animals whose caloric intake was equal to that of the control group, no accelerating effect of ethanol on NNN tumorigenicity was observed
1981	Hoffmann et al. (1710) reported that, in a study involving subcutaneous injections into Syrian golden hamsters, the tumor production data indicated NNK was a more potent carcinogen than NNN. The authors stressed the importance of this finding because of the relatively high exposure (approximately 1 µg/cig for an 85 mm filtered cigarette) of smokers to NNK [see also Table 9 in (1710)] which they described: "As a carcinogen more potent than the strongly carcinogenic *N*′-nitrosonornicotine… Exposure to NNK in tobacco and tobacco smoke should certainly be minimized."
1981	In the U.S. Surgeon General's 1981 report (4009), the relative tumorigenicities of NNN, NNK, and NAT were discussed: "NNN is a moderately active carcinogen in mice, rats, and Syrian golden hamsters, whereas NNK is a strong carcinogen to the respiratory tract of all three species; NAT has so far not been bioassayed." After it was noted that conclusive epidemiologic data were not available to define the precise effect of NNN in humans, the following statement was cited from a 1978 IARC report: "NNN should be regarded for practical purposes as if it were carcinogenic to humans."
1982	Brunnemann et al. (471) described the environmental occurrence of NNAs derived from foods and other consumer items, including tobacco products. They also discussed the possibility of the *in vivo* formation of NNAs in blood serum, gastric secretions, and urine
1982	The IARC (1867) concluded that there was sufficient laboratory evidence to categorize NNN as carcinogenic in laboratory animals

TABLE 15.4 (continued)
A Brief Chronology of the Research on TSNAs

Year	Investigation
1982	In the Third Annual Report on Carcinogens by the National Technical Information Service (2686), the National Toxicology Program officials noted: "Cigarette smokers, tobacco chewers, cancer researchers, and organic chemists are at greatest risk of exposure to *N*-nitrosonornicotine… Smokers and persons breathing tobacco smoke may inhale a significant amount of *N*-nitrosonornicotine. The amount of this substance in commercial U.S. tobacco products varies from 1.9 to 88.5 ppm; this is one of the highest values of an experimental nitroso compound reported in the literature
1982	In the U.S. Surgeon General's 1982 report (4011), it was stated: "At this time, there is no experimental evidence on the formation of TSN (tobacco-specific nitrosamines) in the lung upon inhalation of tobacco smoke. However, a smoker of one or two packs of cigarettes daily retains…1 to 4 milligrams of nornicotine…thus, *in vivo* formation of tobacco-specific NNAs is a real possibility. The report also concluded that NNK is "…by far the most potent carcinogens of the TSNAs." In this 1982 report, NNK was included in a list of "toxic and tumorigenic agents of cigarette smoke." It was noted that the level of NAT in MSS of U.S. cigarettes ranged from 0.15 to 4.6 ng/cig. It was also pointed out that no carcinogenicity bioassay data were currently available for NAT in 1982
1982	In their review on MSS and SSS composition and SSS/MSS ratios, Klus and Kuhn (2142) summarized the published data [Hoffmann et al. (1679)] on MSS and SSS yields of several tobacco-specific NNAs (NNN, NNK, NAT)
1983	Using radiolabeled compounds, Adams et al. (29) conducted a detailed study on the formation and transfer of NNK: It was reported that 6.9%–11.0% of the tobacco component transferred to MSS; this amount represented 26%–37% of the NNK in MSS, the remainder (63%–74%) was considered to be formed from nicotine during the smoking process. However, conflicting data were later presented by Fischer et al. (1193, 1199) who reported that NNN and NNK in cigarette MSS arose only by transfer from the tobacco rod and were not formed pyrogenetically during the smoking process
1983	Hecht et al. (15A16) reported the induction of lung tumors in Syrian golden hamsters treated with a single dose of 1 mg of 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)
1983	Castonguay et al. (15A08) reported: "As a result of tobacco smoking, NNN [*N′*-nitrosonornicotine] and NNK [4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone] are among the most ubiquitous procarcinogens detected in the human environment." In their carcinogenicity study, Castonguay et al. found that a total dose of 0.1 mmol of NNK induced 3.76 lung tumor/mouse or a total of 86.5 lung tumors. This value was 29 times higher than that found in the similarly treated NNN group. The number of lung carcinomas in the NNK group was 41 times higher than that in the NNN group
1983	Brunnemann et al. (499) studied the influence of stem (and their nitrate content) on the volatile and tobacco-specific NNAs in MSS and SSS. They reported that the MSS yields of "tar," nicotine, carbon monoxide, and carbon dioxide were *not* greatly influenced by filler nitrate content. This should be contrasted with previous reports from the same laboratory—at a time when nitrate addition or high-nitrate tobacco use was touted as beneficial—on the reduction in smoke yields of "tar," nicotine, PAHs, phenols, and carbon monoxide as a result of nitrate addition [Wynder and Hoffmann (4332), Hoffmann and Wynder (1797, 1798)]. The SSS yield of NDMA was extremely high (>1000 ng/cig). SSS yields of NDMA and NNN were dependent on filler nitrate content
1983–1984	Hecht et al. (15A17, 15A22) and Hecht and Lin (15A21) demonstrated the genotoxicity (Ames test with *S. typhimurium*) of NNK and NNN [Hecht et al. (1984)]
1984	As noted previously, since the early 1980s, Hoffmann et al. at the American Health Foundation have presented or published numerous reviews, many repetitious in content, of their views on NNAs. In particular, they have emphasized the TSNAs, their levels in tobacco, in MSS and SSSs, and in ETS, their tumorigenicity in laboratory animals, and their supposed involvement in tumor induction in tobacco users, e.g., Hecht et al. (15A17), Hoffmann et al. (1688, 1730, 1731, 1746, 1770, 1772, 15A26, 15A27), Djordjevic et al. (1014), Hecht and Hoffmann (1571, 1571a, 15A20), Hoffmann and Hecht (1727), and Brunnemann and Hoffmann (15A03)
1984	Although their data showed that an increase in the nitrate content of cigarette tobacco reduced the MSS levels of FTC "tar," nicotine, carbon monoxide, catechol, and B[*a*]P, Adams et al. (28) emphasized that significantly higher yields of volatile NNAs and TSNAs were found in the MSS of an 85 mm nonfiltered cigarettes whose nitrate contents were increased by sodium nitrate addition. Despite reductions in MSS levels of "tar," nicotine, B[*a*]P, and catechol, Adams et al. considered that the "carcinogenic potential" of the whole MSS from the enhanced nitrate cigarettes was increased primarily due to elevated yields of nitrogen oxides (NO_x), volatile NNAs, and TSNAs. They stressed the importance of the NO_x as a precursor in the endogenous formation of NNAs during tobacco smoke inhalation. However, they ignored the fact that (1) only traces of nitrogen dioxide NO_2 exist in cigarette MSS, (2) over 95% of its NO_x content is nitric oxide, NO, and (3) other components in tobacco smoke reduce the nitric-oxide-to-nitrogen-dioxide conversion ($NO \rightarrow NO_2$) [Cooper (815), Cooper and Hege (816)]. On the basis of their findings, Adams et al. concluded: "The findings of this study support the recommendation that the nitrate content of tobacco products should be reduced."
1984	Hoffmann et al. (1769) reported the following results from the MSS and SSS analyses of U.S. commercial cigarettes:

	Ng/cig	
TSNA	**MSS**	**SSS**
NNN	120–1000	150–1700
NNK	80–770	170–410
NAT	140–1000	150–270

(*continued*)

TABLE 15.4 (continued)
A Brief Chronology of the Research on TSNAs

Year	Investigation
	In this study, subcutaneous injection of NNN (three levels: 9.0, 3.0, and 1.0 mmol/kg, thrice weekly for 20 weeks) into F344 rats showed a dose response with respect to nasal tumors (60% and 100% at the higher two levels) and carcinoma of the nasal cavity. Lung adenomas were observed at all three dose levels. In a parallel experiment with NNK, relatively high carcinogenicity in the rats was observed. They wrote: "Perhaps the most important finding was that even the lowest dose of NNK induced a high percentage of lung tumors in males (85%) and a significant yield of lung tumors in females (30%). These lung tumors included squamous cell carcinomas."
	In an NAT experiment, similar to those for NNN and NNK, NAT was not carcinogenic at any of the three dose levels
1986	IARC (1870) concluded that the TSNAs are the most abundant suspected carcinogens in tobacco smoke. It considered NNN and NNK to be proven carcinogens for laboratory animals. It considered the evidence limited for defining the carcinogenicity of NAB in laboratory animals and inadequate to label NAT as a carcinogen for laboratory animals
1987	Adams et al. (31) presented data on the levels of TSNAs in MSSs and SSSs from different types of cigarette. TSNAs comprised NNN, NNK, NAB, and NAT. For the latter three, the per cigarette SSS levels substantially exceeded the MSS levels
1987	Brunnemann et al. (469) identified a new TSNA 4-(*N*-methyl-nitrosamino)-4-(3-pyridinyl)-1-butanol (*iso*-NNAL) in snuff and cigarette tobaccos. It was not detected in either cigarette MSS or SSS. In a study involving iso-NNAL, NNN, and NNK, LaVoie et al. (15A34) determined the tumorigenicity of the three in mice
1987	Klus et al. (15A32) measured several ETS-related TSNAs in indoor air of an 83 m^3 office under various smoking conditions. NNN varied from 0.7 to 6 pg/L, NNK varied from 0.2 to 10.7 pg/L. They found no correlation with the carbon monoxide levels
1988	Tricker et al. (3945) reported that nicotine was not *N*-nitrosated to NNN under simulated gastric conditions. However, nornicotine, anabasine, and anatabine were *N*-nitrosated to NNN, NAB, and NAT, respectively, under such conditions. They also reported that NNK decomposed slightly under these conditions
1989	Hecht and Hoffmann (15A19) considered both NNN and NNK as powerful carcinogens because they induced benign and malignant tumors of the lung, nasal cavity, esophagus, pancreas, and/or liver in mice, rats, and hamsters
1989–1990	Caldwell and Conner (573) reported: "The methodology previously reported [by others] leads to significant overestimation of NNA concentrations in cigarette smoke."
	The overestimations were true for both volatile NNAs and TSNAs in MSS and SSS for the Kentucky Reference Cigarette K1R4F used in their study: MSS data indicate the levels found were 380% high for NPYR and 83%, 38%, 27%, and 19% for NAB, NAT, NNK, and NNN, respectively. Thus, it is highly probable that the levels of NNAs in smoke tabulated in articles such as those by Hoffmann and Hecht (1727) and frequently cited by the EPA and the Surgeon General are incorrect
1990	Hoffmann and Hecht (1727) reviewed the evidence supporting the roles of various classes of tobacco smoke components in cancer induction by tobacco smoke. They concluded that PAHs and NNK are the major carcinogens involved in lung cancer induction by cigarette smoke. In their 1990 publication, they stated: "These exposure estimates [for benzo[*a*]pyrene] and the determinations of the tumorigenic potential of [polycyclic aromatic hydrocarbons] in bioassays strongly suggest that [polycyclic aromatic hydrocarbons] play a significant role in the induction of respiratory tract cancer in smokers… Human exposure to [4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)] is consistent with its potential role as a causative agent for lung cancer… These calculations [relating smoker exposure to 4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK) to dose level needed to induce respiratory tract tumors in hamsters], which ignore the probable endogenous formation of [4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)…], point to a significant risk for the smoker and strongly support the role of [4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)] as an important etiological factor in lung cancer."
	However, they also noted: "The organospecificity of [4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)] for the lung is consistent with its role in tobacco smoke-induced respiratory carcinogenesis. The lung is the main target organ for [4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)] administered [per os] or [subcutaneously] to rats and hamsters… Lung tumors[a] have also been induced in mice after topical applications of high doses of [4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)]… It has not been tested by inhalation."
1990	In their list of 43 "tumorigenic agents in tobacco and tobacco smoke," a list cited frequently in reports issued by various governmental agencies (EPA, USPHS), Hoffmann and Hecht (1727) listed three TSNAs: NNN, NNK, and NAB, the same three listed previously in 1986 by Hoffmann and Wynder (1808) and IARC (1870) and subsequently by Hoffmann et al. (1740, 1741, 1743, 1744, 1773)
1991	In the introduction to their publication on lung and pancreatic cancer, Hecht and Hoffmann (1571a) reiterated their previous conclusion on the role of PAHs and NNK in cancer causation in tobacco smokers: "Polynuclear aromatic hydrocarbons and NNK [4-(N-methyl-nitrosamino)-1-(3-pyridinyl)-1-butanone] are the major carcinogens involved in lung cancer induction by cigarette smoke and that NNK [4-(N-methylnitrosamino)-1-(3-pyridinyl)-1-butanone] is a likely candidate for induction of pancreatic cancer in smokers."
1992	Mimicking intragastric conditions, Caldwell et al. (575, 576) studied nicotine *N*-nitrosation and found it to be extremely slow. They concluded: "It is unlikely that nicotine itself contributes to exposure to nitroso compounds [*N′*-nitrosonornicotine (NNN), 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-1-butanal, and 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)] due to chemically mediated intragastric nitrosation."
	Caldwell et al. confirmed, in part, the 1988 findings of Tricker et al. (3945) who had previously studied the potential endogenous formation of TSNAs under conditions simulating normal human gastric conditions

TABLE 15.4 (continued)
A Brief Chronology of the Research on TSNAs

Year	Investigation
1991–1992	Brunnemann et al. (459, 460) sampled indoor air in bars, restaurants, and trains; the levels found for NNN ranged from 0 to 23 pg/L; for NNK, 1–29 pg/L; for NAT, 0–9 pg/L
1992	In 1992, Chung et al. (793a) demonstrated that components, e.g., phenethyl isothiocyanate, indole-3-carbinol, in green tea and cruciferous vegetables inhibited lung tumorigenesis induced by NNK
1992	Klus et al. (4711) described the level s of TSNAs in ETS
1993	Carmella et al. (15A05) identified 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanol (NNAL) and its glucuronide in the urine of cigarette smokers, thus providing the first evidence for metabolites of TSNAs in human urine. No NNK was detected. Results with smokers' urine were consistent with those found previously with monkeys' urine
1993	Hoffmann et al. (1773) again cited the list of 43 tumorigens in tobacco and smoke from Hoffmann and Hecht (1727). Despite the fact that in 1991, Hecht and Hoffmann (1571a) concluded that "polynuclear aromatic hydrocarbons and NNK [4-(*N*-methyl-nitrosamino)-1-(3-pyridinyl)-1-butanone] are the major carcinogens involved in lung cancer induction by cigarette smoke and that NNK is a likely candidate for induction of pancreatic cancer in smokers," they listed NNK, NNN, and NNAL in this publication only as "likely causative agents for tobacco-related cancers."
1993	Castonguay (15A07) described the inhibition in A/J mice of NNK-induced lung tumorigenesis by ellagic acid, a polyphenolic dilactone
2006	Stepanov et al. (5566) listed the levels of TSNAs in smokeless tobacco products
2007	Chwoidak et al. (4547) described an improved LC/MS/MS method for the determination of TSNAs in tobacco and tobacco-related products
2007	The influence of curing on TSNA production in dark fire-cured tobacco was outlined by Bailey (4991)
2008	Moldoveanu and Borgerding (5008) outlined the formation of TSNAs in cigarette MSS
2009	Wang et al. (5091) described the control of TSNAs in cigarette MSS by a filter-tip additive
2010	Zhu et al. (5589) reported the control of TSNAs in cigarette MSS by a filter-tip additive
2010	The effect of agronomy and curing of burley tobacco on its TSNA content was described by Peek et al. (5550)
2010	Suzuki et al. (5569) reported the control of TSNAs and NO_x in tobacco smoke by nitrate control
2010	Yoshida et al. (5584) outlined an improved analytical method for the determination of TSNAs in cigarette MSS, cf. their report with that of the 2009 presentation by Mathis and Yeung (5063)

[a] The tumor type was the adenoma, not the squamous cell carcinoma supposedly associated with cigarette smoking in smokers.

and the common TSNAs, the following *N*-nitrosamino acids were identified: 4-(*N*-methylnitrosamino)-4-(3-pyridinyl) butanoic acid (*iso*-NNAC), NMBA, NMPA [*N*-methyl-*N*-nitroso-β-alanine], 2-(methylnitrosamino)acetic acid [*N*-methyl-*N*-nitrosoglycine, *N*-nitrosarcosine] (NSAR), 1-nitroso-2-piperidinecarboxylic acid, and NPRO. Djordjevic et al. considered these NNA compounds important in cancer causation, particularly in snuff and chewing tobacco users. Djordjevic et al. (992) confirmed the findings of Ohshima et al. (2852) on the presence of *N*-nitrosamino acids in tobacco. In addition to the *N*-nitrosamino acids identified by Ohshima et al., Djordjevic et al. identified 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-1-butanoic acid (*iso*-NNAC). The highest concentrations of these *N*-nitrosamino acids were found in snuffs and black tobacco. They also identified NMPA in tobacco and MSS and estimated its transfer from tobacco to MSS to be 0.85%.

In studies with *N*-nitrosamino-acid-spiked cigarettes, Brunnemann et al. (466) reported that added NMPA did not completely decarboxylate. Some was esterified to the methyl ester. Some of the intact acid, its methyl ester, and its decarboxylation product, NEMA, appeared in the MSS. Similarly with NMBA, some NMBA transferred intact from the tobacco to the MSS, some formed the methyl ester which appeared in the MSS, and some decarboxylated to yield *N*-nitrosomethylpropylamine which also appeared in the MSS. NPRO primarily decarboxylated to NPYR. NSAR primarily decarboxylated to NDMA.

Djordjevic et al. (1012) identified *iso*-NNAC in tobacco and in MSS. This acid was found only in the MSS from cigarettes containing tobacco spiked (2 mg/cig) with cotinine. From the results of *in vitro* nitrosation studies with radiolabeled cotinine and nicotine, Djordjevic et al. (995) proposed that the formation of *iso*-NNAC in tobacco proceeds *via* cotinine and its hydrolysis product 4-methyl-4-(3-pyridinyl)-1-butanoic acid rather than via nicotine.

Brunnemann et al. (464) presented a more detailed exposition of their 1989 findings on the fate in "spiked" cigarettes of several *N*-nitrosamino acids [NSAR, NMPA, NMBA, NPRO]. These acids are delivered intact to MSS, undergo esterification to the methyl ester and are delivered as such to MSS, and/or decarboxylate and are delivered to MSS as the NNAs NDMA, NEMA, NMPA, and NPYR, respectively.

Djordjevic et al. (1013) described in greater detail their identification of *iso*-NNAC in tobacco and in MSS. They reported that *iso*-NNAC was found only in the smoke from cigarettes containing cotinine-spiked tobacco (2 mg/cig) (*cf.* Djordjevic et al., 1989b). Djordjevic et al. (1005, 1008) identified three new *N*-nitrosamino acids

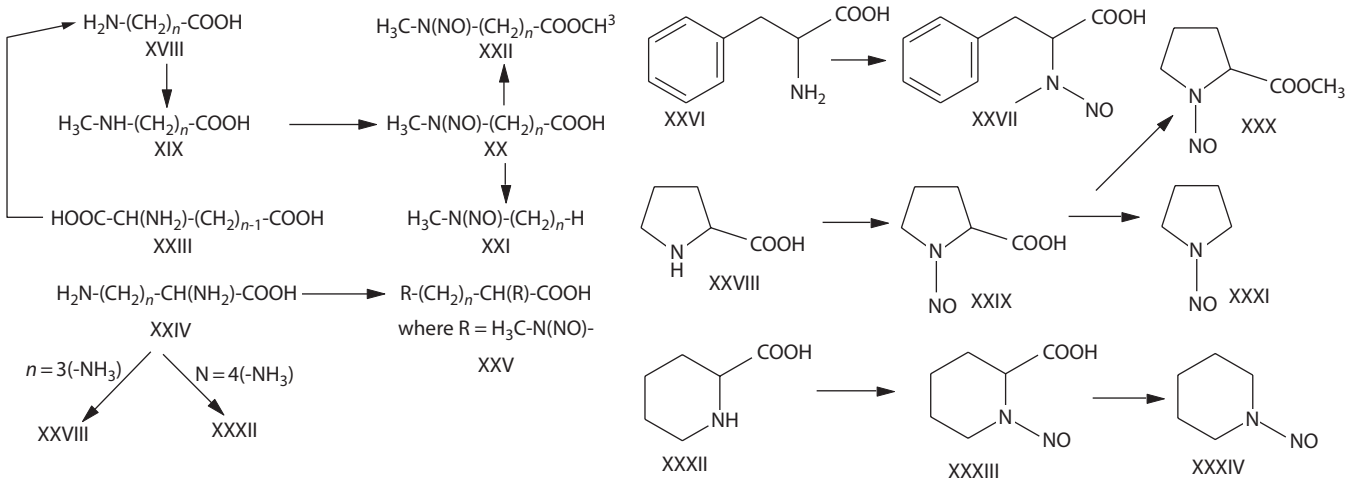
Ref. No.	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993–1994	1995–1996	1997–1998	1999–2000	2001–2002	2003–2004
									15A56							
									15A20							
							15A19	**15A06**	**15A03**							
							3954	**3181**	**4405**							
							3948	**2995**	3944							
							3374	**1770**	**3182**							
	15A22[a]						3373	**1688**	**2994**							
	15A16				**15A44**		2917b	1198	2235						15A45	
	15A08				15A34		2674	1197	1771						4128	
	3179				15A04		**1676**	1193	**1750**						4077	
	2728	15A43			656		1196	1191	**1571a**	3953					3943b	
	1724	**15A27**			**469**		1195	1036	1200	**2168**				3342	3816	
	1559	**15A17**			379	3947	1194	**1014**	1199	**1777**	15A05			2916	3176a	4129
	1558	**3184**	2852		324	3945	1192	**995**	**1013**	**1005**	3177			2915	2917	3343
	1003	2990	**1746**		70	3184	**1012**	720	**486**	739a	**2996**			2637	1305	2700
	667	2441	**1725**	**15A23**	67	**3180**	**1002**	573	**484**	549	**2992**	4161		**2561**	1304	2638
	650	2437	728	**15A21**	65	2436	573	484	**464**	542	**1702**	**2997**		2051	951	2618
	99	**1696**	**595**	2559b	64	**1571**	547	**483**	459	**501**	**1573a**	**2993**		1988	557	2588
	98	**1694**	**468**	657	63	572	543	326	325	**487**	**1562a**	**1775**	2943a	1016	**505**	2362
	29	660	**26**	99	62	**508**	**466**	205	202	**463**	554	502	**2169**	**1011**	279	2052
	22	**25**	**24**	**36**	**33**	**19**	204	201	**76**	**460**	313	**59**	**1001**	670	50	507

Year

Reference numbers listed in bold print represent conference presentations and/or journal publications by Hoffmann and his American Health Foundation colleagues.

[a] References listed as 15A22, etc., may be found at the end of the chapter in the list of additional references to Chapter 15.

FIGURE 15.3 References pertinent to TSNAs, 1983–2004.



Legend

Aliphatic Compounds

No.	*n* = 1	*n* = 2	*n* = 3	*n* = 4
XVIII	Glycine [2-aminoacetic acid]	β-Alanine [3-aminopropanoic acid]	4-Aminobutanoic acid	
XIX	Sarcosine [*N*-methylaminoacetic acid]	3-(*N*-Methylamino)-propanoic acid	4-(*N*-Methylamino)-butanoic acid	
XX	2-(Methylnitrosamino)-acetic acid (NSAR) [*N*-nitrosarcosine]	3-(Methylnitrosamino)-propanoic acid (NMPA)	4-(Methylnitrosamino)-butanoic acid (NMBA)	
XXI	*N*-Nitrosodimethylamine (NDMA)	*N*-Nitrosoethyl-methylamine (NEMA)	*N*-Nitrosomethylpropyl-amine	
XXII	2-(Methylnitrosamino)-acetic acid, methyl ester	3-(Methylnitrosamino)-propanoic acid, methyl ester	4-(Methylnitrosamino)-butanoic acid, methyl ester	
XXIII			Glutamic acid	
XXIV			Ornithine [2,5-diaminopentanoic acid]	Lysine [2,6-diaminohexanoic acid]
XXV			2,5-Di-(methylnitrosamino)pentanoic acid	2,6-Di-(methylnitrosamino) hexanoic acid

Aromatic and Heterocyclic Compounds

XXVI	2-Amino-3-phenylpropanoic acid [phenylalanine]	XIX	NPRO [1-nitroso-2-pyrrolidinecarboxylic acid]	XXXII	2-Piperidinecarboxylic acid [pipecolic acid]
XXVII	2-(Methylnitrosamino)-3-phenylpropanoic acid	XXX	1-Nitroso-2-pyrrolidinecarboxylic acid, methyl ester	XXXIII	1-Nitroso-2-piperidinecarboxylic acid
XXVIII	2-Pyrrolidinecarboxylic acid [proline]	XXXI	*N*-Nitrosopyrrolidine (NPYR)	XXXIV	*N*-Nitrosopiperidine (NPIP)

FIGURE 15.4 Relationships among amino acids, *N*-nitrosamino acids, their esters, and NNAs.

in snuff tobacco: 2-(methylnitrosamino)-3-phenylpropanoic acid, 2,5-di(methylnitrosamino)pentanoic acid, and 2,6-di(methylnitrosamino)hexanoic acid. They discussed not only the identification of the three new *N*-nitrosamino acids but also the carcinogenic potential of these and other *N*-nitrosamino acids, particularly in the context of tobacco chewing or snuff dipping.

Djordjevic et al. (993) reported that the levels of *N*-nitrosamino acids in snuff tobaccos were often 150 times those found in cigarette tobaccos (usually about 1 ppm).

Examination of the results of the studies on *N*-nitrosamino acids in tobacco smoke reveals the importance of amino acids (and their precursors, the tobacco proteins) in *N*-nitrosamino acid formation before and during the smoking process. Figure 15.4 illustrates some of the relationships among the amino acids, *N*-nitrosamino acids, their methyl esters, and NNAs.

15.5 TOBACCO-SPECIFIC NNAs: AN EXCEPTION AMONG THE MAJOR MSS TOXICANTS

Since the mid-1950s, various MSS toxicants, either as an individual component or a class of components, have had their moment of publicity, but one by one, their importance

gradually faded. Chronologically, the first toxicants to become infamous were the tumorigenic PAHs with B[*a*]P at the pinnacle because of its potent tumorigenicity to mouse skin and its per cigarette MSS yield. The chronology of the rise to notoriety of the various individual and/or class of toxicants has been previously depicted [see Figure 1 in Rodgman et al. (3307)] but not shown is when the prominence of most of them declined.

In the mouse-skin-painting bioassay, neither B[*a*]P nor the total tumorigenic PAHs accounted for the observed specific tumorigenicity (4354). The B[*a*]P content of CSC accounted for less than 2.5%, and the total tumorigenic PAH content of CSC accounted for less than 3.5% of the CSC specific tumorigenicity [1056, 4312, see p. 626 in (4332)]. Inclusion of tumorigenic aza-arenes reported by Van Duuren et al. (4027) did not improve the situation. Hoffmann and Wynder (1798) reported that doubling or tripling the level of 17 tumorigenic PAHs in CSC significantly increased the % TBAs, whereas others reported that a 10-fold (3311) or 30-fold (2320) increase in the B[*a*]P level in CSC produced no change in the % TBA. In the early 1960s, the promoting effect of MSS phenols on tumorigenic PAHs was advanced to explain the tumorigenic response observed in CSC-painted mice. Inclusion of this effect in the assessment accounted for about 5% of the % TBA. In addition, reports of no change in the tumorigenicity of CSC when significant amounts (75%–90%) of the phenols were removed from MSS (and the CSC) by selective filtration [see p. 626 in (55), 4344] and the inhibition of the specific tumorigenicity of B[*a*]P by phenol (149) diminished the alleged importance of the promoting effect of phenols.

To offset the decrease in importance of the PAHs, aza-arenes, and phenols, ciliastatic components in MSS then became the in-vogue toxicants. It was asserted, based on studies with clam cilia and mammalian ciliated tissue, that certain MSS toxicants impair lung ciliary activity thus preventing removal of tumorigen-containing smoke particles from the lung. MSS components proposed as significant ciliastats included formaldehyde, acetaldehyde, acrolein, HCN, formic and acetic acids, and phenol. However, after the reported findings of Dalhamn et al. in 1968, the ciliary assertion faded because of the demonstration that less than a third of the ciliastats reach the lung cilia in human smokers (892, 893).

In the mid-1960s, several other MSS toxicants had their brief moment of infamy, e.g., ^{210}Po, NO_2, CO, Ni. In their comparison of lung cancer incidence in uranium miners exposed to ^{210}Po *vs*. cigarette smokers exposed to MSS ^{210}Po, Harley et al. (75) questioned the significance of ^{210}Po in tobacco-induced lung cancer. Concern over NO_2 diminished with the demonstration that over 95% of the NO_x in MSS was NO, not NO_2, and the conversion of NO to NO_2 was impeded by other MSS components (94).

In the early 1960s, the formation of NNAs during tobacco smoking was suggested (423) as well as the possible presence of NNN and NAB in MSS (423, 3313). Between 1964 and the early 1970s, several volatile NNAs were identified in MSS. It was also reported that 60%–85% of the volatile NNAs, like the phenols, are selectively filtered from MSS (514, 1236, 1761, 2635). The identification of several TSNAs, including NNN and NAB, then followed.

Why have TSNAs maintained their status as important MSS toxicants while the importance of other individual and/or classes of toxicants has faded?

Alternate exposures are possible with other toxicant classes including NNAs other than the TSNAs, but the TSNAs, as defined, are "tobacco-specific." In other words, no alternate exposure exists for TSNAs. In the detailed 1984 outline of chemical carcinogenesis edited by Searle (3568), the only class of MSS tumorigens discussed in 22 chapters comprising nearly 1400 pages was the NNAs [see pp. 839–844 in Preusmann and Eisenbrand (2990)]. Most of the data cited [see Tables VII through IX, pp. 841, 843, 844 in (2990)] are those from publications by Hoffmann et al. (514, 1677, 1680, 1685).

Since the early 1960s, a "less hazardous" cigarette has been defined on the basis of three criteria: (1) the per cigarette delivery of a specific toxicant has been lowered, (2) the ratio of the specific toxicant to MSS "tar" has been lowered, and (3) the specific tumorigenicity of the MSS "tar" as measured in the mouse-skin-painting bioassay has been lowered.

From bioassay results of more than 330 NNAs plus knowledge of fewer than 60 specific NNAs in MSS, it is obvious that the MSS NNAs cannot meet criterion 3. Over 330 *N*-nitroso compounds variously administered to 40 different species have been reported as tumorigenic. No laboratory species is resistant to NNAs. In their summary of the results from 323 *N*-nitroso compounds bioassayed from 1956 to 1984, Preussmann and Stewart (2991) reported that 87% of the *N*-nitroso compounds are tumorigenic. Over 70% of the *N*-nitroso compounds studied were NNAs; the remainder was *N*-nitrosamides.

Administration of most NNAs to laboratory animals via skin painting seldom results in carcinoma induction at the application site. Generally, tumors develop at site(s) remote from the painting site, and various organs may be involved. This major difference between PAH and NNA tumorigenicity led to defining NNAs as organ-specific tumorigens. Failure to produce tumors with NNAs at the painting site subsequently led to studies of NNAs administered by alternate routes (injection [subcutaneous, intravenous, intraperitoneal], per os, intratracheal instillation, etc.). Administration of NNAs by inhalation was studied infrequently.

Skin-painting studies with six NNAs (*N*-nitrosobutylmethylamine, NDEA, NDELA, *iso*-NNAL, NNK, NNN) present in tobacco and/or tobacco smoke were reported by Brune and Henning (15A02), F. Hoffmann and Graffi (15A30), Herrold (15A24), Herrold and Dunham (15A25), IARC (1870), Hoffmann et al. (1786a), and LaVoie et al. (15A34). Tumors developed elsewhere in the test animals but none at the painting site. In a painting study by Deutsch-WenzeL et al. (956a), NNN induced a few skin tumors, but

no dose–response relationship was observed over a 12.5–200 µg range. In the same study, the tumorigenic potency to skin of *N*-nitroso-*N*-methylurea was estimated to be about 4% of that of B[*a*]P. In painting studies with *N*-nitroso-*N*-alkylureas, tumors did develop at the skin-painting site, but to date, no *N*-nitroso-*N*-alkylurea has been identified in tobacco or MSS.

15.6 DIRECT TRANSFER OF TSNAs FROM TOBACCO *VS.* THEIR FORMATION DURING THE SMOKING PROCESS

Nicotine, nornicotine, anabasine, and anatabine are precursors of TSNAs in tobacco and tobacco smoke (29, 1564). Both nicotine and nornicotine are considered to be NNN precursors. Since NNAs (both volatile and tobacco-specific) occur in tobacco, part of the NNAs in cigarette MSS was reported to be due to direct transfer of NNAs from tobacco to MSS, the remainder due to formation and transport during the smoking process (201). For NNK, the transfer from tobacco to MSS ranges from 6.9% to 11.0% of the amount in the tobacco; this represents about 30% of the NNK in MSS. Similarly, about 40% of the NNN in MSS is transferred from the tobacco. Hoffmann et al. maintain that the remainder of NNN and NNK in MSS is formed during the smoking process (1558, 1734). Both the levels of volatile NNAs and TSNAs in MSS are proportional to the nitrate content of the tobacco filler (3985). However, the premise of the pyrogenesis of NNN and NNK has been challenged by Fischer et al. (1193, 1199) who reported that these compounds occur in cigarette MSS only by transfer from the tobacco rod. Castonguay (15A07) stated that NNK is transferred from tobacco to smoke during the smoking process. In agreement with Fischer et al., Renaud et al. (15A46) concluded that direct tobacco-to-smoke transfer was the dominant factor explaining the presence of TSNAs in MSS. From their study of the contribution of ^{13}C-nicotine to ^{13}C-NNN and ^{13}C-NNK levels in MSS CSC, Moldoveanu et al. concluded that NNN and NNK are generated during the smoking process (2599), thus contradicting the views of Fischer et al. (1193, 1199), Castonguay (15A07), and Renaud et al. (15A46). Moreover, the pyrogenesis situation was further clouded by data on the effect of tobacco nitrate on the MSS TSNA yields (1552). Analysis of MSS TSNAs indicated that NNN and NAT yields increased when nitrate was added to the tobacco but the NNK yield did not.

15.7 INFREQUENTLY STUDIED TOBACCO AND/OR TOBACCO SMOKE SECONDARY AMINES AND THEIR *N*-NITROAMINES

During extensive investigations of the composition of tobacco smoke in general and cigarette MSS in particular, much effort was expended in the early 1960s to define the nature of *N*-nitrosation during curing and the smoking process. As more and more NNAs were identified in tobacco and/or tobacco smoke, they were categorized as follows: volatile NNAs, nonvolatile NNAs, TSNAs, and *N*-nitrosamino acids. Within these four categories, only about 60 NNAs have been identified to date as tobacco and/or tobacco smoke components. Except for an excursion into the identification of *N*-nitrosamino acids, identification of NNAs in MSS almost ceased when NNK and to some extent NNN became the toxicants of choice. This situation raises the question: If a detailed study similar to those conducted on the PAHs and aza-arenes were conducted, how many additional NNAs could be identified in tobacco and/or tobacco smoke?

Table 15.5 lists several NNAs reported as tobacco components that are seldom discussed. To date, none of them have been identified in tobacco smoke.

While Table 15.6 is not necessarily complete, it suffices for the following discussion: In Table 15.6 are listed 22

TABLE 15.5
NNAs in Tobacco and/or Tobacco Smoke

		Identified in Smoke (S) and/or Tobacco (T)		
NNAs	CAS No.	S	T	Activity
1-Nitroso-2-azetidinecarboxylic acid	55556-98-4	–	+	
4-(*N*-Methylnitrosamino)-1-(3-pyridinyl) butanone oxide	76014-82-9	–	+	Yes[a]
1-Nitroso-4-hydroxyproline	2443-30-3	–	+	
1-Nitroso-3-piperidinecarboxylic acid	65445-62-7	–	+	
1-Nitroso-4-piperidinecarboxylic acid	6238-69-3	–	+	No [173][b]
3-Nitroso-4-thiazolidinecarboxylic acid	88381-44-6	–	+	

[a] Bioassay results reported by Castonguay et al. (15A08).

[b] Bioassay results in laboratory animals are summarized in Preussmann and Stewart (2991); yes, tumor induction; no, negative response. Number in [] represents catalog number in Preussmann and Stewart (2991).

TABLE 15.6
Aliphatic Secondary Amines and VNAs in Tobacco and Tobacco Smoke

R_1-N(R)-R_2		R = H			R = NO			
		Identified in Smoke (S) or Tobacco (T)			Identified in Smoke (S) or Tobacco (T)			
R_1 =	R_2 =	CAS No.	S	T	CAS No.	S	T	Biological Activity
CH_3-	CH_3-	124-40-3	+	+	62-75-9[a]	+	+	Yes [1][b]
CH_3-	CH_3CH_2-	624-78-2	+	+	10595-95-6[a]	+	+	Yes [52][b]
CH_3-	$CH_3(CH_2)_2$-	627-35-0	+	+	924-46-9	+	+	Yes [66][b]
CH_3-	$(CH_3)_2CH$-	4747-21-1	+	+		+	–	
CH_3-	$CH_3(CH_2)_3$-	110-68-9	+	+	7068-83-9[a]	+	–	Yes [71][b]
CH_3-	$(CH_3)_2CHCH_2$-		–	–	2504-18-9	+	–	
CH_3-	$(CH_3)(C_2H_5)CH$-		+	–		–	–	
CH_3-	$(CH_3)_2CH(CH_2)_2$-		+	–		–	–	
CH_3-	$CH_2 = C(CH_3)$-	22023-64-9	+	–		–	–	
CH_2CH_3-	CH_2CH_3-	109-89-7	+	+	55-18-5[a]	+	+	Yes [7][b]
CH_2CH_3-	$CH_3(CH_2)_2$-	20193-20-8	–	–	25413-61-0	+	+	
CH_2CH_3-	$(CH_3)_2CHCH_2$-		–	–	71607-99-3	+	+	
CH_2CH_3-	$CH_3(CH_2)_3$-	13360-63-9	–	–		+	–	Yes [122][b]
$CH_3(CH_2)_2$-	$CH_3(CH_2)_2$-	142-84-7	+	+	621-64-7[a]	+	+	Yes [21][b]
$CH_3(CH_2)_2$-	$(CH_3)_2CH$-	21968-17-2	+	+		–	–	
$CH_3(CH_2)_2$-	$(CH_3)(C_2H_5)CH$-		+	–		–	–	
$(CH_3)_2CH$-	$(CH_3)_2CH$-	108-18-9	+	–	601-77-4	+	–	Yes [34][b]
$(CH_3)_2CH$-	$CH_3(CH_2)_3$-	39099-23-5	+	–		–	–	
$CH_3(CH_2)_3$-	$CH_3(CH_2)_3$-	111-92-2	–	+	924-16-3[a]	+	+	Yes [36][b]
$CH_3(CH_2)_3$-	$(CH_3)_2CHCH_2$-	20810-06-4	+	–		+	–	
$(CH_3)(C_2H_5)CH$-	$(CH_3)(C_2H_5)CH$-	626-23-3	–	+		–	–	Yes [45][b]
$(CH_3)_3C$-	$(CH_3)_2CH$-		+	–		–	–	

[a] Compound listed as a toxicant in one or more lists published since 1986 (1217, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1870, 2825).

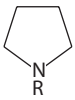
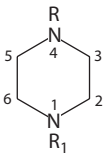
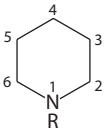
[b] Bioassay results in laboratory animals are summarized in Preussmann and Stewart (2991); yes, tumor induction; no, negative response. Number in [] is catalog number in Preussmann and Stewart (2991).

dialkylamines, identified in tobacco and/or smoke as the amine or the NNA. For four NNAs (*N*-nitrosoisobutylmethylamine, *N*-nitrosoethylpropylamine, *N*-nitrosoethylisobutylamine, and *N*-nitroso-*n*-butylethylamine), the corresponding amines have not been identified in tobacco smoke. It is highly probable that the four amines are present as MSS components. Alternatively, NNAs corresponding to the other 10 dialkylamines identified in tobacco and/or tobacco smoke have not yet been identified in smoke; e.g., no NNA corresponding to *sec*-butylmethylamine, isopentylmethylamine, or isopropylidenemethylamine identified as MSS components has been identified in MSS. Synthetically, the corresponding NNAs are as easily prepared as *N*-nitrosodimethylamine or *N*-nitrosodiethylamine, so their pyrogenesis during the smoking process should not be hindered. Thus, it is highly probable that the 10 NNAs are present in tobacco smoke.

Many other secondary amines have been identified in tobacco smoke, but for most of them, no corresponding NNA has been identified in smoke. These include a series of *N*-substituted anilines, all amenable to *N*-nitrosation {XXXV}. Others include the alkyl derivatives of pyrrolidine {XXXVI}, piperazine {XXXVII}, and piperidine {XXXVIII}. The amines pyrrolidine {XXXVI}, piperazine {XXXVII}, and 1,2,3,6-tetrahydropyridine {XXXIX} have been identified in cigarette MSS but not piperazine {XXXVII} (see structures in Table 15.7). For each piperazine, mono- and di-*N*-nitroso derivatives are possible. Morpholine {XL} and an alkyl derivative have also been identified in tobacco. For completeness, azetidine {XLI} is included in Table 15.7. In many instances, the NNAs listed in Table 15.7 are readily synthesized and have been tested for tumorigenicity in laboratory animals [see Preussmann and Stewart (2991)].

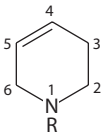
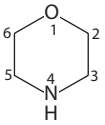
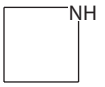
Table 15.7 lists 46 secondary amines, most of which have been identified as components of tobacco and/or its smoke. In only a few cases have the corresponding NNAs been identified as tobacco and/or smoke components.

TABLE 15.7
Aromatic and Cyclic Secondary Amines and NNAs in Tobacco and Tobacco Smoke

Amine		R = H			R = NO			
		Identified in Smoke (S) or Tobacco (T)			Identified in Smoke (S) or Tobacco (T)			Biological Activity
R_1 =	R_2 =	CAS No.	S	T	CAS No.	S	T	
Aromatic amine {XXXV} R_1-N< R R_2		R = H			R = NO			
CH_3-	C_6H_5-	100-61-8	+	–	614-00-6	+	+	Yes [108][a]
CH_3-	2-CH_3-C_6H_4-	611-21-2	+	–		–	–	
CH_3-	4-CH_3-C_6H_4-	623-08-5	+	–		–	–	
CH_3-	2-C_2H_5-C_6H_4-	1821-38-1	+	–		–	–	
CH_3-	3-C_2H_5-C_6H_4-	71265-20-8	+	–		–	–	
CH_3-	4-C_2H_5-C_6H_4-	37846-06-3	+	–		–	–	
CH_3-	C_6H_5-$(CH_2)_2$-	589-08-2	+	–		–	–	
CH_3-	4-NH_2-C_6H_4-		+	–		–	–	
C_2H_5-	C_6H_5-	103-69-5	+	–	612-64-6	–	–	
C_2H_5-	2-CH_3-C_6H_4-	94-68-8	+	–		–	–	
C_6H_5-	C_6H_5-	122-39-5	+	–	86-30-6	+	–	No [55][a]
C_6H_5-	4-$(CH_3)_2CH$-C_6H_4-	5650-10-2	+	–		–	–	
Pyrrolidine {XXXVI}		123-75-1	+	–	930-55-2	+	–	Yes [146][a]
2-CH_3-		765-38-8	+	+		–	+	
3-CH_3-		34375-89-8	+	–		–	–	
2,4-diCH_3-		13603-04-8	+	–		–	–	
2,5-diCH_3-		3378-71-0	+	–	55556-86-0	–	–	Yes [148][a]
2-CH_3CH_2-		1003-28-7	+	–		–	–	
2-COOH		147085-3	+	+	7519-36-0	+	+	
2-$COOCH_3$			–	–		+	+	
2-keto-		616-45-5	+	+		–	–	No [301][a]
2-keto-3-CH_3-		2555-05-7	+	–		–	–	
2-keto-4-CH_3-		2996-58-9	+	+		–	–	
2-keto-5-CH_3-		108-27-0	+	–		–	–	No [302][a]
Piperazine {XXXVII}		110-85-0	–	–	5632-47-3	–	–	Yes [200][a]
					140-79-4[b]	–	–	Yes [207][a]
1-CH_3-		109-01-3	+	–	16339-07-4	–	–	Yes [201][a]
2-CH_3-		109-07-9	+	–	55556-94-0	–	–	Yes [208][a]
2,5-diCH_3-		106-55-8	+	–	55556-88-2[b]	–	–	Yes [209][a]
Piperidine {XXXVIII}		110-89-4	+	+	100-75-4	+	+	Yes [160][a]
2-CH_3-		109-05-7	+	–	7247-89-4	–	–	Yes [174–176][a,c]
3-CH_3-		626-56-2	+	–	13603-07-1	–	–	Yes [177][a]
4-CH_3-			–	–		+	–	Yes [179][a]
2-COOH		535-75-1	+	–	4515-18-8	+	–	No [172][a]
3-COOH			–	–	65445-62-7	+	–	

(*continued*)

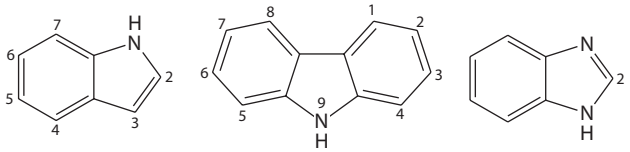
TABLE 15.7 (continued)
Aromatic and Cyclic Secondary Amines and NNAs in Tobacco and Tobacco Smoke

Amine		R = H			R = NO			
		Identified in Smoke (S) or Tobacco (T)			Identified in Smoke (S) or Tobacco (T)			Biological Activity
R_1 =	R_2 =	CAS No.	S	T	CAS No.	S	T	
4-COOH			–	–	6238-69-3	+	–	No [173][a]
2,3-diCH_3-		23513-39-5	+	–		–	–	
2,4-diCH_3-		6287-19-0	+	–		–	–	
2,6-diCH_3-		504-03-0	+	–	17721-95-8	–	–	No [180][a]
2-C_2H_5-		1484-80-6	+	–		–	–	
2-$(CH_3)_2$CH-			+	–		–	–	
2-keto-6-CH_3-		4775-98-8	+	–		–	–	Yes [178][a]
4-keto-2,6-diCH_3- (*Z*)-		13200-35-6	+	–		–	–	
4-keto-2,6-diCH_3- (*E*)-		69135-98-4	+	–		–	–	
Pyridine, 1,2,3,6-tetrahydro- {XXXIX}		694-05-3	+	+		–	–	Yes [168][a]
Morpholine {XL}		110-91-8	–	+	59-89-2	+	+	Yes [192][a]
2,2-diCH_3-		147688-58-2	–	+		–	–	
Azetidine {XLI}		503-29-7	+	+	55556-98-4	–	+	

[a] Bioassay results in laboratory animals are summarized in Preussmann and Stewart (2991); yes, tumor induction; no, negative response. Number in [] is catalog number in Preussmann and Stewart (2991).

[b] *N,N′*-Dinitroso derivative, i.e., R = R_1 = NO.

[c] The *cis*- and *trans*-isomers were tested individually as well as mixture of them.



XLII XLIII XLIV

FIGURE 15.5 Indole {XLII}, carbazole {XLIII}, and 1*H*-benzimidazole {XLIV}.

It is highly probable that the NNAs corresponding to the remaining secondary amines may also be tobacco smoke components.

Among the numerous classes of smoke components are several other types of secondary amines, e.g., the pyrroles, indoles, carbazoles, and imidazoles. However, their highly aromatic nature and the acidity of the imino hydrogen probably preclude any significant *N*-nitrosation either in the tobacco or during the smoking process. Despite the fact that a dozen or so theoretically *N*-nitrosatable substituted pyrroles; nearly 50 alkyl derivatives of indole {XLII}; carbazole {XLIII} and several of its alkyl derivatives, benzocarbazoles, and dibenzocarbazoles; and several alkyl derivatives of imidazole and benzimidazole {XLIV} have been identified in

tobacco smoke, no NNA corresponding to any of them has been identified to date in tobacco smoke (Figure 15.5).

It is obvious that the number of NNAs in tobacco and/or tobacco smoke might be substantially greater than the 60 or so NNAs now known to be present. Since the per cigarette yields of the yet unidentified NNAs may be at the picogram or femtogram levels, their contribution to MSS toxicological properties may not be particularly meaningful or important. However, they may be just as important from a biological point of view as those MSS components repeatedly listed as toxicants for which no or questionable quantitative data are available, e.g., the much discussed dibenzo[*def*,*p*]chrysene (dibenzo[*a,l*]pyrene) (1557, 1727, 1740, 1741, 1743).

To put the NNAs in perspective and to determine how many more are actually present in MSS, what may be needed is an extensive study corresponding to the excellent studies on PAHs (3756–3758) and aza-arenes (3750) conducted and reported by U.S. Department of Agriculture (USDA) personnel in the late 1970s and early 1980s.

It is also interesting to note that 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL), the major metabolite of NNK (1557), is usually not listed as a cigarette MSS toxicant even though NNAL has been reported to be both tumorigenic to several rodent species (15A08) and mutagenic in the Ames *S. typhimurium* test.

15.8 FLUE CURING AND TSNAs

As described by Williams (4247), there is general agreement among tobacco scientists that TSNAs are not present in either freshly harvested, i.e., green flue-cured and burley tobaccos. As the tobaccos are cured either by air curing in the case of burley or in heated barns for flue-cured varieties, the amounts of TSNAs rise to their final levels. In the case of air curing, the process has changed little over the past 50 years. However, for flue curing, the process changed drastically in the United States during the 1960s and 1970s due to the introduction of energy-efficient bulk-curing barns heated by exhaust gases of liquid propane gas or similar burners. It is at this point that a breakdown must have occurred between tobacco agriculturists and chemists. The emission of NO_2 during the combustion of liquid propane or natural gas is well known. In fact, the North Carolina Department of Environment and Natural Resources (NCDENR) has electronic spreadsheets available for download from its website that North Carolina industries may use in estimating their NO_2 emissions during natural gas or liquid propane combustion. In retrospect, any competent chemist would predict the potential nitrosation of tobacco alkaloids during flue curing in the presence of combustion exhaust gases. However, without the knowledge of TSNA formation during direct heating of green tobaccos, the agricultural community adopted the new energy-efficient technique. It appears that prior to this "technological advance," the formation of TSNAs during flue curing by traditional methods was not a problem.

Earlier, at least two research groups discovered the problem with direct heating flue curing of tobacco. Peele et al. (2917) demonstrated that modification of the curing process for flue-cured tobacco permitted significant control of its TSNA levels. The curing process was altered from one involving direct fired burners to one involving a heat exchange system. During approximately the same period, Williams (258) applied for and was granted a U.S. patent on essentially the same modification of the flue-curing barns to achieve the same significant reduction in TSNAs. An example of the TSNA reductions in flue-cured tobacco and its smoke was shown by Rodgman and Green [see Figure 3, p. 522 in (3300)]. The tobacco data were from Williams (4247), and the smoke data were from Doolittle et al. (1051).

During the past few years, advances have been made to reduce NNAs, specifically TSNAs in tobacco and tobacco smoke. The agronomic community with the help of the tobacco industry has made significant headway in discontinuing direct heating for flue curing as a means to reduce TSNAs in tobacco and tobacco smoke. This advancement is desirable from a product stewardship perspective and has little if any effect on tobacco quality. Biological response data on individual TSNAs indicate that TSNAs play a minor role in MSS carcinogenesis [see Tables 1 and 5 in Rodgman and Green (3300)]. Comparisons of the biological effects (neutral red cytotoxicity, mutagenicity in the Ames test with several *S. typhimurium* strains) of mainstream CSCs from flue-cured tobacco cigarettes with normal and reduced levels of TSNAs indicated no significant difference between the biological activity of the two CSCs [Doolittle et al. (1051)]. Although the Doolittle et al. data appear to support the hypothesis on a whole-smoke basis that mainstream TSNAs are of relatively minor toxicological importance, the sensitivity of the Ames assay is not sufficient to differentiate between the cigarettes tested. For example, consider the following points published by Doolittle et al. (1051):

- The minimum amount of NNK needed for a mutagenic response in the Ames assay is 200 µg.
- The maximum amount of CSC that can be tested is 250 µg.
- In 250 µg of CSC, there is 1.33 and 0.13 ng of NNK from direct fired and heat exchanged flue-cured tobacco, respectively.
- The amount of NNK in the CSC from either flue-cured tobacco smoke is too low for a response.

Every practical effort should be made to reduce the amounts of alleged human carcinogens from tobacco products. However, whether the reduction or elimination of TSNAs from MSS will result in a "less hazardous" cigarette is unknown.

Table 15.8 lists the 66 NNAs identified to date in tobacco and/or tobacco smoke. Of the 66, 53 NNAs have been identified in tobacco smoke, 53 in tobacco, and 41 in both tobacco and tobacco smoke.

TABLE 15.8
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

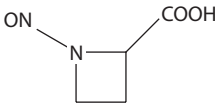
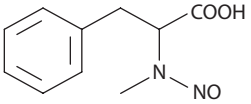
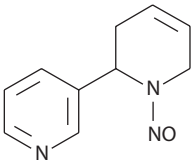
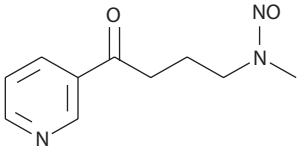
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	10478-42-9	β-Alanine, *N*-methyl-*N*-nitroso- {NMPA} {propanoic acid, 3-(methylnitrosamino)-} $H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOH$	3256, 3300, 3943a, 3944–3946, 5811b	464, 466, 485, 503, 982, 2852, 3943a, 3944–3946, 3971, 3973, 5811b	
2.	133201-38-4	β-Alanine, *N*-(nitrosomethyl)-	4249	4249	
3.		β-Alanine, *N*-methyl-*N*-nitroso-, methyl ester $H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOCH_3$	3300, 4249	4249	
4.	55556-98-4	2-Azetidinecarboxylic acid, 1-nitroso- 		486, 4249, 5811b	
5.	614-00-6	Benzenamine, *N*-methyl-*N*-nitroso-	2884	2139	
6.	86-30-6	Benzenamine, *N*-nitroso-*N*-phenyl-	746c		
7.		Benzenepropanoic acid, 2-(methylnitrosamino)- 	1013	1008, 1009	
8.	71267-22-6 71608-13-4	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-nitroso-, (S)- {NAT} 	24, 28–31, 34, 59, 174b, 174c, 239, 402, 459, 463, 478, 483, 484, 486, 501, 502, 514, 568b, 572, 573, 603, 688, 895, 1002, 1015, 1051, 1192–1196, 1198, 1199, 1217, 1304, 1386, 1437, 1445, 1569–1571, 1584, 1672, 1685, 1692, 1694, 1696, 1702, 1725, 1736, 1751, 1769, 1870, 1871, 1987, 1988, 2142, 2235, 2354, 2407, 2516, 2588, 2617, 2618, 2879, 2949, 2991, 3007, 3080, 3094, 3190, 3255, 3265, 3300, 3342, 3343, 3370, 3844, 3943a, 3944–3946, 3952, 3976, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5494, 5531, 5569, 5679, 5692, 5811b, 5836	29, 33, 34, 64, 174c, 201, 324, 404, 468, 478, 483, 484, 486, 501, 502, 505, 514, 548–550, 557, 568b, 655, 720, 895, 951, 995, 998, 1002, 1010, 1015, 1175a, 1192–1196, 1198, 1199, 1206a, 1385, 1569–1571, 1576, 1679, 1685, 1694, 1696, 1702, 1712, 1725, 1733, 1916a, 1988, 2050–2052, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2637, 2638, 2674, 2700, 2914, 2949, 3144a, 3176a, 3177, 3661, 3773, 3774, 3816, 3943a, 3944–3948, 3973, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5063, 5518, 5531, 5579, 5584, 5811b	
	64091-90-3	Butanal, 4-(methylnitrosamino)-4-3-(pyridyl)-	See 3-pyridinebutanal, γ-(methylnitrosoamino)-		

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

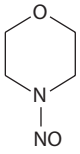
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
9.	924-16-3	1-Butanamine, *N*-butyl-*N*-nitroso- {NDBA} $[CH_3\text{-}(CH_2)_3]_2$=N-NO	203, 239, 486, 572, 573, 746c, 1058, 1217, 1740, 1741, 1743, 1744, 1781, 1870, 1871, 1952, 2442, 2443, 2516, 2561, 2751, 2825, 2884, 3219, 3257, 3265, 3300, 3308, 3491, 3711, 3713, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	5811b	
10.	7068-83-9	1-Butanamine, *N*-methyl-*N*-nitroso- $CH_3\text{-}(CH_2)_3\text{-}N(NO)\text{-}CH_3$	486, 568b, 572, 573, 1058, 1428, 2205, 2724, 2750, 2751, 3123, 3300, 3308, 3491, 3994, 4249, 4332, 5811b	5811b	
11.	56375-33-8	1-Butanamine, *N*-nitroso-	2041		
12.	61445-55-4 133201-39-5	Butanoic acid, 4-(methylnitrosoamino)- Butanoic acid, 4-[(nitrosomethyl) amino]-(NMBA) $CH_3\text{-}N(NO)\text{-}(CH_2)_3\text{-}COOH$	486, 982, 2852, 3256, 3300, 3943a, 3944–3946, 3973, 5811b	464, 466, 486, 982, 992, 2852, 3943a, 3944–3948, 3973, 5001, 5811b	
13.	67557-56-6	Butanoic acid, 4-(methylnitrosoamino)-, methyl ester $CH_3\text{-}N(NO)\text{-}(CH_2)_3\text{-}COOCH_3$	466, 470, 3256, 3300		
14.	64091-91-4 110053-55-9 121268-99-3 126165-82-0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}  {1-Butanone, 4-[(nitrosomethyl) amino]-1-(3-pyridinyl)-}	7, 23–26, 28–31, 34, 59, 70, 75, 97–99, 126, 126a, 126b, 172, 174b, 174c, 237, 239, 402, 458–460, 463, 478, 483, 484, 486, 501, 502, 508, 514, 568b, 572, 573, 595, 603, 688, 728, 772, 895, 998, 1001, 1002, 1004, 1006a, 1011, 1013–1016, 1016a, 1051, 1058, 1099, 1148, 1191–1200, 1373, 1386, 1445, 1557, 1564, 1566, 1567, 1567a, 1569–1571, 1571a, 1572, 1573a, 1580, 1584, 1674, 1679, 1685, 1692, 1696, 1702, 1710, 1725, 1727, 1728, 1730, 1731, 1736, 1741, 1744, 1746, 1750, 1751, 1768, 1769, 1781, 1842, 1870–1872, 1987, 1988, 2133, 2134a, 2142, 2168, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2879, 2949, 2991, 2992, 2993, 3007, 3094, 3178, 3179, 3180, 3181, 3182, 3184, 3190, 3255–3257, 3265, 3300, 3342, 3343, 3365, 3370, 3376, 3378, 3844, 3952, 3973, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5070, 5087, 5494, 5508, 5512, 5531, 5546, 5556, 5569, 5679, 5692, 5811, 5811a, 5811b, 5836	29, 33, 34, 64, 70, 97–99, 174c, 201, 324–326, 458, 463, 465, 468, 478, 483, 484, 486, 498, 501, 505, 508, 510, 548–550, 553, 554, 557, 568b, 595, 655, 720, 772, 895, 998, 1002, 1004, 1010, 1014, 1015, 1051, 1156, 1191–1200, 1385, 1564, 1566, 1567, 1567a, 1569–1571, 1573a, 1576, 1577, 1584, 1679, 1685, 1696, 1702, 1712, 1722, 1725, 1728, 1730, 1731, 1746, 1750, 1768, 1771, 1870–1872, 1988, 2050–2052, 2169, 2235, 2326c, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2638, 2674, 2700, 2914–2917, 2949, 2992, 2996, 2997, 3144a, 3176a, 3177, 3183, 3441a, 3491, 3773, 3774, 3816,	

(*continued*)

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK} (cont.)		3943b, 3947, 3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4090, 4128, 4161, 4236, 4247, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5531, 5579, 5584, 5589, 5811, 5811a, 5811b	
15.	76014-82-9	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-, *N*-oxide		4249	
16.	30533-08-5	Ethanamine, *N*,1-dimethyl-*N*-nitroso-	3256		
17.	55-18-5	Ethanamine, *N*-ethyl-*N*-nitroso- {NDEA} $(H_3C\text{-}CH_2)_2$=N-NO	31, 126, 126a, 126b, 172, 203, 239, 379, 457, 470, 480, 486, 510, 568b, 572, 573, 649, 746c, 1058, 1148, 1217, 1236, 1428, 1445, 1557, 1580, 1674, 1727, 1736, 1740, 1741, 1743, 1744, 1761, 1773, 1808, 1842, 1870–1872, 1952, 2118, 2129, 2142, 2440–2443, 2516, 2635, 2686, 2722, 2724, 2825, 2884, 2990, 2991, 3123, 3255–3257, 3265, 3300, 3308, 3343, 3378, 3491, 3595–3598, 3713, 3994, 4010, 4011, 4249, 4332, 5512, 5811b, 5869a	465, 468, 486, 568b, 1712, 1727, 1870–1872, 2516, 2655, 3973, 4010, 4010, 4011, 4249, 5496	
18.	10595-95-6	Ethanamine, *N*-methyl-*N*-nitroso- {NEMA} $H_3C\text{-}CH_2\text{-}N(NO)\text{-}CH_3$	31, 126a, 239, 457, 467, 480, 470, 486, 572, 573, 746c, 1058, 1148, 1217, 1236, 1428, 1445, 1580, 1725, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1784, 1808, 1842, 1870–1872, 1953, 2142, 2158, 2516, 2537, 2884, 2990, 2991, 3190, 3256, 3265, 3300, 2993, 3491, 3493, 3714, 3943a, 3944–3946, 3951, 3952, 3992, 3994, 4010, 4010, 4011, 4249, 5512, 5811b	486, 498, 1712, 1727, 1870–1872, 2516, 2655, 3943a, 3944–3948, 4249, 5496, 5811b	
19.	1116-54-7	Ethanol, 2,2′-(nitrosoimino) bis- {NDELA} $(HO\text{-}CH_2CH_2)_2$=N-NO	126, 126a, 126b, 172, 237, 239, 458, 471, 477–479, 481, 482, 485, 486, 510, 603, 1058, 1148, 1159, 1217, 1445, 1674, 1704, 1705, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1867, 1870–1872, 2516, 2825, 2655, 3190, 3255–3257, 3265, 3300, 3370, 3480, 3714, 3973, 3992, 4010, 4011, 5512, 5869a	458, 468, 471, 477-479, 481, 482, 485, 486, 490, 498, 1704, 1705, 1727, 1867, 1870–1872, 2990, 3265, 3300, 3480, 3481, 3491, 3947, 3948, 3973, 4010, 4011, 4249, 5001, 5811b	
20.	88476-94-2	Glycine, *N*-(1-nitroso-*L*-prolyl)-		3951, 4249	
21.	13256-22-9	Glycine, *N*-methyl-*N*-nitroso- {NSAR} $H_3C\text{-}N(NO)\text{-}CH_2\text{-}COOH$	1058, 2442, 3256, 3300	464, 466, 485, 486, 498, 2442, 3947, 3948, 5001, 5811b	

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
22.		Glycine, *N*-methyl-*N*-nitroso-, methyl ester H_3C-N(NO)-CH_2-$COOCH_3$	3256, 3300	466	
23.		Hexanoic acid, 2,6-di-(methylnitrosamino)- R-$(CH_2)_4$-CH(R)-COOH where R = CH_3-N(NO)-	1008, 1009, 1012, 3256, 3300	1008, 1009	
24.	62-75-9	Methanamine, *N*-methyl-*N*-nitroso- {NDMA} $(H_3C)_2$=N-NO$(H_3C)_2$=NH	28, 30, 31, 50, 59, 126, 126a, 126b, 158a, 167, 172, 185, 191, 192, 203, 226, 237, 239, 241, 379, 380, 463, 466, 467, 471, 478, 480, 488, 489, 499, 514, 572, 573, 603, 649, 677b, 746c, 1057–1059, 1099, 1217, 1236, 1428, 1437, 1442, 1443, 1580, 1445, 1674, 1685, 1692, 1693, 1725, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1781, 1784, 1808, 1842, 1870, 1871, 1885, 1952, 1953, 2008, 2057a, 2118, 2129, 2133, 2135, 2134a, 2142, 2205, 2206, 2404, 2405, 2440–2443, 2472, 2516, 2537, 2561, 2635, 2686, 2724, 2750, 2751, 2825, 2884, 2990, 2991, 3123, 3124, 3190, 3255–3257, 3265, 3300, 3308, 3343, 3366, 3370, 3378, 3441a, 3491, 3493, 3595–3598, 3713, 3777, 3812, 3943a, 3944–3946, 3951, 3952, 3985, 3992, 3994, 4010, 4011, 4249, 5508, 5512, 5811b, 5869a	468, 478, 498, 499, 677b, 1685, 1712, 1727, 1870, 1871, 2313a, 2686, 2990, 3811a, 3943a, 3944–3948, 3973, 3974b, 4010, 4011, 4249, 5001, 5029, 5053. 5496, 5811b	45
25.	59-89-2	Morpholine, 4-nitroso- {NMOR} 	31, 126a, 203, 471, 478, 485, 510, 746c, 1058, 1059, 1727, 1842, 2442, 2443, 3255, 3257, 4010, 4011, 5811b	468, 478, 498, 510, 1217, 1727, 1740, 1741, 1773, 3256, 3265, 3300, 3973, 3974b, 4010, 4011, 4249, 5001, 5496, 5811b	
26.	35576-91-1	Nitrosamide H_2N-N=O NNAs {general discussion}	1726, 5811b 1678, 1680, 1681, 1683, 1688, 1690, 1698, 1708, 1711, 1714, 1718, 1721, 1724, 1745, 1770–1772, 1775–1777, 5091, 5093	1677, 1680, 1681, 1683, 1684, 1697, 1698, 1702, 1707, 1708, 1711, 1713, 1714, 1715, 1720, 1721, 1726, 1729, 4991, 5000, 5001, 5004, 5007, 5020, 5024	
27.		Pentanoic acid, 2,5-di-(methylnitrosoamino)- R-$(CH_2)_3$-CH(R)-COOH where R = CH_3-N(NO)-	1008, 1009, 1013, 3256, 3300	1008, 1009	
28.	17721-95-8	Piperidine,2,6-dimethyl-1-nitroso-	2884, 4249		
29.	14300-04-0	Piperidine, 2-ethyl-1-nitroso-	2884, 4249		
30.	13603-07-1	Piperidine, 3-methyl-1-nitroso-	2884, 4249		
31.	15104-03-7	Piperidine, 4-methyl-1-nitroso-	2884, 4249		

(*continued*)

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

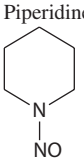
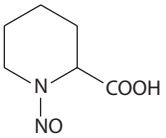
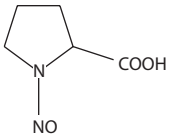
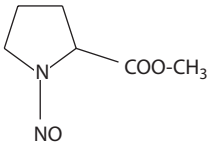
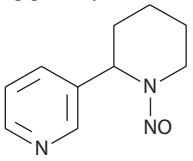
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
32.	100-75-4	Piperidine, 1-nitroso- {NPIP} 	30, 31, 203–206, 239, 457, 568b, 572, 573, 746c, 1058, 1428, 1740, 1741, 1743, 1744, 1781, 1784, 1808, 1870–1872, 1952, 2118, 2205, 2442, 2443, 2516, 2724, 2825, 2884, 3255–3257, 3265, 3300, 3302, 3308, 3491, 3595–3598, 3714, 3994, 4010, 4011, 4249, 5512, 5811b 5869a	498, 568b, 1870–1872, 2139, 2205, 2516, 3947, 3948, 3994, 4249, 5001, 5496, 5811b	
33.		2-Piperidineaceticacid, 1-nitroso- {NPIPAC}		486	
34.	4515-18-8 30310-81-7	2-Piperidinecarboxylic acid, 1-nitroso- {*N*-nitrosopipecolic acid; NPIC} 	3256, 3300, 3943a, 3944–3946, 5811, 5811a, 5811b	486, 992, 3943a, 3944–3948, 811, 5811a, 5811b	
35.	65445-62-7	3-Piperidinecarboxylic acid, 1-nitroso-	3951	3300, 4249	
36.	6238-69-3	4-Piperidinecarboxylic acid, 1-nitroso-		3300, 4249	
37.	7519-36-0	*L*-Proline, 1-nitroso- {NPRO} 	204–206, 486, 499, 509, 1058, 1673, 1695, 1719, 1870, 1871, 3256, 3260, 3300, 3943a, 3944–3946, 3951, 4249	464, 466, 468, 485, 486, 498, 499, 511, 992, 1870, 1871, 3256, 3566, 3943a, 3944–3948, 3973, 4130, 4249, 5811b	
38.	35909-01-4	*L*-Proline, 1-nitroso-, methyl ester 	3256, 3300	466, 485, 3256	
39.	30310-80-6	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}		486, 3300, 3947, 3948, 5811b	
40.	85502-23-4	Propanal, 3-(nitrosomethylamino)- CH_3-N(NO)-$(CH_2)_2$-CHO		2791	
41.	2504-18-9 34419-76-6	1-Propanamine, *N*,2-dimethyl-*N*-nitroso- $CH_3CH(CH_3)CH_2$-N(NO)-CH_3	568b, 2884, 2885, 3256, 3300, 4249	568b, 3561, 4249	
42.	71607-99-3	1-Propanamine, *N*-ethyl-2-methyl-*N*-nitroso- $CH_3CH(CH_3)$ CH_2-N(NO)-CH_2CH_3	2726, 2884, 2885, 3256, 3300, 4249	2726	
43.	25413-61-0	1-Propanamine, *N*-ethyl-*N*-nitroso- $CH_3CH_2CH_2$-N(NO)-CH_2CH_3	514, 568b, 2726, 3256, 3300, 4249, 5811b	514, 568b, 4249	

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
44.		1-Propanamine, 2-methyl-, *N*-(2-methylpropyl)-*N*-nitroso-	2726, 2884, 4249		
45.	924-46-9	1-Propanamine, *N*-methyl-*N*-nitroso- {NMPA} $CH_3CH_2CH_2$-N(NO)-CH_3	457, 470, 486, 1058, 1428, 3256, 3300, 3302, 4249, 5811b	466, 486	
46.	621-64-7	1-Propanamine, *N*-nitroso-*N*-propyl- {NDPA} $(CH_3CH_2CH_2)_2$=N-NO	203, 239, 379, 457, 486, 572, 573, 746c, 1058, 1428, 1740, 1741, 1743, 1744, 1870–1872, 2442, 2443, 2516, 2825, 2884, 3255–3257, 3265, 3300, 3491, 3711, 3713, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	486, 498, 1870–1872	
47.	16339-04-1	2-Propanamine, *N*-methyl-*N*-nitroso-	568b, 4249		
48.	601-77-4	2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso- $[(CH_3)_2 = CH]_2$-N-NO	2884		
49.	60153-49-3	Propanenitrile, 3-(methylnitrosoamino)- {MNPN} CH_3-N(NO)-$(CH_2)_2$-CN	3256	2994, 3947, 3948	
50.	10478-42-9	Propanoic acid, 3-(methylnitrosoamino)- Also listed as β-Alanine, *N*-methyl-*N*-nitroso- {NMPA} CH_3-N(NO)-$(CH_2)_2$-COOH	3256, 3300, 3943a, 3944–3946	466, 485, 503, 982, 2852, 3943a, 3944–3946, 3971, 3973, 5001	
51.	1133-64-8 37620-20-5	Pyridine, 3-(1-nitroso-2-piperidinyl)-, (*S*)-{NAB} 	28–31, 174b, 174c, 239, 422, 423, 460, 478, 483, 484, 486, 568b, 572, 573, 576, 603, 688, 890, 895, 1148, 1193–1196, 1199–1200, 1216, 1217, 1304, 1373, 1386, 1445, 1559, 1566, 1567, 1567a, 1569–1571, 1576, 1578, 1584, 1653, 1672, 1696, 1702, 1725, 1727, 1732, 1736, 1740, 1741, 1751, 1753, 1773, 1808, 1842, 1870–1872, 1987, 1988, 2235, 2354, 2407, 2442, 2443, 2516, 2588, 2617, 2618, 2730, 2879, 3007, 3080, 3094, 3190, 3255–3257, 3265, 3300, 3302, 3308, 3313, 3342, 3343, 3370, 3943a, 3944–3946, 3992, 4010, 4011, 4059, 4078, 4128, 4249, 4319, 4547, 5008, 5049, 5494, 5531, 5569, 5679, 5692, 5811b, 5836	29, 33, 174c, 201, 324, 468, 478, 483, 484, 486, 505, 510, 557, 568b, 655, 720, 890, 895, 922, 995, 998, 1002, 1192, 1206a, 1216, 1566, 1567, 1567a, 1569–1571, 1575, 1578, 1579, 1584, 1679, 1696, 1702, 1725, 1727, 1732, 1870–1872, 1988, 2050–2052, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2637, 2638, 2700, 2724, 2822a, 2914, 3144a, 3176a, 3661, 3773, 3774, 3816, 3943a, 3943b, 3944–3948, 3973, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5063, 5531, 5584, 5811b	

(*continued*)

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

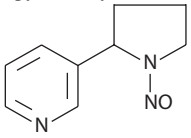
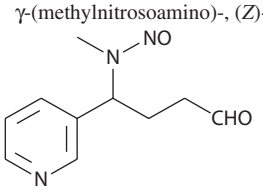
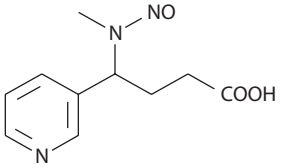
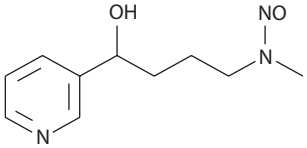
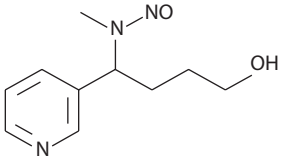
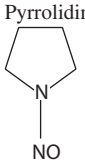
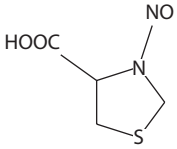
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
52.	16543-55-8	Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-, (S)- {NNN} 	24–26, 28–31, 59, 76, 97–99, 126, 126a, 126b, 167, 172, 174b, 174c, 203, 226, 237, 239, 313, 368, 402, 422, 423, 458–460, 463, 471, 478, 483, 484, 486, 488, 489, 499, 501, 568b, 572, 573, 575, 576, 595, 603, 632, 651, 684, 688, 772, 895, 1011, 1015, 1016, 1051, 1057, 1058, 1099, 1148, 1191–1200, 1216, 1217, 1304, 1373, 1386, 1437, 1442, 1445, 1559, 1564, 1567a, 1568–1571, 1580, 1569, 1574, 1578, 1584, 1585, 1653, 1672, 1674, 1692, 1696, 1702, 1710, 1712, 1717, 1725, 1727, 1722, 1730–1732, 1734, 1736, 1740, 1741, 1743, 1744, 1746, 1750, 1751, 1753, 1761, 1769, 1773, 1781, 1808, 1842, 1870–1872, 1987, 1988, 2128, 2133, 2134a, 2136, 2138, 2142, 2168, 2169, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2730, 2799a, 2825, 2879, 2949, 2991, 3007, 3050, 3080, 3094, 3190, 3255–3257, 3265, 3300, 3302, 3308, 3313, 3342, 3343, 3364, 3370, 3491, 3493, 3654, 3714, 3844, 3943a, 3944–3946, 3952, 3976, 3992, 4009–4011, 4059, 4078, 4128, 4249, 4547, 4683, 4885, 5008, 5049, 5071, 5494, 5508, 5512, 5518, 5531, 5569, 5679, 5692, 5811b, 5836, 5869a	29, 33, 64, 97–99, 174c, 201, 313, 322, 324, 326, 368, 458, 468, 478, 483, 484, 486, 498, 501, 503, 505, 507, 548–550, 557, 568b, 595, 650, 653–657, 660, 667, 677a, 685, 720, 772, 895, 951, 988a, 994, 995, 997, 1003, 1010, 1015, 1051, 1175a, 1191–1200, 1206a, 1216, 1385, 1564, 1567a, 1568–1571, 1576, 1577, 1579, 1569, 1575, 1577, 1579, 1580, 1584, 1585, 1679, 1696, 1702, 1704, 1712, 1725, 1727, 1731–1734, 1742–1744, 1750, 1753, 1771, 1870–1872, 1916a, 1988, 2050–2052, 2138, 2139, 2235, 2362, 2363, 2406, 2441, 2637, 2637, 2638, 2660, 2674, 2700, 2914–2917, 2949, 2996, 2997, 3144a, 3176a, 3177, 3491, 3654, 3670a, 3773, 3774, 3816, 3943a, 3943b, 3944–3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4247, 4249, 4410b, 4413, 4547, 4683, 4885, 5001, 5005, 5007, 5008, 5018, 5023, 5033, 5038, 5053, 5063, 5531, 5561, 5579, 5584, 5811b	
53.	53844-45-4	Pyridine, 3-(1-nitroso-2-pyrrolidinyl-2-^{14}C)-, (S)-	683b	683b	
54.	64091-90-3	3-Pyridinebutanal, γ-(methylnitrosoamino)- {NNA}	772, 1568, 1584, 4249	554, 772, 1565, 1584, 3973, 3974b, 4249, 5577, 5811b	
55.	64142-45-6	3-Pyridinebutanal, γ-(methylnitrosoamino)-, (*Z*)- 	1012, 1563–1565, 1567a, 1569, 1702, 1751, 3256, 3491, 4249	466, 992, 1012, 1563–1565, 1567a, 1569, 1576, 1577, 1567a, 1702, 3491, 5811b	
56.	152720-16-6	3-Pyridinebutanoic acid, γ-(methylnitroamino)-		3444, 4249	

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
57.	123743-84-0 133201-36-2	3-Pyridinebutanoic acid, γ-(methylnitrosoamino)-{iso-NNAC} 	59, 486, 1008, 1009, 1012, 1013, 1584, 1702, 1751, 3256, 3300, 4249, 5811, 5811a, 5811b	465, 486, 992, 993, 995, 1008, 1009, 1012, 1013, 1584, 1702, 1750, 3973, 4236, 4249, 5811, 5811a, 5811b	
58.	59578-66-4 76014-81-8	3-Pyridinebutanol, δ-(methylnitrosoamino)-{NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-; 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-} 	24, 25, 59, 486, 991, 1565, 1571a, 1573a, 1584, 1702, 1751, 3184, 3256, 3300, 5508, 5565, 5811b	469, 486, 507a, 728, 995, 1562a, 1565, 1571a, 1573a, 1584, 1702, 1771, 3943b, 3973, 4236, 4249, 5577, 5811b	
59.	133201-37-3	3-Pyridinebutanol, δ-(methylnitrosoamino)-{iso-NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-} 	59, 486, 508, 1584, 1702, 1751, 3256, 3943a, 3944–3946	486, 1562a, 1584, 1679, 1702, 3943a, 3944–3948, 3973, 4236, 5577	
60.	55557-02-3	3-Pyridinecarboxylic acid, 1,2,5,6-tetrahydro-1-nitroso-, methyl ester		5811, 5811b	
61.	76014-81-8	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-		4249	
62.	85352-99-4	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-, 1-oxide		4249	
63.		Pyrrolidine,2,5-dimethyl-,1-nitroso-	2884		

(*continued*)

TABLE 15.8 (continued)
NNAs in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
64.	930-55-2	Pyrrolidine, 1-nitroso- {NPYR} 	28, 30, 31, 50, 64, 126, 126a, 126b, 172, 203, 237, 239, 467, 478, 480, 486, 514, 572, 573, 576, 603, 649, 746c, 1058, 1099, 1148, 1217, 1373, 1428, 1445, 1567a, 1580, 1674, 1685, 1691–1693, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 1885, 2118, 2133, 2134a, 2142, 2325, 2404, 2405, 2516, 2561, 2686, 2724, 2750, 2825, 2879, 2884, 2990, 2991, 3190, 3255–3257, 3260, 3265, 3300, 3308, 3343, 3370, 3378, 3491, 3714, 3943a, 3944–3946, 3951, 3952, 3976, 3992, 3994, 4010, 4011, 4332, 5508, 5512, 5811b, 5869a	172, 463, 468, 466, 478, 486, 498, 514, 993, 1567a, 1685, 1712, 1727, 1740, 1741, 1743, 1744, 1870, 1871, 2139, 2686, 2990, 3943a, 3944–3948, 4010, 4249, 5001, 5496, 5811b	50 (0)
65.		2-Pyrrolidineaceticacid, 1-nitroso-		486, 4249	
66.	88381-44-6	4-Thiazolidinecarboxylic acid, 3-nitroso- {*N*-nitrosothioproline} 		486, 3300, 5811b	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

16 Nitroalkanes, Nitroarenes, and Nitrophenols

In his 1954 catalog of tobacco smoke components, Kosak (2170) listed no organic nitro-containing component. In 1959, Johnstone and Plimmer (1971) in their compilation of tobacco and tobacco smoke components also listed no organic nitro-containing component.

In their 1964 review (4319) and 1967 book (4332) on tobacco smoke carcinogenicity, Wynder and Hoffmann did not mention a nitroalkane or a nitroarene. In his 1968 review, Stedman (3797) listed no organic nitro-containing component identified in tobacco and tobacco smoke composition. His list of the agricultural chemicals used in tobacco agronomy [see Table XVI in (3797)] also contained no nitro-containing compound.

In their review of the *N*-containing components in tobacco and smoke, Schmeltz and Hoffmann listed 30 nitro components [see Table X in (3491)] separated into 6 nitroalkanes identified by Hoffmann and Rathkamp (1755) and Rathkamp et al. (3086) in the late 1960s, 8 monocyclic nitroarenes identified by Hoffmann and Rathkamp in 1970 (1758), and 16 nitrophenols, including a methylnitro-1-naphthol, reported by Klus and Kuhn in 1975 (2137).

In their 1980 catalog (1884), Ishiguro and Sugawara also listed 30 nitro components in tobacco smoke. All the nitro components they listed were those tabulated in the 1977 article by Schmeltz and Hoffmann (3491).

With the limiting analytical technology available in 1982, Lee et al. (2329) at the American Health Foundation reported that they were unable to measure significant quantities of 4-nitro-1,2-benzenediol (4-nitrocatechol) in cigarette MSS. El-Bayoumy et al. in a conference presentation (1122) and a journal publication (1124) reported that 1-nitronaphthalene, 1-nitropyrene, and 6-nitrochrysene, if present in cigarette smoke, were at yields lower than their analytical capability.

In its 1986 monograph on tobacco smoking, the International Agency for Research on Cancer (IARC) discussed many of the details of *N*-nitrosamines and tobacco-specific *N*-nitrosamines in tobacco smoke. Despite the reports prior to 1985 on the identification in tobacco smoke of many nitro components (1755, 1758, 2137, 3086), the IARC listed only one nitro compound, 2-nitropropane, as a biologically active smoke component [see Table 19, pp. 86–87 in (1870)]. In its listing of the evaluation of tobacco smoke components for carcinogenicity, IARC defined the evidence in 1986 of the carcinogenicity in animals and humans of 2-nitropropane as sufficient [see Appendix 2, p. 393 in (1870)]. Hoffmann and Wynder (1808) included 2-nitropropane in their list of major toxic and tumorigenic agents in nonfiltered cigarette MSS. Although not dealing with cigarette smoke in this particular 1987 study, Grimmer et al. (1406a) identified 1-nitropyrene in diesel exhaust.

Of the many nitro components in tobacco smoke, only nitrobenzene, nitromethane, and 2-nitropropane have been discussed repetitively since 1986. In reports primarily dealing with commercial cigarettes, these three nitro compounds were listed periodically in various publications as toxic smoke components, biologically active smoke components, tumorigenic smoke components, or carcinogenic smoke components: nitrobenzene (1741, 1743, 1744, 5512), nitromethane (1743, 1744, 5512), 2-nitropropane (1217, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 2825, 5512). 2-Nitropropane was also described as a known carcinogen in the MSS from all-flue-cured or all-burley cigarettes (1716).

In 2003, Cheng et al. (692, 693) reported the identification in CSC of five nitro-polycyclic aromatic hydrocarbons. They included 1- and 4-nitropyrene, 1,6- and 1,8-dinitropyrene, and 6-nitrochrysene. In 2004, Cheely et al. (683) described an analytical procedure which enabled the identification of 1-nitronaphthalene, 1-nitropyrene, and 6-nitrochrysene in cigarette MSS.

Although 2-nitropropane was much discussed as a tumorigen or carcinogen in cigarette smoke and its categorization by IARC as having yielded sufficient evidence to rate it as both an animal and a human carcinogen, it seldom was designated as a "Hoffmann analyte." While it did not use the term "Hoffmann analyte" in its report, the Department of Health (Canada) proposed that analytical data on the per cigarette yields of over 40 components in tobacco smoke should be a requirement to indicate the hazardous nature of cigarette smoke (16A01). No nitroalkane was included in its list. Neither nitrobenzene nor nitromethane appeared in any "Hoffmann analyte" list.

Table 16.1 lists the nitroalkanes, nitroarenes, and nitrophenols identified in tobacco, tobacco smoke, and tobacco substitute smoke. The list also contains over a dozen complex nitro components such as Butralin® and Imidacloprid® that are used in tobacco agronomy.

TABLE 16.1
Nitroalkanes, Nitroarenes, and Nitrophenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

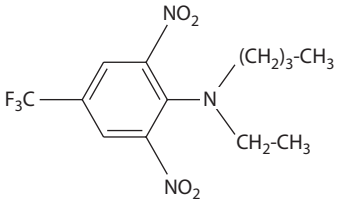
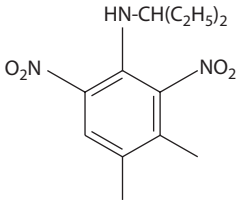
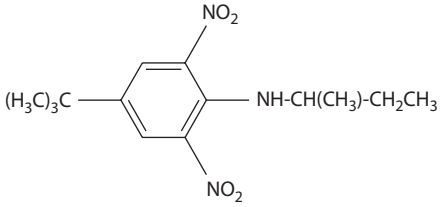
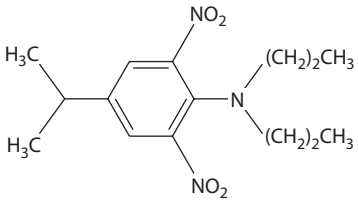
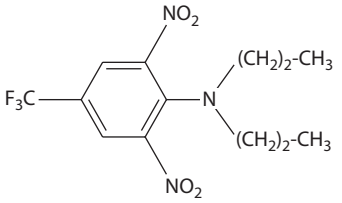
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	1861-40-1	Benzenamine, *N*-butyl-2,6-dinitro-*N*-ethyl-4-(trifluoromethyl)- {Benefin®; Benfluralin®} 		2892a, 3633	
2.	99-30-9	Benzenamine, 2,6-dichloro-4-nitro- {Dicloran®}		3633	
3.	40487-42-1	Benzenamine, 3,4-dimethyl-2,6-dinitro-*N*-(1-ethylpropyl)- {Pendimethalin®} 		2650b, 2913a, 3633, 3811a, 4271a	
4.	33629-47-9	Benzenamine, 4-(1,1-dimethylethyl)-2,6-dinitro-*N*-(1-methylpropyl)- {Butralin®} 		2913a, 3585c, 3633, 3811a, 3973, 5568	
5.	33820-53-0	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(1-methylethyl)- {Isopropalin®} 		2892a, 3633, 4271a	
6.	1582-09-8	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)- {Trifluralin®} 		1219c, 2650a	
7.	103-33-3	Benzene, azobis- C_6H_5-N=N-C_6H_5		3476	

TABLE 16.1 (continued)
Nitroalkanes, Nitroarenes, and Nitrophenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
8.	81-15-2	Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro- {musk xylene}		5811, 5811b	
9.	83-66-9	Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro- {musk ambrette}		5811, 5811b	
10.	99-51-4	Benzene, 1,2-dimethyl-4-nitro-	480, 1580, 1758, 3491, 4010, 4011, 4249, 5811b		
11.	89-58-7	Benzene, 1,4-dimethyl-2-nitro- {2,5-dimethyl-1-nitrobenzene}	480, 1580, 1758, 1884, 3491, 4010, 4011, 4249, 5811b		
12.	89-87-2	Benzene, 2,4-dimethyl-1-nitro- {1,3-dimethyl-4-nitrobenzene}	480, 1580, 1758, 1884, 3491, 4010, 4011, 4249, 5811b		
13.	1817-47-6	Benzene, 1-(1-methylethyl)-4-nitro-{4-nitrocumene}	480, 1580, 1758, 1884, 3491, 4010, 4011, 4249, 5811b		
14.	88-72-2	Benzene, 1-methyl-2-nitro-	480, 1580, 1758, 1781, 1884, 2329, 3491, 4010, 4011, 4249, 4594		
15.	99-08-1	Benzene, 1-methyl-3-nitro-	480, 1580, 1758, 1884, 2329, 3491, 4010, 4011, 4249, 4594, 5811b		
16.	99-99-0	Benzene, 1-methyl-4-nitro-	480, 1580, 1758, 1884, 2329, 3491, 4010, 4011, 4249, 5811b		
17.	98-95-3	Benzene, nitro- C_6H_5-NO_2	480, 1428, 1580, 1741, 1743, 1744, 1758, 1884, 2329, 3081, 3082, 3265, 3300, 3493, 3714, 4010, 4011, 4249, 5512, 5811b		
18.	15457-05-3	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)- {Fluorodifen®}		3633	
19.	82-68-8	Benzene, nitropentachloro- {Quintocen®}		3770	
20.	71630-70-1	Benzenediol, ethyl-nitro-	1884, 2137, 3491, 4249		
21.		Benzenediol, methyl-nitro-	1884, 2137, 3491		
22.	62726-14-1	Benzenediol, nitro- {at least four isomers were detected}	1884, 2137, 3491, 4249		
23.	71608-02-1	1,2-Benzenediol, 5-ethyl-3-nitro-	2137, 3712, 4249		
24.	6665-98-1	1,2-Benzenediol, 3-nitro-	2137, 3712, 4249		
25.	3316-09-4	1,2-Benzenediol, 4-nitro-	1884, 2016, 2137, 2329, 3308, 3491, 3712, 4010, 4011, 4249, 5811b		
26.	71608-03-2	1,3-Benzenediol, 4-methyl-6-nitro-	2137, 3712, 4249		
27.	3163-07-3	1,3-Benzenediol, 4-nitro-	2137, 3712, 4249		
28.	62924-70-3	Benzenemethanamine, 2-chloro-*N*-(2,6-dinitro-4-(trifluoromethyl)phenyl)-*N*-ethyl-6-fluoro- {Flumetralin®}		2913a, 3633. 5568, 5811b	
29.	19044-88-3	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro- {Oryzalin®}		4271a	
30.	92-93-3	1,1′-Biphenyl, 4-nitro-	3081, 4249		
31.	627-05-4	Butane, 1-nitro- H_3C-$(CH_2)_2$-CH_2-NO_2	1755, 1884, 2724, 2977, 3086, 3491, 4249, 5811b		
32.	600-24-8	Butane, 2-nitro- H_3C-CH_2-$CH(NO_2)$-CH_3	2977, 3086, 4249		
33.	39300-45-3	2-Butenoic acid, 2-(1-methylheptyl)-4,6-dinitrophenyl ester {Dinocap®}		3661a, 3633, 4271a	
34.	7496-02-8	Chrysene, 6-nitro-	692, 1122 (0), 1124 (0)		
35.	79-24-3	Ethane, nitro- C_2H_5-NO_2	1755, 1756, 1884, 2724, 2799a, 3081, 3082, 3086, 3491, 3493, 4249, 4342, 5811b		

(*continued*)

TABLE 16.1 (continued)
Nitroalkanes, Nitroarenes, and Nitrophenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

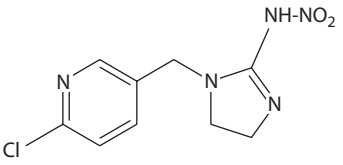
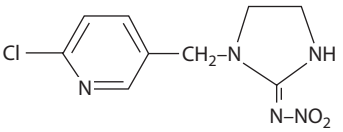
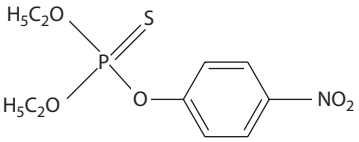
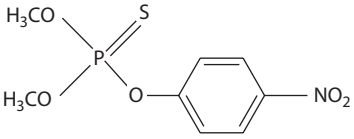
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
36.	20661-60-3	Glycine, *N*-methyl-*N*-nitro-		992	
37.	105827-78-9	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl)methyl)-4,5-dihydro-*N*-nitro- {Admire®} 		2892a, 4249	
38.	138261-41-3	Imidazolidinimine, 1-((6-chloro-3-pyridinyl)methyl)-*N*-nitro- {Imidacloprid®} 	568b, 4249, 21A19	568b, 4249, 5064, 5568, 21A19	
39.	61010-32-0	Isoquinoline, 1-[(4-methoxy-3-nitrophenyl)methyl]-, mononitrate		4249	
40.	75-52-5	Methane, nitro- $H_3C\text{-}NO_2$	112, 172, 480, 1663a, 1667, 1743, 1744, 1755, 1756, 1884, 2724, 3081, 3082, 3086, 3265, 3300, 3491, 3493, 4249, 4342, 5512, 5811b		
41.	76-06-2	Methane, nitrotrichloro- {Chloropicrin®}		3633, 3646a, 3973	
42.	86-57-7	Naphthalene, 1-nitro-	683, 1122 (0), 1124 (0)		
43.	23245-64-9	1-Naphthalenecarbonitrile, 5-nitro-	4249		
44.		1-Naphthalenol, methyl-nitro-	1884, 2137, 3746, 3747, 4249		
45.	628-05-7	Pentane, 1-nitro- $H_3C\text{-}(CH_2)_3\text{-}CH_2\text{-}NO_2$	1755, 1758, 1884, 2724, 3086, 3491, 5811b		
46.	4609-89-6	Pentane, 2-nitro- $H_3C\text{-}(CH_2)_2\text{-}CH(NO_2)\text{-}CH_3$	1758, 3086		
47.		Phenol, dimethyl-2-nitro-	1884, 2137, 3491, 4249		
48.		Phenol, ethyl-methyl-nitro-	1884, 2137, 3491, 4249		
49.		Phenol, ethyl-nitro-	1884, 2137, 3491, 4249		
50.	12167-20-3	Phenol, methyl-nitro-	1884, 2137, 3491, 4249		
51.	71607-97-1	Phenol, 2-ethyl-3-nitro-	2137, 3797, 4249		
52.		Phenol, 2-ethyl-4-nitro-	3712		
53.	99-53-6	Phenol, 2-methyl-4-nitro-	2137, 3491, 3712, 4249, 5811b		
54.	88-75-5	Phenol, 2-nitro-	414, 1884, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
55.	4920-77-8	Phenol, 3-methyl-2-nitro-	1884, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
56.	2581-34-2	Phenol, 3-methyl-4-nitro-	1884, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
57.	554-84-7	Phenol, 3-nitro-	1884, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
58.	71607-98-2	Phenol, 4-ethyl-3-nitro-	2137, 3712, 4249		
59.	119-33-5	Phenol, 4-methyl-2-nitro-	1884, 2137, 3712, 4010, 4011, 4249, 5811b		

TABLE 16.1 (continued)
Nitroalkanes, Nitroarenes, and Nitrophenols in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
60.	2042-14-0	Phenol, 4-methyl-3-nitro-	2137, 3712, 4249		
61.	100-02-7	Phenol, 4-nitro-	414, 1884, 2137, 3491, 3712, 4010, 4011, 4249, 5811b		
62.	71278-12-1	Phenol, 5-ethyl-2-methyl-4-nitro- {phenol, 3-ethyl-6-methyl-4-nitro-}	2137, 3712, 4249		
63.	6665-95-8	Phenol, 2,3-dimethyl-6-nitro- {phenol, 5,6-dimethyl-2-nitro-}	1884, 2137, 3491, 3712, 4010, 4011, 4249		
64.		Phenol, 2,5-dimethyl-6-nitro-	2137, 3712, 4249		
65.	71608-10-1	Phenol, 3,6-dimethyl-2-nitro- {phenol, 2,5-dimethyl-6-nitro-}	2137, 3712, 4249		
66.	56-38-2	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®} 	21A19	2058a, 3381, 3633, 3634, 3973, 4249, 4271a, 5079, 5439, 5811b, 21A19	
67.	298-00-0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-nitrophenyl) ester{Parathion-methyl®} 	5811b	2058a, 3381, 3633, 3973, 4271a	
68.	122-14-5	Phosphorothioic acid, *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester {Fenitrothion®}		3633, 3973, 4249, 4271a, 4917	
69.	108-03-2	Propane, 1-nitro- $H_3C\text{-}(CH_2)_2\text{-}NO_2$	1673, 1755, 1884, 2329, 2724, 2977, 3086, 3255, 3257, 3491, 4249, 5811b, 5869a		
70.	79-46-9	Propane, 2-nitro- $(H_3C)_2{=}CH\text{-}NO_2$	126a, 239, 566, 567, 568b, 1148, 1217, 1373, 1727, 1740, 1741, 1743, 1744, 1755, 1773, 1781, 1808, 1842, 1870, 1871, 1884, 2329, 2724, 2799a, 2825, 2977, 3086, 3265, 3300, 3491, 3714, 4009–4011, 4249, 5512, 5811b, 5869a		
71.	127-06-0	2-Propanone oxime $(H_3C)_2\text{-}C{=}N\text{-}OH$	568b, 4249		
72.	42397-64-8	Pyrene, 1,6-dinitro-	692, 693		
73.	42397-65-9	Pyrene, 1,8-dinitro-	692, 693		
74.	5522-43-0	Pyrene, 1-nitro-	683, 692, 693, 1122 (0), 1124 (0)		
75.	57835-92-4	Pyrene, 4-nitro-	692, 693		
76.	18368-73-5	Pyridine, 3-methyl-2-nitro-	1360, 1375a, 2761, 2762, 2765, 2766, 4249		1360, 1375a
77.	152720-16-6	3-Pyridinebutanoic acid, γ-(methylnitroamino)-		3444, 4249	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

17 Nitrogen Heterocyclic Components

17.1 MONOCYCLIC FOUR- AND FIVE-MEMBERED *N*-CONTAINING RING COMPOUNDS

17.1.1 Background

Tobacco (*Nicotiana tabacum*) is a unique agricultural crop used to prepare a variety of commercial products (cigarettes, pipe tobacco, cigars, chewing tobacco, snuff, etc.). Consumers enjoy tobacco by placing it into their mouth or nasal cavity (in the case of oral and snuff products) or by lighting the tobacco article (cigarette, cigarillo, cigar, etc.) and inhaling the tobacco smoke produced. As a result, the chemical composition of both leaf and the tobacco smoke is important to consumers (for its flavor and appeal) and to scientists attempting to understand the chemical organoleptic, pharmacological, and toxicological properties of this extremely complex consumer product.

Tobacco is a natural product that contains numerous classes of chemical compounds. As a living entity, tobacco contains all of the complex biological machinery necessary to sustain life. Chemical constituents in the tobacco leaf are influenced by numerous factors as the tobacco plant develops from seed to cured leaf. These factors include genetic potential, environmental conditions, cultural practices, and curing methods. Interactions among the factors also influence the chemical composition of the cured leaf. The genetic makeup of the plant provides the potential to produce or not to produce certain compounds, and the realization of these potentials depends on environmental variations that the plant endures during growth and processing conditions employed to manufacture the finished tobacco product (677a).

Although the chemical composition of the tobacco leaf is important, tobacco smoke also contains an extensive variety of chemical compounds. The presence and relative concentrations of these tobacco smoke components depend upon (1) the composition of the tobacco leaf, (2) tobacco additives, (3) manufacturing processes, (4) the physical form and materials used to construct the different smoking articles, and (5) the smoking procedure.

An elemental analysis for carbon, hydrogen, and nitrogen in foods (2439) and tobacco indicates that there is only about 5% nitrogen in dry tobacco. The percent carbon, hydrogen, and oxygen (by difference) of dry tobacco leaf are about 43%, 6%, and 43%, respectively (2798), with the remainder being trace levels of metals and nonmetals. The majority of the nitrogen in tobacco leaf resides in the proteins, alkaloids, nitrates, and amino acids. The *N*-containing compounds in tobacco leaf have often been associated with the quality of the leaf. This is especially true with burley tobacco (3973). Nitrogenous compounds in tobacco and smoke have an enormous range of taste and odor quality and intensity. Many are odorless and tasteless (proteins, nitrates), some have extremely pleasant tastes and odors, e.g., some pyrazines (2439) and imidazoles, while others are very strong, pungent, and offensive, e.g., some pyridines (1803).

In this section, we present information on four- and five-membered *N*-containing ring compounds identified in tobacco, tobacco smoke, and tobacco substitute smoke. The classes of compounds include azetidines, pyrrolidines, 2- and 3-pyrrolines, pyrroles, pyrazoles, imidazolidines, imidazolines, imidazoles, and 1,2,4-triazoles (Figure 17.1).

17.1.2 Four-Membered *N*-Containing Rings

Few four-membered *N*-containing ring compounds have been identified in tobacco or tobacco smoke. These compounds are classified as azetidines. Nicotianamine, first isolated from tobacco by Noma et al. in 1971 (2796a), has also been identified in numerous other plant species (3528a). Nicotianamine is a derivative of 2-azetidinecarboxylic acid, an amino acid identified in numerous plant species, including *N. tabacum* (2330b). The precursor for the biosynthesis of azetidine in tobacco and azetidine-2-carboxylic acid, in particular, is considered to be methionine (2330b). The bacterial plant pathogen tabtoxin (*L*-threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]-) was isolated from wildfire tobacco (a wild species of *N. tabacum*) in 1971 (3819a).

The scant information on azetidine compounds can be found in several review articles on the chemistry of compounds identified in tobacco and tobacco smoke. In their 1977 review, Schmeltz and Hoffmann (3491) reported the presence of 2-azetidinecarboxylic acid and nicotianamine in tobacco. Hecht et al. (1580) reported the identification of azetidine in both tobacco and smoke in 1977. Brunnemann and Hoffmann (486) reported the presence of the nitrosamine and 1-nitroso-2-azetidinecarboxylic acid in tobacco in 1991.

Table 17.1 lists the four-membered *N*-containing ring compounds identified in tobacco, tobacco smoke, and tobacco substitute smoke. Only five compounds are known to exist in tobacco and tobacco smoke that contain an

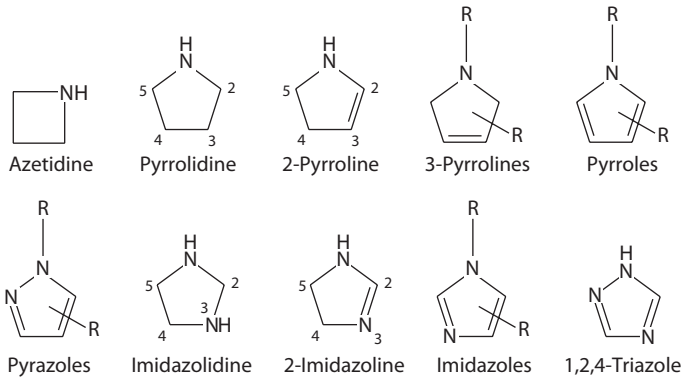
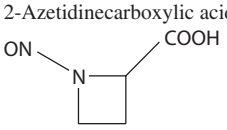


FIGURE 17.1 Representative structures of the four- and five-membered *N*-containing ring compounds in tobacco, tobacco smoke, and tobacco substitute smoke.

TABLE 17.1
Four-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	503-29-7	Azetidine 	568b, 1580, 4249	568b, 1580, 4249	
2.	34441-14-0	1-Azetidinebutanoic acid, α-[(3-amino-3-carboxypropyl)amino]-2-carboxy-, [2S-[1[αR*(R*)],2R*]]- {nicotianamine}		3491, 4249, 5811b	
3.	2517-04-6	2-Azetidinecarboxylic acid		3491, 4249, 5811b	
4.	55556-98-4	2-Azetidinecarboxylic acid, 1-nitroso- 		486, 4249, 5811b	
5.	32190-57-1	*L*-Threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]- {tabtoxin}		3819a, 4249	

azetidine ring. All five have been identified in tobacco. Azetidine has been identified in tobacco and tobacco smoke.

17.1.3 Five-Membered *N*-Containing Rings

Tobacco and smoke chemists have shown an intense interest in the chemistry and biochemistry of this diverse class of compounds. Numerous studies on the presence of nitrogenous compounds in tobacco and tobacco smoke have appeared over the past 45 years, and various aspects of the origin of these compounds in tobacco and their presence in tobacco smoke by direct transfer, pyrosynthesis, and combustion processes have been examined. Books, reviews, and articles by Wynder and Hoffmann (4332), Stedman (3797), Neurath (2724), Tso (3972, 3973), Chaplin (677a), Leffingwell (2337), Schmeltz and Hoffmann (3491), Hecht et al. (1580), Leete (2330c), Bush and Saunders (557a), Green (1351), Newell et al. (2769), Ishiguru and Sugawara (1884), Heckman and Best (1587), Gorrod and Wahren (1334d), Davis and Nielsen (910a), and Gorrod and Jacob (1334c) contain synopses of much of the information we know today on *N*-containing ring compounds in tobacco and tobacco smoke.

During the 1970s and 1980s, an exceptional amount of research on tobacco and smoke component isolation and identification was conducted and published. This was largely due to many scientific advancements that occurred in chromatographic methods during this period. The results of several excellent studies on tobacco leaf composition by Lloyd et al. (2389), Dickerson et al. (965), Roberts and Rohde (3219), Takahara et al. (3858), Demole et al. (937–939, 941, 943, 943a), Fujimori et al. (1247, 1249, 1250), Chuman et al.

(731–739), Schumacher (3550), and Schumacher and Vestal (3561) are included here for reference. Swedish Tobacco Company published nearly 100 articles on the composition of tobacco, primarily Oriental tobacco. Many Swedish Tobacco Company investigators included Aasen, Almqvist, Behr, Enzell, Hlubucek, Kimland, Nishida, and Wahlberg, all of whom coauthored many tobacco composition articles (1–13, 52, 53, 84, 91–94, 227, 229–236, 1149–1157a, 1205a, 1660–1662, 2092–2095, 3315, 4083–4102). Excellent detailed summaries of their identification of hundreds of tobacco components and the generation of them from various terpenoid structures were presented and published in the late 1970s and the early 1980s by Enzell (1149, 1150), Enzell and Wahlberg (1156), and Wahlberg and Enzell (4089, 4090).

The basic five-membered *N*-containing ring compounds found in tobacco, whether they contain one or more nitrogens, arise from several metabolic and catabolic pathways. Additionally, many *N*-containing ring compounds are formed via nonenzymatic browning reactions.

Amino acids and proteins are produced in living species and are essential compounds of tobacco plants. One of the most important metabolic pathways in plants is the Krebs tricarboxylic acid cycle (2337, 3973). The Krebs cycle controls the metabolic carbon–nitrogen balance in living plants by converting carbon dioxide via photosynthesis to such intermediates as oxaloacetic, α-ketoglutaric, and pyruvic acids. Concurrently, inorganic nitrogen as nitrates is assimilated through the plant roots and is subsequently reduced to ammonia by hydrogen originating from reactions occurring in the Krebs cycle. Ammonia then reacts with oxaloacetic, α-ketoglutaric, and pyruvic acids to form aspartic and glutamic acids and alanine which provide the nitrogen for further synthesis of other amino acids (1351). These amino acids are then used as the nitrogen pool from which many of the other nitrogenous compounds of the tobacco plant are formed. For example, the pyrrolidine ring can be formed from arginine or ornithine via a series of metabolic reactions involving arginine decarboxylase or ornithine decarboxylase to form putrescine (1,4-diaminobutane) which is then converted to 4-methylaminobutanal via putrescine *N*-methyltransferase, *S*-adenosine-methionine, and methylputrescine oxidase. Via cyclization and demethylation, pyrrolidine is produced (3973). Numerous other metabolic reactions occur that produce five-membered *N*-containing ring compounds such as the pyrrolines, pyrroles, pyrazolines, pyrazole, imidazolidines, imidazolines, and imidazoles.

From the time of harvest through curing and aging, many changes take place in the concentrations of tobacco leaf amino acids and proteins (3972). According to Gaines and Miles (1270a), one of the extremely important aims of this process is to accomplish a degradation of tobacco proteins. This degradation produces numerous types of short-chained amino acid oligomers, free amino acids, and many functionalized *N*-containing compounds such as alcohols, aldehydes, acids, aldehydes, and esters. Among these catabolic breakdown products are the simple four-membered, five-membered, and six-membered *N*-containing ring compounds and a variety of alkaloids and alkaloid-type compounds that are oxidized, reduced, or otherwise functionalized.

The origins of the five-membered *N*-containing ring compounds in leaf are also attributed at least partially to nonenzymatic browning or Maillard reactions between sugars and amino acids (965). Many compounds formed by nonenzymatic browning reactions have desirable flavor and aroma characteristics that taken together form the characteristic bouquet and taste associated with tobacco (2337).

A wide variety of five-membered *N*-containing ring compounds have been isolated and identified in tobacco smoke. Two general mechanisms are involved: direct transfer of tobacco components to tobacco smoke and the generation of smoke components by combustion and pyrolysis of tobacco. In 1977, it was estimated that the direct transfer of components from leaf to smoke accounted for about one-third of the smoke constituents identified in tobacco smoke at that time (1351). This process is relatively simple, and many of its factors are understood. This process has been discussed in some length by Wakeham (4103). The second mechanism involves the pyrolysis, combustion, and subsequent pyrogenesis of smoke components. This process is complex and involves the tobacco, the means and materials used in constructing the smoking article, and the actual smoking process (puff volume, duration, puff interval, etc.). The relationships between various leaf constituents and their pyrolysis products are the ones most difficult to trace yet they are the most necessary to understand (1351).

In contrast to the number of leaf components that generally transfer directly to smoke (~33%), only about 16% of the 313 tobacco and tobacco smoke compounds that contain a five-membered *N*-containing ring were found in both tobacco and tobacco smoke. A considerable portion of the smoke yields from these compounds was no doubt due to transfer of the compounds directly from tobacco, although some of the yield of these compounds is produced by pyrolysis, combustion, and pyrogenesis of a variety of compounds in tobacco.

As mentioned previously, the largest contributors of organic leaf nitrogen are the leaf proteins, alkaloids, and amino acids. A majority of the protein in the tobacco consists of the enzymes associated with photosynthesis. The single most abundant protein in tobacco is called Fraction I and is designated functionally as ribulose-l,5-diphosphate carboxylase. Our knowledge of the genomic makeup of tobacco has advanced tremendously in the last 20 years. Once the Tobacco Genome Initiative is completed, over 90% of the genetic map of tobacco will be known (429b, 429c). Numerous databases of genes, enzymes, and reactions occurring in *Nicotiana* species are already available.

The identities of the free amino acids of cured leaf are well known (1351). Of the 44 amino acids reported in leaf,

a majority have also been found in tobacco smoke. Proline and asparagine are the major amino acids in flue-cured tobacco, whereas asparagine and aspartic acid are the major amino acids in burley tobacco. These plus glutamine and histidine are the principal amino acid precursors of the five-membered *N*-containing ring compounds in tobacco.

High-temperature pyrolysis studies of protein and amino acids have been described in a series of papers by Smith et al. (3724, 3727a, 3728a, 3729), Patterson et al. (2902–2905), Higman et al. (1647), Schmeltz (3477–3479), Sugimura et al. (3829), and Yamamoto et al. (4365a). Under these pyrolytic conditions, pyrodegradation and pyrosynthesis were extensive. In general, pyrolysis gave complex mixtures which were qualitatively similar regardless of the specific amino acid being pyrolyzed. Compounds identified included aromatic hydrocarbons such as benzene and naphthalene, their *N*-containing analogs such as pyridine and quinoline, pyrrole, aromatic nitriles such as benzonitrile and 1-naphthonitrile, aniline, and phenols. As suggested by Patterson et al. (2904), this similarity of results indicates that the amino acids and proteins undergo degradation into common intermediates of 2-, 3-, and 4-carbon types which subsequently recombine to form more thermally stable aromatic systems. To be discussed in a subsequent chapter is the pyrogenesis of the potent mutagens 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) and 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) from tryptophan (3829) and 2-aminodipyrido[1,2-*a*:3′,2′-d]imidazole (Glu-P-2) and 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) from glutamic acid (3828a, 4365a), all four of which were subsequently identified in tobacco smoke (3828c). Table 17.2 catalogs many of the pyrolysis studies conducted on amino acids.

Pyrolysis and smoke studies of amino acids indicate that they are potential precursors of several nitrogen heterocyclic ring systems found in tobacco smoke. Proline has been shown to be efficiently converted to pyrrole upon pyrolysis (3219, 3724) and in addition has been proposed as a possible precursor of pyrocoll (2593, 4336). γ-Amino acids and dicarboxylic amino acids are capable, under pyrolytic conditions, of forming 2-pyrrolidones (1967, 3079), and by a similar mechanism, δ-amino acids can form 2-piperidones (1967, 3079). A side effect of the pyrolysis of amino acids is the formation of hydrogen cyanide.

Johnson, Kang, and Wakeham (1967) studied the hydrogen cyanide yields from pyrolysis of compounds containing ring nitrogen and found that these heterocycles, particularly those with five-membered rings, produced the highest yields of hydrogen cyanide. These results are in accord with those of Smith et al. (3724) in which proline was found to give high yields of hydrogen cyanide. The pathway seems to be through pyrrole which is formed in excellent yield (67%) on pyrolysis of proline. Patterson et al. (2908) had previously found that pyrrole on pyrolysis at 850°C is converted in 49% yield to hydrogen cyanide. This may not be the only pathway for the formation of hydrogen cyanide from proline because Johnson and Kang (1967) found that proline can generate hydrogen cyanide more readily than pyrrole.

Protein and free amino acids found in tobacco leaf contribute significantly through pyrodegradation and pyrosynthesis to the formation of many nitrogenous compounds found in tobacco smoke. The nonvolatility of these compounds either as free acids, proteins, or as members of

TABLE 17.2
Studies on the Pyrolysis of Amino Acids

Amino Acid	CAS No.	References
Amino acids		Kato et al. (2048, 2049), Kosuge et al. (2178a), Masuda et al. (2486), Nebert et al. (2688a)
Alanine	107-95-9	Matsumoto et al. (2491b)
Arginine	74-79-3	Matsumoto et al. (2491b)
Asparagine	7006-34-0	Matsumoto et al. (2491b)
Cysteine	52-90-4	Matsumoto et al. (2491b)
Cystine	24645-67-8	Matsumoto et al. (2491b)
Glutamic acid	6899-05-4	Matsumoto et al. (2491b), Ohgaki et al. (2849b), Sugimura (3828a), Takeda et al. (3863a), Takayama et al. (3862b), Yamamoto et al. (4365a)
Glutamine	56-85-9	Matsumoto et al. (2491b)
Histidine	71-00-1	Matsumoto et al. (2491b), Smith et al. (3722a)
Histidine, 3-methyl-		Smith et al. (3722a)
Lysine	56-87-1	Matsumoto et al. (2491b), Wakabayashi et al. (4102a)
Methionine	63-68-3	Matsumoto et al. (2491b)
Ornithine	70-26-8	Matsumoto et al. (2491b)
Ornithine, *N*5-(aminocarbonyl)-{citrulline}	372-75-8	Matsumoto et al. (2491b)
Phenylalanine	63-91-2	Matsumoto et al. (2491b), Sugimura et al. (3829)
Serine	6898-95-9	Kato et al. (2048), Matsumoto et al. (2491b)
Threonine	72-19-5	Matsumoto et al. (2491b)
Tryptophan	73-22-3	Hosaka et al. (1835a), Matsukura et al. (2491a), Matsumoto et al. (2491b), Negishi and Hayatsu (2689a), Sugimura et al. (3829), Takayama et al. (3862d), Yamazoe et al. (4370a), Yoshida and Matsumoto (4390)
Tyrosine	60-18-4	Matsumoto et al. (2491b)
Valine	7004-03-7	Matsumoto et al. (2491b)

tobacco pigment, e.g., porphyrins, makes them particularly liable to pyrolytic destruction because they, unlike nicotine and the other plant alkaloids, are not readily volatilized and swept away as the more intense heat of the cigarette coal approaches (3724).

There are also interactions that occur among amino acids, proteins, and carbohydrates during plant growth and during smoke formation. These interactions form complex mixtures of leaf constituents and complex mixtures resulting from the pyrodegradation and pyrosynthesis of reaction products of amino acids, proteins, and carbohydrates.

In freshly harvested leaf, both reducing sugars and amino acids are present, and these are known to react to form nonvolatile sugar–amino acid compounds, known as Amadori compounds (1671b). A number of these Amadori compounds have been isolated from flue-cured tobacco leaf by Cousins (841a), Tomita et al. (3923), Yamamoto et al. (4362), and Wahl (4081a). Noguchi et al. (2794a) have shown how the free amino acid concentration of leaf decreases during aging and the Amadori compound levels initially increase and then slowly decrease. These changes, especially the decrease in Amadori compounds, indicated the possible progress of Maillard-type reactions during natural aging of leaf tobaccos.

Dickerson et al. (965) found evidence for progress of the Maillard reaction in their studies on aged flue-cured leaf where a number of formylpyrroles were isolated. Dickerson et al. (965) followed the formation of several formylpyrroles from a specific Amadori compound. The Amadori compound was converted via the Maillard reaction to a 3-deoxyosulose which further reacted with either an amino acid or an amine to form the isolated formylpyrroles. In addition to the formylpyrroles, a number of pyrazines and furans, characteristic of nonenzymatic browning reactions, were also isolated from flue-cured tobacco. Thus, there is evidence for the Maillard reaction occurring even before smoking.

Sometimes in sugar–amine browning systems where pyrazines are isolated, there is also found another class of nitrogen heterocyclic compounds, the imidazoles (1835b, 1947a). These compounds have been reported in tobacco smoke by Schumacher and coworkers (3553). In contrast to the pyrazines, only a few imidazoles have been isolated from nonenzymatic browning reactions of foods. This might be due to the unusually high boiling points and polarity of these compounds. Grimmett (1410b) has reviewed the formation of imidazoles from the interaction of carbohydrates and amine sources, and many of the same compounds found to be pyrazine precursors can also form imidazoles. Simple sugars, starches, and cellulose—all known tobacco leaf constituents—are reported to react with amines, including ammonia, to form imidazoles (1351).

Many of the reactions producing imidazoles in tobacco and tobacco smoke involve the interaction of carbohydrates with ammonia which has several precursors in tobacco. Amino acids and proteins can contribute to the formation of smoke amines and the formation of ammonia. Johnson et al. (1964) conclusively demonstrated through experiments with ^{15}N-glycine that it is an ammonia source. In addition to amino acids, nitrates have been shown to be efficiently converted during the smoking of a cigarette to ammonia (1964). This ammonia from nitrates was shown to participate in the formation of many nitrogenous compounds in smoke. Thus, leaf nitrates as well as amino acids and proteins are considered the major sources of ammonia in tobacco smoke.

As to the mode by which certain leaf constituents may form imidazoles, it is commonly recognized that α-dicarbonyl compounds may react with aldehydes in the presence of ammonia to form nitrogen heterocyclic compounds such as imidazoles. The required α-dicarbonyl compounds and aldehydes are well known pyrolysis products of carbohydrates either through thermal (1170a) or Maillard-type (1671a) degradations, and many of these compounds have been isolated from tobacco smoke (3797). It is possible that α-aminoketones, such as those proposed as intermediates in the formation of pyrazines, may also be involved with the formation of imidazoles because reactions producing imidazoles from these compounds have been reported (1410b). Although the formation of imidazoles through carbohydrate and amino acid or protein interaction is especially appealing due to the analogies which can be made with pyrazines, a second origin is also possible. Tobacco leaf contains an appreciable amount of the amino acid, histidine, either in its free form or as part of tobacco protein. Pyrodegradation of this compound in a manner similar to that of tryptophan (2047) could also be a source of some imidazoles in tobacco smoke.

The contribution of the five-membered *N*-containing ring compounds in tobacco and tobacco smoke to smoke flavor is not as well known. The flavor evaluations of some tobacco-derived imidazoles have been described by Schumacher et al. (3553a). The flavors of these compounds are an example of how relatively nonvolatile, flavorless compounds in tobacco leaf can be transformed during the smoking process into a part of the characteristic aroma of tobacco smoke. Leffingwell et al. (2341) and Roberts (3215) in his review of natural tobacco flavor reported that several acetylpyrroles provided a nutty, woody, and sweet taste to tobacco smoke but that formylpyrroles often added harshness to the tobacco smoke aroma. Imidazoles have been reported to provide a sweet chocolate or nutty character to tobacco smoke at low levels but can be bitter at high levels (3215).

The principal precursor for the biosynthesis of ring structures of pyrrolidine, pyrroline, and pyrrole is glutamine (2056b, 2659a, 2848a). Pyrrole structures can also be produced in plants from arginine or ornithine (2056b). The biosynthetic pathway for the production of the imidazole ring structure involves the biosynthesis of histidine through

a series of 10 enzymatic reactions (57a). The first intermediate of the pathway (phosphoribosyl pyrophosphate) is also the starting point for purine and pyrimidine biosynthesis. The amino acid glutamine provides much of the backbone for imidazole which is an intermediate in histidine biosynthesis (429d). From imidazole glycerol phosphate, five additional enzymatic steps are needed to the plant to produce histidine. The imidazoline and imidazolidine rings can be produced by enzymatic hydrogenation of the imidazole ring. The imidazolidine ring is also believed to be produced biosynthetically when glutamate condenses with carbamoyl phosphate to form hydantoin or imidazolidine-2,4-dione. The hydantoin can be enzymatically reduced to imidazolidines (225a). Additionally, hydantoin can be produced in plants by hydrogenation of allantoin (2,5-dioxo-4-imidazolidinyl urea), a cyclic amide naturally occurring in many plants (4068a). Pyrazolidine, pyrazoline, and pyrazoles are produced in plants from 1,3-diaminopropane via pyrazole synthase (C_3) (437a).

The five-membered *N*-containing ring compounds with three nitrogens are the 1,2,3-triazoles and the 1,2,4-triazoles. Triazoles are not produced in plants naturally but are found as structural components of many pesticides and herbicides. Seven herbicides containing a five-membered *N*-containing ring have been identified in tobacco as residues. The pesticides containing a 1,2,4-triazole ring include three fungicides (Triadimefon®, Penconazole®, and Triadimenol®), one herbicide (Sulfentrazone®), and one insecticide (Triazophos®). Two 1,2,3-triazoles (as benzotriazoles) have been identified in tobacco and tobacco smoke to date, Azinphos-Methyl-Oxon® and Azinphos-Methyl®. Both of these pesticides are insecticides. Azinphos-Methyl-Oxon has also been identified as a degradation product of Azinphos-Methyl. All of these triazoles were reported as tobacco pesticide residues (928a, 2913a, 3663, 2650a). The remaining fungicide in this series of five-membered *N*-containing ring compounds with three nitrogens is Iprodione®. Iprodione is an imidazolidinecarboxamide and has been reported as a fungicide residue on tobacco (3585, 3633, 3661a).

Table 17.3 lists the distribution of five-membered *N*-containing ring compounds identified in tobacco, tobacco smoke, and tobacco substitute smoke.

Table 17.4 contains 358 compounds. One hundred and sixteen are pyrroles, 79 are pyrrolidines, and 28 are pyrrolines. There are 16 pyrazoles in Table 17.4. Sixty-two imidazoles, 10 imidazolidines, and 3 imidazolines have been identified in tobacco and tobacco smoke. Five compounds with a 1,2,4-triazole ring have been identified in tobacco. Two compounds with a 1,2,3-triazole ring (as benzotriazoles) have been identified in tobacco and tobacco smoke. The compounds in Table 17.4 exhibit a great deal of functionality. Although each contains a five-membered *N*-containing ring, some are alcohols, ketones, sugar–amines, acids, esters, and imides. Of the 358 compounds listed in Table 17.4, 289 were identified in tobacco smoke, 151 identified in tobacco, and 82 identified in both tobacco and tobacco smoke.

TABLE 17.3
Distribution of Five-Membered *N*-Containing Ring Compounds between Tobacco and Tobacco Smoke

	Number of Identified Five-Membered *N*-Containing Ring Compounds in Tobacco and Tobacco Smoke			
Component	**Total**	**Smoke**	**Tobacco**	**Smoke and Tobacco**
Pyrroles	116	88	50	22
Pyrrolidines	79	64	36	21
Pyrrolines	28	23	7	2
Pyrazoles	16	13	3	0
Imidazoles	62	57	8	3
Imidazolidines	10	8	3	1
Imidazolines	3	1	2	0
Triazoles	7	2	8	3
Totals	321	256	117	52

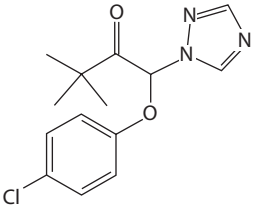
17.1.4 Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Multiple Five-Membered *N*-Containing Rings

Porphyrins are a class of biologically important heterocyclic compounds with a characteristic chemical structure that includes four pyrrole groups (five-membered organic rings each containing a nitrogen atom) linked on opposite sides (α position) through four methine bridges (=CH–) to form a large flat ring structure (see Figure 17.2). A porphyrin in which no metal is inserted in its cavity is called a free base.

Many organic analogs that contain a porphyrin ring are biological pigments and are closely related molecules responsible for many of the vivid colors in living organisms. They often occur combined with metal ions and various substituents as coordination complexes. Chlorophylls are magnesium complexes of porphyrin derivatives (also called phorbines). In plants, these pigments are responsible for photosynthesis and play important roles as respiratory pigments, electron transport carriers, and oxidative enzymes. Several chlorophylls have been identified in tobacco, the most common being chlorophyll *a* and chlorophyll *b*. Chlorophyll a is a waxy blue-black microcrystalline green-plant pigment, $C_{55}H_{72}MgN_4O_5$, with a characteristic blue-green alcohol solution. Chlorophyll *b* is a similar green-plant pigment, $C_{55}H_{70}MgN_4O_6$, having a brilliant green alcohol solution. Several other chlorophyll derivatives have also been isolated from tobacco (3770a).

The biosynthesis of porphyrin involves glycine and succinyl-CoA (from the citric acid cycle) to form *d*-aminolevulinic acid (dALA). Two dALA molecules are combined into porphobilinogen (PBG), which contains the pyrrole ring. Four PBGs are then combined through deamination into hydroxymethylbilane (HMB), which is hydrolyzed to

TABLE 17.4
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	43121-43-3	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)- {Triadimefon®} 		3633	
2.	2433-57-0	3-Buten-2-one, 4-(1*H*-pyrrol-2-yl)-, (*E*)-	2775, 4249		
3.		Ethanone, 1-(alkyl-1*H*-pyrrolyl)-	2773, 4249		
4.		Ethanone, 1-(1,2-dihydro-1*H*-pyrrolyl)-	568b, 4249		
5.		Ethanone, 1-(1-ethyl-1*H*-pyrrol-3-yl)-	568b, 4249		
6.		Ethanone, 1-(methyl-1*H*-pyrrolyl)-	2543, 2761, 2765–2767, 2773, 3557, 4249		
7.	13678-73-4	Ethanone, 1-[1-(2-furanylmethyl)-1*H*-pyrrol-2-yl]-		404, 568b, 3547, 3555, 4249	
8.	20583-33-9	Ethanone, 1-(1*H*-pyrazol-3-yl)-		4249	
9.	25016-16-4	Ethanone, 1-(1*H*-pyrazol-4-yl)-		984, 4249	
10.	1072-83-9	Ethanone, 1-(1*H*-pyrrol-2-yl)- {2-acetylpyrrole; methyl 2-pyrrolyl ketone}	568b, 1360, 1371, 1375a, 1375, 1375b, 1428, 1586, 1587a, 2337, 2387, 2543, 2545, 2570, 2731, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3059, 3266, 3397, 3410, 3444, 3553, 3555, 3557, 4249, 4407, 5811b	120, 404, 568b, 937, 965, 1063–1066, 1068–1074, 1590a, 1854, 2337, 2386, 2389, 2544, 2861a, 2862, 2917a, 2939, 3188, 3198, 3215, 3217, 3266, 3354, 3543, 3545, 3547, 3555, 3560, 3561, 3797, 3905, 3974a, 4249, 5811b	1360, 1375a, 2387
11.	1072-82-8	Ethanone, 1-(1*H*-pyrrol-3-yl)- {3-acetylpyrrole; methyl 3-pyrrolyl ketone}	568b, 1371, 1586, 1587, 2543, 2767, 2769, 2773, 2775, 3255, 3410, 3553, 3557, 4249	568b, 3549, 4249	
12.	20970-50-7	Ethanone, 1-(1-methyl-1*H*-imidazol-5-yl)-	568b, 1587, 1590, 2775, 4249, 5811b		
13.	37687-18-6	Ethanone, 1-(1-methyl-1*H*-pyrazol-4-yl)-	3553, 4249		
14.	932-16-1	Ethanone, 1-(1-methyl-1*H*-pyrrol-2-yl)-	568b, 1360, 1375a, 2387, 3491, 4249, 4570a, 5811b	568b, 984, 1248, 3201, 3215, 3491, 3974a, 4249	1360, 1375a, 2387
15.	932-62-7	Ethanone, 1-(1-methyl-1*H*-pyrrol-3-yl)-	568b, 1587, 3491, 4249, 4570a, 5811b	568b, 937, 1248, 3491, 3974a, 4249	
16.	55041-85-5	Ethanone, 1-(2,3-dihydro-1*H*-pyrrolizin-5-yl)-	568b, 2543, 2773, 4249	568b, 3547, 4249	
17.	19005-95-9	Ethanone, 1-(2,4,5-trimethyl-1*H*-pyrrol-3-yl)-	2543, 2773, 4249		
18.	85213-22-5	Ethanone, 1-(2,5-dihydro-1*H*-pyrrol-2-yl)- {2-acetylpyrroline}		2917a, 4249	
19.		Ethanone, 1-(2,5-dihydro-5-methyl-1*H*-pyrrol-3-yl)-	2767, 4249		
20.	1500-94-3	Ethanone, 1-(2,5-dimethyl-1*H*-pyrrol-3-yl)-	1375, 1375b, 2767, 3410, 3557, 4249		
21.	78210-66-9	Ethanone, 1-(2-methyl-1*H*-imidazol-4-yl)-	568b, 1587, 4249, 5811b		

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

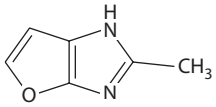
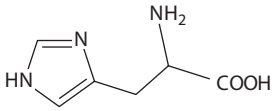
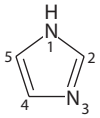
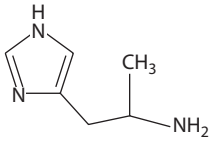
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
22.	60026-20-2	Ethanone, 1-(2-pyrrolidinyl)- {2-acetylpyrrolidine}	2727, 2775, 3410, 3491, 3650, 4159, 4249	937, 1154, 2095, 2389, 2544, 3219, 3491, 3550, 3560, 3561, 3974a, 4249	
23.	72693-15-3	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-	3553, 4249, 5811b		
24.	72709-76-3	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-	3553, 4249		
25.	2524-90-5	Ethanone, 1-(4-methyl-1*H*-imidazol-2-yl)-	568b, 1351, 3553, 4249, 5811b		
26.	23328-91-8	Ethanone, 1-(5-methyl-1*H*-imidazol-2-yl)-	568b, 4249		
27.	6982-72-5	Ethanone, 1-(5-methyl-1*H*-pyrrol-2-yl)- {2-acetyl-5-methylpyrrole}	568b, 1375, 1375b, 1586, 1587a, 2337, 2570, 2767, 2775, 3553, 3557, 4159, 4249, 5811b	568b, 2337, 2389, 2544, 3205, 3219, 3491, 3543, 3560, 3561, 4249, 5811b	
28.	78210-67-0	Ethanone, 1-(5-propyl-1*H*-imidazol-4-yl)-	568b, 1587, 4249, 5811b		
29.	61891-76-7	Ethanone, 1-(dihydro-3,4-dimethylpyrrol-2-yl)-	568b, 3553, 4249		
30.		Formamide, *N*-(3-methylpyrrolyl-2-ethyl)-	568b, 4249		
31.	29118-61-4	*D*-Fructose, 1-(2-carboxy-1-pyrrolidinyl)-1-deoxy-, (S)-		434, 1063–1066, 1068–1074, 1351, 2337, 2339b, 3555, 3639, 3923, 3973, 3974a, 4159, 4249, 5811b	
32.	61481-02-5	2-Furanmethanol, 5-(1-pyrrolidinylmethyl)-	3553, 4249		
33.	61893-05-8	1*H*-Furo[2,3-*d*]imidazole, 2-methyl- 	1351, 3553, 4249		
34.	88476-94-2	Glycine, *N*-(1-nitroso-*L*-prolyl)-		3951, 4249	
35.	7006-35-1	Histidine		429b, 3797, 4249, 5699, 5785, 5831	
36.	71-00-1	*L*-Histidine 		120, 158, 553, 622, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5478, 5699, 5785, 5811b, 5831	
37.	332-80-9	*L*-Histidine, 1-methyl-	1083, 4249	1086, 1351, 2337, 2597a, 3491, 3797, 3972, 3974a, 4249	
38.	368-16-1	*L*-Histidine, 3-methyl-	1083, 4249	1086, 2597a, 4249	
39.	62504-27-2	*L*-Histidine, *N*-(1-carboxyethyl)-, (R)-		3565, 4249	
40.	288-32-4	1*H*-Imidazole {1,3-diazole} 	568b, 1124a, 1360, 1375a, 1590, 2543, 2761, 2762, 2765–2767, 2773, 3255, 3553, 3559, 4249, 5811b	568b, 2079, 3215, 4249	1360, 1375a

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
41.	2466-76-4	1*H*-Imidazole, 1-acetyl-		568b, 937, 3219, 3491, 4249	
42.		1*H*-Imidazole, C_3-alkyl- {three isomers detected}	568b, 3559, 4249		
43.		1*H*-Imidazole, C_4-alkyl- {five isomers detected}	568b, 3559, 4249		
44.		1*H*-Imidazole, C_5-alkyl- {four isomers detected}	568b, 3559, 4249		
45.	50790-93-7	1*H*-Imidazole, butyl-	568b, 1124a, 4249		
46.		1*H*-Imidazole, 2-butyl-	568b, 1351, 3255, 4249		
47.	931-35-1	1*H*-Imidazole, 4,5-dihydro-2-ethyl-4-methyl-		2359, 4249	
48.	1739-84-0	1*H*-Imidazole, 1,2-dimethyl-	568b, 1371, 2543, 2773, 2775, 3386, 3410, 3559, 4249		
49.	6338-45-0	1*H*-Imidazole, 1,4-dimethyl-	568b, 3255, 3559, 4249		
50.	10447-93-5	1*H*-Imidazole, 1,5-dimethyl-	568b, 3559, 4249		
51.	930-62-1	1*H*-Imidazole, 2,4-dimethyl-	568b, 1351, 1371, 1590, 2775, 3255, 3410, 3553, 3559, 4249, 5811b		
52.	2302-39-8	1*H*-Imidazole, 4,5-dimethyl-	568b, 1351, 1371, 3255, 3410, 3553, 3559, 4249, 5811b		
53.	37455-73-5	1*H*-Imidazole, 1,4-dimethyl-2-(1-methylethyl)-	3559, 4249		
54.	40688-28-6	1*H*-Imidazole, 2,4-dimethyl-5-(1-methylethyl)-	568b, 3553, 4249, 5811b		
55.		1*H*-Imidazole, 2,5-dimethyl-4-(1-methylethyl)-	1351, 4249		
56.		1*H*-Imidazole, 1,4-dimethyl-5-phenyl-	2601a, 4249		
57.	51-45-6	1*H*-Imidazole, 4-ethanamine		568b, 4249, 4437	
58.	75614-87-8	1*H*-Imidazole-4-ethanamine, α-methyl- 		5603, 5777	
59.		1*H*-Imidazole, ethyl-	1124a, 4249		
60.	7098-07-9	1*H*-Imidazole, 1-ethyl-	568b, 3559, 4249		
61.	1072-62-4	1*H*-Imidazole, 2-ethyl-	568b, 3386, 3559, 4249, 5811b		
62.	19141-85-6	1*H*-Imidazole, 4-ethyl-	568b, 1351, 2543, 2773, 3255, 3553, 3559, 4249		
63.	21202-52-8	1*H*-Imidazole, 1-ethyl-2-methyl-	3559, 4249		
64.	931-36-2	1*H*-Imidazole, 2-ethyl-4-methyl-	568b, 3559, 4249		
65.		1*H*-Imidazole, 2-ethyl-4-(1-methylethyl)-	568b, 4249		
66.	29239-89-2	1*H*-Imidazole, 4-ethyl-2-methyl-	1351, 1590, 3553, 3559, 4249, 5811b		
67.	37455-59-7	1*H*-Imidazole, 4-ethyl-2-(1-methylethyl)-	568b, 1351, 3410, 3553, 3559, 4249, 5811b		
68.	37455-56-4	1*H*-Imidazole, 4-ethyl-2-propyl-	3553, 4249		
69.		1*H*-Imidazole, methyl-	1371, 4249		
70.	616-47-7	1*H*-Imidazole, 1-methyl-	568b, 1351, 2543, 2767, 3255, 3386, 3410, 3553, 3559, 4249, 4570a, 5811b		
71.	693-98-1	1*H*-Imidazole, 2-methyl-	568b, 2773, 2775, 3255, 3386, 3398, 3410, 3559, 4249		
72.	822-36-6	1*H*-Imidazole, 4-methyl-	568b, 1351, 1590, 3255, 3398, 3410, 3553, 3559, 4249, 5811b		
73.	37455-55-3	1*H*-Imidazole, 4-methyl-2-propyl-	5553b, 5811, 5811a, 5811b		

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

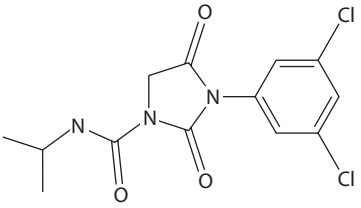
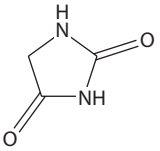
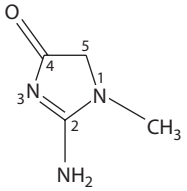
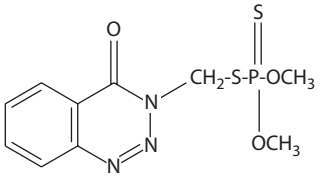
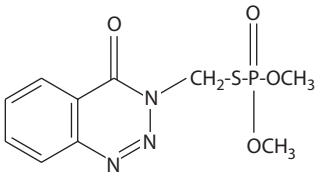
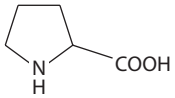
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
74.	36947-68-9	1*H*-Imidazole, 2-(1-methylethyl)-	568b, 1351, 3553, 3559, 4249, 5811b		
75.	58650-48-9	1*H*-Imidazole, 4-(1-methylethyl)-	568b, 1351, 3553, 3559, 4249, 5811b		
76.	22509-02-0	1*H*-Imidazole, 1-methyl-2-(1-methylethyl)-	3559, 4249		
77.	37455-52-0	1*H*-Imidazole, 2-methyl-4-(1-methylethyl)-	3559, 4249		
78.	37455-58-6	1*H*-Imidazole, 4-methyl-2-(1-methylethyl)-	568b, 1351, 3410, 3553, 4249, 5811b		
79.	61893-07-0	1*H*-Imidazole, 4-methyl-2-(1-methylpropyl)-	568b, 1351, 3553, 4249, 5811b		
80.	61893-06-9	1*H*-Imidazole, 2-(1-methylpropyl)-	568b, 3553, 3559, 4249, 5811b		
81.	61893-08-1	1*H*-Imidazole, 4-(2-methylpropyl)-	1351, 3553, 4249, 5811b		
82.		1*H*-Imidazole, pentyl-	1124a		
83.	91491-09-7	1*H*-Imidazole, propyl-	1124a, 4249, 5811b		
84.	1842-63-3	1*H*-Imidazole, 1,2,4-trimethyl-	3255, 3559, 4249		
85.	20185-22-2	1*H*-Imidazole, 1,4,5-trimethyl-	3559, 4249		
86.	822-90-2	1*H*-Imidazole, 2,4,5-trimethyl-	568b, 1351, 1590, 2775, 3255, 3553, 3559, 4249, 5811b		
87.	10111-08-7	1*H*-Imidazole-2-carboxaldehyde	568b, 4249		
88.	36734-19-7	1-Imidazolidinecarboxamide,3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®} 		3585c, 3633, 3661a	
89.	461-72-3	2,4-Imidazolidinedione {hydantoin} 	568b, 3553, 4249, 5811b		
90.	61893-10-5	2,4-Imidazolidinedione, 1-(1-methylethyl)-	3553, 4249, 5811b		
91.	17374-27-5	2,4-Imidazolidinedione, 1,5-dimethyl-	568b, 3553, 4249, 5811b		
92.	61893-09-2	2,4-Imidazolidinedione, 1-ethyl-	568b, 3553, 4249, 5811b		
93.	63637-90-1	2,4-Imidazolidinedione, 3-(1-methylethyl)-	568b, 4249		
94.	16935-34-5	2,4-Imidazolidinedione, 5-(1-methylethyl)-	568b, 2767, 3553, 4249, 5811b		
95.	15414-82-1	2,4-Imidazolidinedione, 5-ethyl-	568b, 2601a, 3553, 4249, 5811b		
96.	616-04-6	2,4-Imidazolidinedione, 1-methyl-	568b, 4249		
97.		2,4-Imidazolidinedione, 3-methyl-	568b, 4249		
98.	616-03-5	2,4-Imidazolidinedione, 5-methyl-	568b, 2767, 3255, 3553, 3557, 4249, 5811b	568b, 3561, 4249	
99.	96-45-7	2-Imidazolidinethione {ethylenethiourea}	124, 568b, 3265, 3300, 3714, 4249, 5811b, 5869a		
100.	61892-75-9	2*H*-Imidazol-2-one, 1,5-dihydro-5-methyl-	568b, 3553, 4249, 5811b		

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
101.	60-27-5	2*H*-Imidazol-2-one, 2-amino-1,5-dihydro-5-methyl- {creatinine} 		751, 755, 756, 4249	
102.	86-50-0	Phosphorodithioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Guthion®; Azinphos-Methyl®} 	417, 419, 1457, 1884, 3302, 4249, 21A19	419, 1219a, 1219c, 1457, 1884, 2650b, 3381, 3973, 4249, 4271a, 21A19	
103.	24017-47-8	Phosphorothioic acid, *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) ester {Triazophos®}		2650a	
104.	961-22-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl) methyl] ester {Azinphos-Methyl-Oxon®} 	419, 3302, 4249	419, 4249	
105.	147-85-3	*L*-Proline 	1351, 1910, 1914, 1933, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249, 4319, 5048	120, 158, 480, 486, 749, 751–756, 826a, 927, 1033, 1053, 1063–1066, 1068–1074, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1933a, 1971, 2133, 2270, 2337, 2394a, 2395, 2453, 2529, 2532, 2592, 2597a, 2795, 2858, 2911c, 2914, 2939, 3059, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4226, 4159, 4224, 4226, 4244, 4249, 4359, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5881, 5896, 5905, 5907	

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

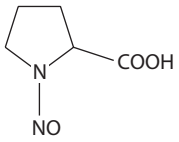
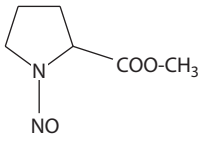
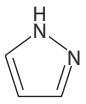
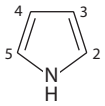
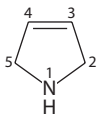
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
106.	147427-29-0	*L*-Proline, 1-[1-[1-(1-*L*-seryl-*L*-prolyl)-*L*-prolyl]-*L*-prolyl]-		4249	
107.		*L*-Proline, *N*-(1-deoxy-*D*-fructos-1-yl)-		3639	
108.		Proline, hydroxy-		5907	
109.	18610-59-8	*L*-Proline, 1-hydroxy-		1063–1066, 1068–1074, 1351, 2337, 2394a, 2597a, 3491, 3797, 3973, 3974a, 4224, 4226, 4249	
110.	7519-36-0	*L*-Proline, 1-nitroso- {NPRO} 	204–206, 486, 499, 509, 1058, 1673, 1695, 1719, 1870, 1871, 3256, 3260, 3300, 3943a, 3944–3946, 3951, 4249	466, 468, 485, 486, 498, 499, 511, 992, 1870, 1871, 3256, 3566, 3943a, 3944–3948, 3973, 4130, 4249	
111.	35909-01-4	*L*-Proline, 1-nitroso-, methyl ester 	3256, 3300	466, 485, 3256	
112.	62137-28-4	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl) oxy]-, *trans*-		4249, 4429	
113.	62137-29-5	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-ar abinofuranosyl)oxy]-, *trans*-		4249, 4429	
114.	51-35-4	*L*-Proline, 4-hydroxy-, *trans*-		120, 1305a, 4249, 5811b	
115.	30310-80-6	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}		486, 3300, 3947, 3948, 4249, 5811b	
116.	1073-26-3	1-Propanone, 1-(1*H*-pyrrol-2-yl)-	568b, 1586, 2767, 3553, 3557, 3650, 4249, 5811b	568b, 2389, 2544, 3547, 4249, 5811b	
117.	496-49-1	2-Propanone, 1-(1-methyl-2-pyrrolidinyl)-		2917a, 4249	
118.	288-13-1	1*H*-Pyrazole 	279, 568b, 1580, 2773, 3410, 3555, 4249	568b, 1580, 4249	
119.		1*H*-Pyrazole, C_2-alkyl-	2773		
120.	13808-64-5	1*H*-Pyrazole, 4-bromo-3-methyl-	568b, 4249		
121.	67771-72-6	1*H*-Pyrazole, dimethyl-	1426, 1427, 3491, 4249		
122.	2820-37-3	1*H*-Pyrazole, 3,4-dimethyl-	568b, 1427, 4249		
123.	67-51-6	1*H*-Pyrazole, 3,5-dimethyl-	568b, 3410, 4249		
124.	1131-16-4	1*H*-Pyrazole, 3,5-dimethyl-1-phenyl-	4407, 4249		
125.	66719-08-2	1*H*-Pyrazole, methyl-	1667, 4249		
126.	930-36-9	1*H*-Pyrazole, 1-methyl-	568b, 4249		
127.	1453-58-3	1*H*-Pyrazole, 3-methyl-	568b, 1371, 2775, 3410, 4249, 5811b		
128.	3347-62-4	1*H*-Pyrazole, 3-methyl-5-phenyl-		3430, 4249, 5811b	
129.	7554-65-6	1*H*-Pyrazole, 4-methyl-	568b, 4249		
130.	1072-91-9	1*H*-Pyrazole, 1,3,5-trimethyl-	4407, 4249		

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

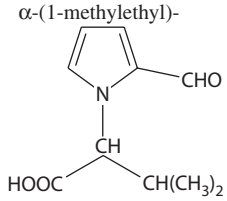
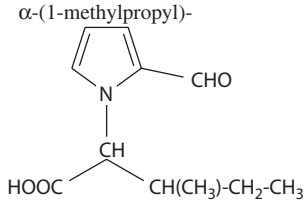
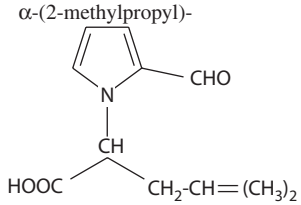
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
131.	5519-42-6	1*H*-Pyrazole, 3,4,5-trimethyl-	568b, 2773, 4249		
132.	106398-69-0	Pyrrole, butyl-	3854, 4249		
133.	71607-59-5	Pyrrole, dihydromethyl-	1153, 4249		
134.		Pyrrole, hydroxymethyl-	1586, 4249		
135.	109-97-7	1*H*-Pyrrole {azole} 	38, 157, 172, 241, 299, 480, 568b, 722, 884, 920, 1078, 1083, 1084, 1099, 1140, 1215, 1244, 1245, 1263, 1339, 1348–1350, 1354, 1361, 1375a, 1416, 1418, 1416–1418, 1426–1428, 1445, 1580, 1586, 1589, 1590, 1634, 1639, 1744, 1842, 1857, 2088, 2170, 2270, 2343, 2382, 2493, 2543, 2545, 2570, 2628, 2629, 2636, 2724, 2765–2767, 2775, 2799a, 2857, 2912, 2939, 3255, 3266, 3324, 3308, 3397, 3398, 3499, 3505, 3530, 3553, 3559, 3797, 3854, 3887, 4159, 4249, 5034, 5079, 5359, 5512, 5811b	568b, 722, 984, 1053, 1063–1066, 1068–1074, 1086, 1244, 1580, 1590a, 2359, 2386, 2724, 2767, 2903, 2908, 2917a, 2939, 3224, 3266, 3797, 3973, 4249, 5079, 5811b	1354, 1375a
136.	609-41-6	1*H*-Pyrrole, 1-acetyl-	4249		
137.	23105-58-0	1*H*-Pyrrole, 1-acetyl-2,3-dihydro-	568b, 1587, 4249, 5811b		
138.	38207-11-3	1*H*-Pyrrole, 1-acetyl-2-methyl-	4249, 4633	2386, 3491, 4249	
139.		1*H*-Pyrrole, 1-acetyl-3-methyl-	4249	937, 3491, 4249	
140.	589-33-3	1*H*-Pyrrole, 1-butyl-	568b, 1587a, 3491, 3854, 4249, 5811b		
141.	50691-30-0	1*H*-Pyrrole, 1-butyl-2-methyl-	568b, 4249		
142.	62672-96-2	1*H*-Pyrrole, 1-(1-cyclohexen-1-yl)-	568b, 2767, 2769, 4249		
143.	28350-87-0	1*H*-Pyrrole, dihydro-	3559, 4249, 5034, 5811b	5811b	
144.	638-31-3	1*H*-Pyrrole, 2,3-dihydro- {2-pyrroline}	568b, 4249		
145.	109-96-6	1*H*-Pyrrole, 2,5-dihydro- {3-pyrroline} 	568b, 1078, 1084, 1140, 2724, 2889, 3491, 3559, 3797, 4249, 5811b	568b, 1877, 3491, 4249, 5811b	
146.	554-15-4	1*H*-Pyrrole, 2,5-dihydro-1-methyl-	5811b	2270, 2939, 3444, 3491, 3797, 4249, 5811b	
147.	5724-81-2	1*H*-Pyrrole, 3,4-dihydro- {1-pyrroline}	568b, 4249		
148.		1*H*-Pyrrole, dimethyl-	5034		
149.	600-28-2	1*H*-Pyrrole, 2,3-dimethyl-	568b, 2079, 4249		
150.	625-82-1	1*H*-Pyrrole, 2,4-dimethyl-	568b, 2079, 4249	568b, 984, 4249	
151.	625-84-3	1*H*-Pyrrole, 2,5-dimethyl-	299, 568b, 1063–1066, 1068–1074, 4249	568b, 984, 4249	
152.	822-51-5	1*H*-Pyrrole, 3,4-dimethyl-	2079, 4249		
153.	2433-66-1	1*H*-Pyrrole, 2-ethenyl-		984, 4249	
154.		1*H*-Pyrrole, ethyl-	5034		
155.	617-92-5	1*H*-Pyrrole, 1-ethyl-	314, 568b, 1587a, 3491, 3559, 3854, 4249	568b, 984, 4249	

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
156.	19983-83-6	1*H*-Pyrrole, 1-ethyl-2-methyl-	568b, 4249		
157.	1551-16-2	1*H*-Pyrrole, 2-ethyl-	5770		
158.	488-92-6	1*H*-Pyrrole, 3-ethyl-4-methyl-	568b, 4249		
159.		1*H*-Pyrrole, 3-ethyl-1-phenyl-	1378, 4249		1378
160.		1*H*-Pyrrole, 4-ethyl-3-methyl-		984, 4249	
161.		1*H*-Pyrrole, 1-(2-furanyl)-	2731, 2735, 4249		
162.	1438-94-4	1*H*-Pyrrole, 1-(2-furanylmethyl)-	568b, 1587a, 2727, 3410, 3491, 4249, 5811b	568b, 2336, 4249	
163.	27417-39-6	1*H*-Pyrrole, methyl-	3553, 3897, 4249, 5811b		
164.	96-54-8	1*H*-Pyrrole, 1-methyl-	299, 314, 568b, 1063–1066, 1068–1074, 1078, 1084, 1140, 1153, 1154, 1313, 1348–1350, 1354, 1375a, 1419, 1587a, 1589, 2387, 2506, 2507, 2543, 2545, 2570, 2724, 2765, 2767, 2777, 3398, 3491, 3530, 3797, 3854, 4249, 4360, 5770	120, 568b, 984, 1087, 1154, 2917a, 3491, 3973, 3974a, 4249, 5811b	1354, 1375a, 2387, 2506, 2507
165.	636-41-9	1*H*-Pyrrole, 2-methyl-	222–224, 299, 1365, 1587, 1590, 3255, 3559, 4249, 5811b	5811b, 5906	
166.		1*H*-Pyrrole, 2-methyl-1-phenyl-	1378, 4249		1378
167.	616-43-3	1*H*-Pyrrole, 3-methyl-	299, 3255, 4249		
168.		1*H*-Pyrrole, 3-methyl-1-phenyl-	1378, 4249		1378
169.	13679-79-3	1*H*-Pyrrole, 1-(3-methylbutyl)-	568b, 1587a, 2731, 2735, 3854, 4249, 5811b	568b, 1154, 3491, 4249	
170.	66309-87-3	1*H*-Pyrrole, 1-(2-methyl-1-cyclohexen-1-yl)-	568b, 2767, 2769, 4249		
171.	7057-97-8	1*H*-Pyrrole, 1-(1-methylethyl)-	1587a, 3491, 3854, 4249		
172.	13678-52-9	1*H*-Pyrrole, 1-[(5-methyl-2-furanyl)methyl]-	568b, 1366, 4249		
173.	78075-83-9	1*H*-Pyrrole, 2-methyl-1-(phenylmethyl)-	568b, 2767, 4249		
174.	20884-13-3	1*H*-Pyrrole, 1-(2-methylpropyl)-	568b, 1587a, 3491, 3854, 4249, 5811b	5811b	
175.	61480-97-5	1*H*-Pyrrole, 1-(1-oxobutyl)-	2767, 3553, 3557, 4249		
176.	699-22-9 1551-12-8	1*H*-Pyrrole, 1-pentyl-	568b, 1587a, 3491, 3854, 4249, 5811, 5811a, 5811b	5811b	
177.	635-90-5	1*H*-Pyrrole, 1-phenyl-	568b, 1375, 1375b, 1378, 2506, 2507, 2767, 4249, 5811b		1378, 2506, 2507
178.	50691-29-7	1*H*-Pyrrole, 1-(2-phenylethyl)-	568b, 1063–1066, 1068–1074, 2769, 3410, 4249		
179.	5145-64-2	1*H*-Pyrrole, 1-propyl-	568b, 1587a, 3491, 3854, 4249		
180.	1551-08-2	1*H*-Pyrrole, 2-propyl-		1157, 4249	
181.	71646-51-0	1*H*-Pyrrolecarbonitrile, methyl-	2526, 2761, 2767, 4249		
182.	89145-04-0	1*H*-Pyrrolecarboxaldehyde		3905, 4249	
183.	72692-79-6	1*H*-Pyrrolecarboxylic acid, ethyl ester	2767, 3553, 4249		
184.	84499-92-3	1*H*-Pyrrole-1-acetic acid, 2-(ethoxymethyl)-5-formyl-		4249, 4573a, 5811b	
185.	61837-43-2	1*H*-Pyrrole-1-acetic acid, 2-ethyl-5-formyl-α-(2-methylpropyl)-		4249, 4573a	

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

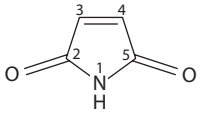
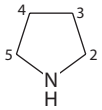
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
186.	60026-07-5	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylethyl)- 		965, 2544, 4249	
187.	60026-08-6	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylpropyl)- 		965, 2544, 4249	
188.	60026-09-7	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(2-methylpropyl)- 		965, 2544, 4249	
189.		1*H*-Pyrrole-1-acetic acid, 2-formyl-5-hydroxymethyl-α-(2-methylpropyl)-	2337, 4249		
190.	61837-42-1	1*H*-Pyrrole-1-acetic acid, 2-formyl-α,5-dimethyl-		2544, 4249	
191.	61837-35-2	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-hexyl-		2544, 4249	
192.	60026-30-4	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-methyl-		2544, 4249	
193.	61837-38-5	1*H*-Pyrrole-1-butanoic acid, 2-formyl-		4249, 4573a	
194.	61837-39-6	1*H*-Pyrrole-1-butanoic acid, 2-formyl-γ-methyl-		4249, 4573a	
195.	61837-44-3	1*H*-Pyrrole-1-butanoic acid, 2-formyl-5-methyl-		4249, 4573a	
196.	78249-88-4	1*H*-Pyrrole-1-carboxaldehyde, 1-methyl-	5811, 5811a, 5811b		
197.	61837-40-9	1*H*-Pyrrole-1-hexanoic acid, 2-formyl-		4249, 4573a	
198.	61837-41-0	1*H*-Pyrrole-1-octanoic acid, 2-formyl-		4249, 4573a	
199.	70898-32-7	1*H*-Pyrrole-1-octanoic acid, 2-formyl-5-methyl-		4249, 4573a	
200.	61837-37-4	1*H*-Pyrrole-1-propanoic acid, β-ethyl-2-formyl-		4249, 4573a	
201.	61837-36-3	1*H*-Pyrrole-1-propanoic acid, 2-formyl-β-methyl-		4249, 4573a	
202.		1*H*-Pyrrole-2-acetaldehyde, α-hydroxy-	1587, 4249		
203.	72693-01-7	1*H*-Pyrrole-2-acetaldehyde, α-oxo-	568b, 1587, 4249, 5811b		
204.	4513-94-4	1*H*-Pyrrole-2-carbonitrile	1365, 1371, 1586, 1587a, 2761, 2762, 2765, 2766, 2773, 3410, 3491, 3650, 4249, 5811b		
205.	133829-71-7	1*H*-Pyrrole-2-carbonitrile, methyl- {two isomers}	1587a, 2761, 2762, 2765, 2766, 4249		

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
206.	26173-92-2	1*H*-Pyrrole-2-carbonitrile, 5-methyl-	568b, 1587, 2543, 2761, 2765, 2766, 2773, 2775, 3491, 3650, 4249, 5811b		
207.	1003-29-8	1*H*-Pyrrole-2-carboxaldehyde	568b, 1075, 1360, 1371, 1375a, 1586, 1587a, 1590, 2337, 2387, 2545, 2570, 2761, 2765–2767, 2773, 2775, 2777, 3255, 3410, 3491, 3553, 3557, 3650, 4249, 5811b	404, 568b, 937, 965, 1590, 2282, 2337, 2386, 2389, 2544, 2917a, 3198, 3219, 3491, 3547, 3549, 3550, 3905, 3974a, 4249	1360, 1375a, 2387
208.	13788-32-4	1*H*-Pyrrole-2-carboxaldehyde, 1-(2-furanylmethyl)-		404, 568b, 3547, 3555, 4249	
209.	13678-79-0	1*H*-Pyrrole-2-carboxaldehyde, 1-(3-methylbutyl)-		568b, 937, 3491, 4249, 5811b	
210.		1*H*-Pyrrole-2-carboxaldehyde, ethyl-	1364, 1371, 4249		
211.	2167-14-8	1*H*-Pyrrole-2-carboxaldehyde, 1-ethyl-	568b, 2767, 3410, 4249		
212.		1*H*-Pyrrole-2-carboxaldehyde, methyl-	1370, 4249	2386, 4249	
213.	1192-58-1	1*H*-Pyrrole-2-carboxaldehyde, 1-methyl-	568b, 1587, 1587a, 1590, 2337, 2767, 3555, 4159, 4249	568b, 937, 965, 2337, 2339a, 2386, 2389, 2544, 3203, 3205, 3219, 3491, 3547, 3555, 3905, 4249	
214.	29813-44-3	1*H*-Pyrrole-2-carboxaldehyde, 5-(hydroxymethyl)-1-methyl-	568b, 1587, 4249, 5811b	404, 568b, 4249	
215.	52115-69-2	1*H*-Pyrrole-2-carboxaldehyde,5-[(acetyloxy)methyl]-		4249, 4786a	
216.	1192-79-6	1*H*-Pyrrole-2-carboxaldehyde, 5-methyl-	568b, 1375, 1375b, 1586, 1587a, 2337, 2387, 2543, 2545, 2767, 2773, 3553, 3555, 3557, 4159, 4249	404, 568b, 2337, 2389, 2544, 3203, 3205, 3219, 3491, 3543, 3547, 3555, 3560, 3561, 4249	2387
217.	4551-72-8	1*H*-Pyrrole-2-carboxamide	568b, 2767, 2775, 3553, 3557, 4249, 5811b		
218.	634-97-9	1*H*-Pyrrole-2-carboxylic acid	568b, 1360, 1375a, 3553, 4249, 5811b		1360, 1375a
219.	3220-74-4	1*H*-Pyrrole-2-carboxylic acid, 2,5-dihydro-		3797, 4249	
220.	3757-53-7	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-	2767, 4249		
221.	3284-51-3	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, ethyl ester	568b, 3553, 4249, 5811b		
222.	1194-97-4	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, methyl ester	568b, 3553, 4249		
223.	1193-62-0	1*H*-Pyrrole-2-carboxylic acid, methyl ester	1587a, 3650, 4249, 5811b	5811b	
224.		1*H*-Pyrrole-3-acetonitrile	1586, 2767, 4249		
225.	7126-38-7	1*H*-Pyrrole-3-carbonitrile	568b, 1375, 1375b, 1586, 2543, 2545, 2761, 2762, 2765, 2766, 2773, 2775, 3557, 4249		
226.	17619-39-5	1*H*-Pyrrole-3-carboxaldehyde, 2-methyl-	568b, 1371, 1586, 2543, 2767, 2773, 3410, 3553, 4249, 5811b	568b, 2544, 3549, 3550, 4249, 5811b	
227.	103002-58-0	1*H*-Pyrrole-3-carboxaldehyde, 4,5-dihydro-2-methyl-		4159b, 4249	
228.	78210-62-5	1*H*-Pyrrole-3-carboxaldehyde, 5-ethyl-	568b, 1587, 4249, 5811b		
229.	936-12-9	1*H*-Pyrrole-3-carboxylic acid, 2-methyl-, ethyl ester	568b, 2543, 2773, 4249		
230.	487-90-1	1*H*-Pyrrole-3-propanoic acid, 5-(aminomethyl)-4-(carboxymethyl)-		4870, 4249	

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
231.	541-59-3	1*H*-Pyrrole-2,5-dione {maleimide} 	568b, 1580, 2775, 3553, 3557, 4249	568b, 1580, 2336, 2389, 2544, 3186, 3188, 3491, 3974a, 4249, 5811b	
232.		1*H*-Pyrrole-2,5-dione, 1,3-dimethyl-4-ethyl-	568b, 4249		
233.	29720-92-1	1*H*-Pyrrole-2,5-dione, ethylmethyl-	1586, 4249	937, 3491, 3560, 3561, 4249	
234.	128-53-0	1*H*-Pyrrole-2,5-dione, 1-ethyl-	568b, 1586, 2767, 4249		
235.	5997-61-5	1*H*-Pyrrole-2,5-dione, 3-ethyl-	568b, 1586, 4249		
236.	15542-97-9	1*H*-Pyrrole-2,5-dione, 3-ethyl-1-methyl-	568b, 4249		
237.	61892-73-7	1*H*-Pyrrole-2,5-dione, 3-(hydroxymethyl)-	3553, 4249		
238.	61892-71-5	1*H*-Pyrrole-2,5-dione, 3,4-bis(hydroxymethyl)-1-methyl-	568b, 3553, 4249	568b, 2544, 3186, 4249	
239.	17825-86-4	1*H*-Pyrrole-2,5-dione, 3,4-dimethyl-	568b, 1075, 1364, 1586, 2545, 2570, 2767, 3553, 3557, 4249, 4407	404, 568b, 2389, 2544, 3215, 3491, 4249, 5811b	
240.	61892-72-6	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-(hydroxymethyl)-	3553, 4249	2544, 3186, 4249	
241.	20189-42-8	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	568b, 1063–1066, 1068–1075, 1364, 2382, 2387, 2545, 2570, 2767, 3553, 3557, 4249, 4407, 5811b	404, 568b, 1590a, 2339a, 2386, 2389, 2544, 3215, 3491, 3543, 3547, 3549, 3550, 3560, 3561, 3905, 4249, 5811b	2387
242.	1072-87-3	1*H*-Pyrrole-2,5-dione, 3-methyl-	1375, 1375b, 1586, 2543, 2767, 2773, 3553, 3557, 4249, 4407, 5811b		
243.	60026-19-9	1*H*-Pyrrole-2,5-dione, 3-propyl-		2389, 2544, 3491, 4249	
244.	3317-61-1	2*H*-Pyrrole, 3,4-dihydro-2,2-dimethyl-, 1-oxide {DMPO}	4249, 17A01		
245.	121197-26-0	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-(2-methylpropyl)-	3429a, 4249	5811b	
246.	121197-16-8	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-propyl-	3429a, 4249	5811b	
247.	121197-27-1	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-bis(2-methylpropyl)-	3429a, 4249		
248.	121197-23-7	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dibutyl-	3429a, 4249	5811b	
249.	121197-14-6	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dipropyl-	3429a, 4249	5811b	
250.	121197-21-5	2*H*-Pyrrole-2,4(3*H*)-dione, 5-(2-methylpropyl)-3-propyl-	3429a, 4249	5811b	
251.	121197-24-8	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-(2-methylpropyl)-	3429a, 4249	5811b	
252.	121213-26-1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-propyl-	3429a, 4249	5811b	
253.	72692-82-1	1*H*-Pyrrolemethanol	1586, 4249		
254.	123-75-1	Pyrrolidine 	222–224, 568b, 1078, 1083, 1084, 1099, 1137, 1140, 1445, 1744, 1842, 1999, 2088, 2724, 2734, 2749, 2799a, 2883, 2889, 3059, 3255, 3302, 3308, 3444, 3491, 3505, 3797, 5034, 5079, 5512, 5811b	120, 289, 480, 568b, 1086, 1087, 2001, 2270, 2283, 2746, 2889, 2939, 3444, 3491, 3973, 3974a, 5079, 5811b, 17B11	

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

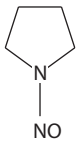
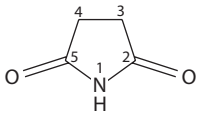
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
255.	71607-78-8	Pyrrolidine, diethyl-	2601a, 4249		
256.	71607-79-9	Pyrrolidine, dimethyl-	2889, 3491, 4249		
257.		Pyrrolidine, 2,5-dimethyl-, 1-nitroso-	2884, 4249		
258.	71607-80-2	Pyrrolidine, ethyl-	2767, 4249		
259.	4030-18-6	Pyrrolidine, 1-acetyl-	568b, 1371, 2543, 2570, 2773, 2775, 3553, 4249, 5811b	568b, 2336, 2386, 2389, 2544, 3491, 4249, 5811b	
260.	767-10-2	Pyrrolidine, 1-butyl-	568b, 4249		
261.	7335-06-0	Pyrrolidine, 1-ethyl-	568b, 2767, 4249		
262.		Pyrrolidine, methyl-	5034		
263.	120-94-5	Pyrrolidine, 1-methyl-	568b, 1078, 1083, 1084, 1099, 1140, 1744, 1842, 2001, 2079, 2170, 2524, 2724, 2889, 3059, 3255, 3444, 3491, 4249, 5079, 5512, 5811b	120, 480, 568b, 984, 1086, 1087, 2001, 2270, 2939, 3444, 3491, 3797, 3973, 3974a, 4249, 4837a, 5079, 5329, 5382, 5403, 5811b	
264.	930-55-2	Pyrrolidine, 1-nitroso- {NPYR} 	28, 30, 31, 50, 64, 126, 126a, 126b, 172, 203, 237, 239, 467, 478, 480, 486, 514, 572, 573, 576, 603, 649, 746c, 1058, 1099, 1148, 1217, 1373, 1428, 1445, 1567a, 1580, 1674, 1685, 1691–1693, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 1885, 2118, 2133, 2134a, 2142, 2325, 2404, 2405, 2516, 2561, 2686, 2724, 2750, 2825, 2879, 2884, 2990, 2991, 3190, 3255–3257, 3260, 3265, 3300, 3308, 3343, 3370, 3378, 3491, 3714, 3943a, 3944–3946, 3951, 3952, 3976, 3992, 3994, 4010, 4011, 4249, 4332, 5508, 5512, 5811b, 5869a	172, 463, 468, 466, 478, 486, 498, 514, 993, 1567a, 1685, 1712, 1727, 1740, 1741, 1743, 1744, 1870, 1871, 2139, 2686, 2990, 3943a, 3944–3948, 4010, 4249, 5001, 5496, 5811b	50 (0)
265.	33527-93-4	Pyrrolidine, 1-(1-oxobutyl)-	568b, 4249		
266.	7335-07-1	Pyrrolidine, 1-propyl-	568b, 2767, 4249		
267.	61893-12-7	Pyrrolidine, 1-(2-furanylmethyl)-	568b, 3410, 3553, 3559, 4249		
268.	78504-05-9	Pyrrolidine, 1-(2-furoyl)-	568b, 4249		
269.		Pyrrolidine, 1-(2-furoyk-5-methyl)-	568b, 4249		
270.	60026-17-7	Pyrrolidine, 1-(3-methyl-1-oxobutyl)-		568b, 2389, 2544, 4249	
271.	61480-99-7	Pyrrolidine, 1-[(5-methyl-2-furanyl)methyl]-	568b, 3410, 3553, 3559, 4249		
272.		Pyrrolidine, 2-acetyloxy-methyl-	2767, 4249		
273.	13603-04-8	Pyrrolidine, 2,4-dimethyl-	2889, 4249		
274.	3378-71-0	Pyrrolidine, 2,5-dimethyl-	568b, 2889, 4249		
275.	1003-28-7	Pyrrolidine, 2-ethyl-	2889, 3491, 4249, 5811b	5811b	
276.		Pyrrolidine, 2-ethyl-1-methyl-	568b, 4249		
277.	765-38-8	Pyrrolidine, 2-methyl-	568b, 1140, 2724, 2734, 2749, 2889, 3308, 3491, 3797, 4249, 5811b	568b, 3797, 3974a, 4249, 5906	
278.	34375-89-8	Pyrrolidine, 3-methyl-	2889, 4249		
279.	28882-68-0	Pyrrolidinecarboxylic acid	2767, 4249		
280.	32389-40-5	Pyrrolidinecarboxylic acid, oxo-, (S)-		4249, 4543	

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
281.	29134-29-0	1-Pyrrolidineacetonitrile	568b, 1063–1066, 1068–1074, 1371, 1587, 3410, 3559, 4249, 5811b		
282.	35543-25-0	1-Pyrrolidinebuyronitrile	568b, 4249		
283.	1530-88-7	1-Pyrrolidinecarbonitrile	568b, 4249		
284.	3760-54-1	1-Pyrrolidinecarboxaldehyde	568b, 1371, 2543, 2773, 2775, 3410, 3553, 4249, 5811b	404, 568b, 2389, 2544, 3491, 4249, 5811b	
285.	78914-62-2	1-Pyrrolidinecarboxaldehyde, 2-methyl-, (R)-	568b, 3553, 4249	568b, 2554, 4249	
286.	56879-46-0	2-Pyrrolidineacetic acid		1351, 2337, 2722, 3491, 3797, 3974a, 4249, 5873	
287.		2-Pyrrolidineacetic acid, 1-nitroso-		486, 4249	
288.	61480-98-6	2-Pyrrolidinecarboxaldehyde		568b, 2544, 4249	
289.	61892-97-5	2-Pyrrolidinemethanol, 5-methyl-	5811, 5811a, 5811b		
290.	28115-37-9	2-Pyrrolidinemethanol, 5-methyl-, *cis*-	568b, 2767, 4249		
291.	14498-44-3	2-Pyrrolidinepropanol, 1-methyl-	2387, 4249		2387
292.	60026-15-5	3-Pyrrolidinecarboxaldehyde, 2-methyl-		2389, 2544, 3491, 4249	
293.	121197-25-9	2,4-Pyrrolidinedione, 3-butyl-5-propylidene-	3429a, 4249	5811b	
294.	121197-20-4	2,4-Pyrrolidinedione, 5-butyl-3-propylidene-	3429a, 4249	5811b	
295.	121197-28-2	2,4-Pyrrolidinedione, 3-butylidene-5-(2-methylpropyl)-	3429a, 4249	5811b	
296.	121197-18-0	2,4-Pyrrolidinedione, 3-butylidene-5-propyl-	3429a, 4249	5811b	
297.	121197-17-9	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-(2-methylpropylidene)-	3429a, 4249	5811b	
298.	121197-22-6	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-propylidene-	3429a, 4249	5811b	
299.	121197-19-1	2,4-Pyrrolidinedione, 3-(2-methylpropylidene)-5-propyl-	3429a, 4249	5811b	
300.	121197-15-7	2,4-Pyrrolidinedione, 5-propyl-3-propylidene-	3429a, 4249	5811b	
301.	123-56-8	2,5-Pyrrolidinedione {succinimide} 	568b, 1360, 1371, 1375, 1375a, 1375b, 1580, 1586, 2387, 2543, 2545, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3410, 3553, 3557, 4249, 4407, 5811b	568b, 1580, 2389, 2544, 3215, 3491, 3550, 3974a, 4249, 5811b	1360, 1375a, 2387
302.	15542-96-8	2,5-Pyrrolidinedione, 1,3-dimethyl-	568b, 1360, 1375, 1375a, 1375b, 1586, 2570, 2767, 3553, 3557, 4249, 5811b		1360, 1375a
303.	33425-47-7	2,5-Pyrrolidinedione, 3,4-dimethyl-	1375, 1375b, 1586, 2761, 2762, 2773, 2775, 3553, 4249, 5811b		
304.	5835-19-8 58467-27-9	2,5-Pyrrolidinedione, 3-ethyl-	568b, 1364, 1375, 1375b, 1586, 2767, 3553, 3557, 4249, 5811b		
305.		2,5-Pyrrolidinedione, ethylmethyl-	1586, 2767, 4249		
306.	15542-97-9	2,5-Pyrrolidinedione, 3-ethyl-1-methyl-	568b, 3255, 3553, 4249, 5811b	568b, 2389, 2544, 3491, 4249, 5811b	
307.	77-67-8	2,5-Pyrrolidinedione, 3-ethyl-3-methyl-	568b, 3553, 4249	404, 568b, 4249	

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

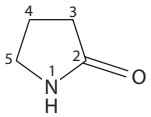
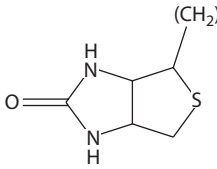
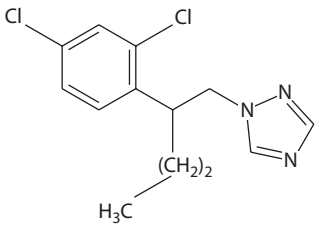
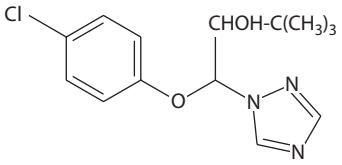
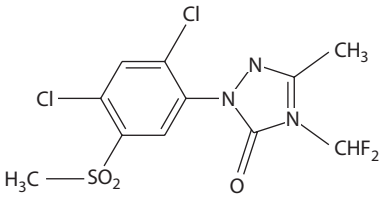
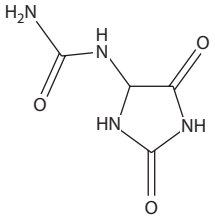
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
308.	58501-92-1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-	568b, 1375, 1375b, 3553, 3557, 4249, 5811, 5811a, 5811b	568b, 937, 2339a, 2389, 2544, 3215, 3491, 3550, 3767a, 4249, 5811, 5811a, 5811b	
309.	16824-61-6	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*Z*)-	1586, 2767, 3553, 3557, 4249	937, 1256, 2544, 3561, 4249	
310.	15510-11-9	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*E*)-		5811b	
311.		2,5-Pyrrolidinedione, 3-ethylene-4-methyl-	568b, 1375, 4249		
312.	14156-12-8	2,5-Pyrrolidinedione, 3-ethylidene-	568b, 3553, 3557, 4249, 5811b		
313.	61892-74-8	2,5-Pyrrolidinedione, 3-ethylidene-1-methyl-	568b, 1375, 1375b, 3553, 4249		
314.	16395-79-2	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-	568b, 1375, 1375b, 2570, 3553, 3557, 4249	568b, 2389, 2544, 3491, 3550, 4249, 5811b	
315.	28098-82-0	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-, (*E*)-		5811b	
316.	18366-19-3	2,5-Pyrrolidinedione, 3-hydroxy- (S)	2767, 3553, 4249		
317.	1121-07-9	2,5-Pyrrolidinedione, 1-methyl-	568b, 1360, 1371, 1375, 1375a, 1375b, 1586, 2570, 2767, 3553, 3557, 4249, 5811b	404, 568b, 2386, 2389, 2544, 3491, 3550, 4249, 5811b	1360, 1375a
318.	5615-90-7	2,5-Pyrrolidinedione, 3-methyl-	568b, 1063–1066, 1068–1074, 1371, 1375, 1375b, 1744, 2545, 2570, 2767, 2773, 2775, 3553, 3557, 4249, 5512, 5811b	568b, 2389, 2544, 3491, 3550, 4249, 5811b	
319.	72693-03-9	2,5-Pyrrolidinedione, 3-(1-methylethyl)-	568b, 2767, 4249	568b, 3550, 4249	
320.	15542-99-1	2,5-Pyrrolidinedione, 1-methyl-3-(1-methylethyl)-	568b, 3553, 4249		
321.	71099-03-1	2,5-Pyrrolidinedione, 1,3,4-trimethyl-	568b, 1586, 2767, 4249	568b, 2336, 4249	
322.	28261-54-3	Pyrrolidinone	1375, 4249		
323.	616-45-5	2-Pyrrolidinone 	568b, 1350, 1354, 1371, 1375, 1375a, 1375b, 1586, 2545, 2570, 2761, 2765, 2766, 2773, 2775, 2857, 3255, 3386, 3398, 3410, 3553, 3557, 3559, 4249	568b, 2389, 2544, 3430, 3491, 3550, 3905, 3974a, 4249	1354, 1375a
324.	932-17-2	2-Pyrrolidinone, 1-acetyl-	568b, 4249		
325.		2-Pyrrolidinone, 1,?-dimethyl-	3553, 4249		
326.	5075-92-3	2-Pyrrolidinone, 1,5-dimethyl-	568b, 4249		
327.	88-12-0	2-Pyrrolidinone, 1-ethenyl-	568b, 4249		
328.	2687-91-4	2-Pyrrolidinone, 1-ethyl-	568b, 4249		
329.	872-50-4	2-Pyrrolidinone, 1-methyl-	568b, 2570, 2775, 3255, 3386, 3410, 3553, 3559, 4249, 5811b	404, 568b, 2339a, 2389, 2544, 3491, 3550, 3905, 4249, 5811b	
330.	2555-05-7	2-Pyrrolidinone, 3-methyl-	568b, 1360, 1375a, 1586, 2767, 3255, 4249		1360, 1375a
331.	2996-58-9	2-Pyrrolidinone, 4-methyl-	3559, 4249	2917a, 4249	
332.	108-27-0	2-Pyrrolidinone, 5-methyl-	568b, 2570, 2767, 3553, 4249, 5811b		
333.	61892-90-8	2-Pyrrolidinone, 1-(2-oxopropyl)-	568b, 3553, 4249		
334.	98-79-3	5-Pyrrolidinone-2-carboxylic acid {5-oxoproline}		2597a, 3052, 4249	
335.	61892-89-5	3-Pyrrolidinone, 1-methyl-5-(2-oxopropyl)-	568b, 3553, 4249		
336.	18028-53-0	2*H*-Pyrrolium, 3,4-dihydro-1-methyl-, chloride	4249, 4791		
337.	54036-77-0	2*H*-Pyrrol-2-one	2387, 4249		2387
338.	61892-80-6	2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-3-ethyl-4-methyl-	568b, 3553, 4249		

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
339.		2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-4-ethyl-3-methyl-	568b, 4249		
340.	4031-15-6	2*H*-Pyrrol-2-one, 1,5-dihydro-	1360, 1375a, 4249		1360, 1375a
341.	13950-21-5	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-		2917a, 4249	
342.	78210-72-7	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-5-(1-methylethylidene)-	568b, 1587, 4249, 5811b		
343.	4030-23-3	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4,5-trimethyl-	568b, 1365, 2767, 3553, 4249, 5811b		
344.	4030-22-2	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4-dimethyl-	568b, 1365, 2767, 2775, 3553, 4249, 5811b		
345.	51088-90-5	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-	568b, 3553, 4249, 5811b		
346.	4030-24-4	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-4-ethyl-	1063–1066, 1068–1074, 3553, 4249, 5811b		
347.		2*H*-Pyrrol-2-one, 1,5-dihydro-4,5-dimethyl-3-ethyl-	568b, 1063–1066, 1068–1074, 2775, 3553, 4249		
348.	27406-77-5	2*H*-Pyrrol-2-one, 1,5-dihydro-3-methyl-	568b, 2767, 2773, 2775, 3553, 3559, 4249, 5811b		
349.	766-36-9	2*H*-Pyrrol-2-one, 1,5-dihydro-3-ethyl-4-methyl-	568b, 1063–1066, 1068–1074, 3553, 3559, 4249, 5811b		
350.	78210-71-6	2*H*-Pyrrol-2-one, 1,5-dihydro-3-ethyl-5-methylene-	568b, 1586, 1587, 3559, 4249, 5811b		
351.	115600-67-4	2*H*-Pyrrol-2-one, 1,5-dihydro-4-ethyl-	3559, 4249		
352.	766-45-0	2*H*-Pyrrol-2-one, 1,5-dihydro-4-ethyl-3-methyl-	568b, 1063–1066, 1068–1074, 3553, 4249, 5811b		
353.	53598-99-5	2*H*-Pyrrol-2-one, 1,5-dihydro-4-methyl-	568b, 4249		
354.	58-85-5	1*H*-Thieno[3,4-*d*]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3aS-(3aα,4β,6aα)]- 		2408a, 4249, 4789	
355.	66246-88-6	1,2,4-Triazole, 1-(2-(2,4-dichlorophenyl)pentyl)- {Penconazole®} 		3633, 4249	

(*continued*)

TABLE 17.4 (continued)
Five-Membered *N*-Containing Ring Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
356.	55219-65-3	1*H*-1,2,4-Triazol-1-ethanol, 8-(4-chlorophenoxy)-α-(1,1-dimethylethyl)- {Triadimenol®} 		928a	
357.	122836-35-5	1*H*-1,2,4-Triazol-1-yl)phenyl) methane-sulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, *N*-(2,4-dichloro-5(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)phenyl)-; Sulfentrazone®} 		2913a	
358.	97-59-6	Urea, (2,5-dioxo-4-imidazolidinyl)- {allantoin} 		120, 2270, 3973, 5079, 5188, 5189, 5436, 5435	

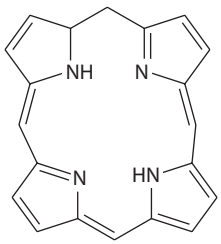


FIGURE 17.2 Porphyrin.

form the circular tetrapyrrole, uroporphyrinogen III. This molecule undergoes a number of further modifications. The biosynthesis is complicated and requires anywhere from 7 to 30 enzymatic reactions involving a variety of catalytic activities including decarboxylation, methylation, metal ion chelation, and porphyrin ring oxidation. Intermediates are used in different species to form particular substances, but, in plants and tobacco in particular, the main end product is protoporphyrin IX, which is combined with magnesium to form chlorophyll (3770a).

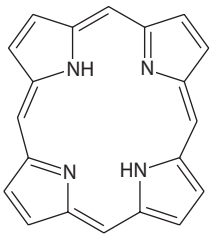
Table 17.5 lists the compounds in tobacco, tobacco smoke, and tobacco substitute smoke with multiple five-membered *N*-containing rings. While 14 porphyrin-containing compounds have been identified in tobacco, only porphyrin itself has been identified in tobacco smoke (1899, 3491).

TABLE 17.5
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Multiple Five-Membered *N*-Containing Rings

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	20298-86-6	21*H*-Biline-8,12-dipropanoic acid-18-ethyl-3-ethylidene-1,2,3,19,22,24-hexahydro-2,7,13,17-tetramethyl-1,19-dioxo-(2R, 3E)		429b, 4249	
2.	479-61-8 42617-16-3	Chlorophyll *a* {also listed under magnesium} {magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]-}		120, 537, 543a, 677b, 830a, 832, 835, 838, 840, 1463, 1941, 2038, 2079, 2236, 2270, 2283, 2649, 2914, 2939, 3616, 3630, 3631, 3632, 3797, 3875, 3973, 3974a, 3974b, 4107, 4108, 4222, 4249, 5079, 5189, 5300, 5539, 5811b	
3.	519-62-0	Chlorophyll *b* {also listed under magnesium} {magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]-}		120, 543a, 677b, 830a, 832, 835, 838, 840, 1941, 2236, 2270, 2914, 2939, 3630, 3631, 3632, 3797, 3875, 3973, 4222, 4249, 5079, 5189, 5300, 5811b	
4.	1406-65-1	Chlorophyll *a* and *b* See magnesium nomenclature in the following		559, 830a, 832, 876, 877, 1927a, 1941, 2038, 2154, 2236, 2394a, 2914, 3448, 3491, 3630, 3631, 3632, 3797, 3973, 3974b, 4222, 4249, 4424, 5067, 5079, 5108, 5109, 5189, 5300, 5413, 5505, 5517, 5811b	
5.		Chlorophyll *a*, phytol		5539	
6.	14428-12-7	Magnesate(1-), [9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(3-)-N23,N24,N25,N26]-, hydrogen, [SP-4-2-[3S-(3α,4β,21β)]]- {chlorophyllide *b*}		4249, 4430, 4473, 4643, 4832a, 4844, 4882, 4884, 4885	
7.	14897-06-4	Magnesate(1-), [9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(3-)-N23,N24,N25,N26]-, hydrogen, [SP-4-2-[3S-(3α,4β,21β)]]- {chlorophyllide *a*}		4249, 4430, 4473, 4643, 4832a, 4844, 4882, 4884, 4885	
8.	11006-34-1 15611- 43-5	Magnesate(3-), [18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12,17-tetramethyl-21*H*,23*H*-porphine-2-propanoato(5-)-N21,N22,N23,N24]-, trihydrogen, [SP-4-2-(2S-*trans*)]- {chlorophyllin}		4249, 4430, 4473, 4643, 4844, 4882, 4884, 4885	
9.	479-61-8 42617-16-3	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]- {chlorophyll *a*}		120, 537, 543a, 677b, 830a, 832, 835, 838, 840, 1463, 1941, 2038, 2079, 2236, 2270, 2283, 2649, 2914, 2939, 3616, 3630, 3631, 3632, 3797, 3875, 3973, 3974a, 3974b, 4107, 4108, 4222, 4249, 5079, 5189, 5300, 5539	

(*continued*)

TABLE 17.5 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Multiple Five-Membered *N*-Containing Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
10.	519-62-0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]- {chlorophyll *b*}		120, 543a, 677b, 830a, 832, 835, 838, 840, 1941, 2236, 2270, 2914, 2939, 3630, 3631, 3632, 3797, 3875, 3973, 4222, 4249, 5079, 5189, 5300	
11.		Pheophorbide**,** hydroxysolanesyl		5517	
12.		Pheophorbide, solanesyl		5517	
13.		Pheophytin, 10-hydroxy-		5517	
14.	24861-47-0	Phorbine		4249, 4885	
15.	20239-99-0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, [3S-(3α,4β,21β)]-		4249, 4844	
16.	3147-18-0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl- 21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2E,7S*,11S*),4β,21β]]- {pheophytin B}		4249, 4445, 5517	
17.	15664-29-6	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, [3S-(3α,4β,21β)]- {pheophorbide A}		4249, 4445, 5517	
18.	603-17-8	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2E,7S*,11S*),4β,21β]]- {pheophytin A}		3626a, 4249, 4445, 5517	
19.	101-60-0	21*H*,23*H*-Porphine {porphyrin} 	1899, 3491, 4249	2571, 3973, 4249	
20.	644-00-8	21*H*,23*H*-Porporphine-2-propanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-		4249, 4466	
21.	1976-85-8	21*H*,23*H*-Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetrakis(carboxymethyl)-5,10,15,20,22,24-hexahydro-		4249, 4430	
22.	147427-29-0	*L*-Proline, 1-[1-[1-(1-*L*-seryl-*L*-prolyl)-*L*-prolyl]-*L*-prolyl]-		4249	

17.2 MONOCYCLIC SIX-MEMBERED *N*-CONTAINING RING COMPOUNDS

17.2.1 Introduction

Over the years, several detailed composition studies on the volatile components in flue-cured [Lloyd et al. (2389) and Dickerson et al. (965)], burley [Roberts and Rohde (3219), Demole et al. (937, 938, 940–942), and Fujimori et al. (1249–1252, 1256)], Maryland [Schumacher (3550)], and Oriental tobaccos [Kimland et al. (2092–2095), Almqvist et al. (52), Aasen et al. (5, 11b), Hlubucek et al. (1660, 1660a, 1661, 1662), Schumacher (3561), Fukuzumi et al. (1257, 1258), and Chuman et al. (731–739)] have been published (2337, 3797). Similarly, the composition of tobacco smoke (3797) has advanced tremendously over the years (1373), notably by the works of Schumacher et al. (3553), Heckman and Best (1587), Grob (1412–1427), Bartle et al. (199, 200), Neurath (2719–2753), Elmenhorst (1129–1140), Newell et al. (2769), Hoffmann and his colleagues (480, 486, 735, 1580), the tobacco research personnel at the U.S. Department of Agriculture, Atlanta, GA, and many others [see additional listing in (2337)].

Tobacco chemists have shown considerable interest in the chemistry and biochemistry of the diverse set of *N*-containing compounds in tobacco and tobacco smoke. Numerous studies on the presence of nitrogenous compounds in tobacco and tobacco smoke have been published. These studies have reported on various aspects of the origins of nitrogenous compounds in tobacco, their synthesis, pyrolysis, and transfer to smoke. Several books and reviews [Tso (3972–3974b), Neurath (2724), Stedman (3797); Wynder and Hoffmann (4332), Schmeltz and Hoffmann (3491), Leffingwell (2337), Hecht et al. (1580)] have been written on *N*-containing compounds in tobacco and tobacco smoke.

The levels of chemical compounds in tobacco are affected by genetics, environmental conditions, and agronomic practices. Considering the six-membered *N*-containing ring compounds and especially the alkaloid-type components (five- and six-membered and multiple six-membered nitrogen heterocycles) of tobacco, this is especially true. There have been numerous reviews on factors affecting plant growth and nicotine/alkaloid accumulation in tobacco [Bush and Saunders (557a), Chaplin and Miner (677a), Bush and Crowe (17B04), Leete (2331a, 2331–2334), Bush (555a), Strunz and Findley (17B56), Bush et al. (17B05)].

Section 17.2.4 provides information on compounds in tobacco and tobacco smoke that contain a six-membered *N*-containing ring (piperidines, tetrahydropyridines, pyridines, piperazines, dihydropyrazines, pyrazines, pyrimidines, pyridazines, and triazines), compounds with a five-membered (pyrrolidine, pyrrole, imidazole) plus a six-membered *N*-containing ring (pyridine), and compounds containing two or more six-membered *N*-containing rings (piperidines, pyridines). The formation of these compounds in tobacco from biosynthetic pathways and from nonenzymatic processes will be presented as well as means of their generation and delivery to tobacco smoke.

17.2.2 Biosynthesis of Six-Membered *N*-Containing Ring Compounds and the Five- and Six-Membered and Multiple Six-Membered Nitrogen Heterocycles of Tobacco

The next few paragraphs will discuss the biosynthesis of the six-membered *N*-containing ring compounds and especially the alkaloid-type components (five- and six-membered and multiple six-membered nitrogen heterocycles) of tobacco. Following the biosynthesis section, information will be provided on the formation of some of the six-membered *N*-containing ring compounds that occurs during tobacco aging and processing. Finally, a discussion of how these six-membered *N*-containing ring compounds and especially the alkaloid-type components arise in tobacco smoke will be presented.

Over 60 species of *Nicotiana* exist that produce nicotine alkaloids (nicotine, nornicotine, anatabine, anabasine). Nicotine is the predominant alkaloid in over 50% of the *Nicotiana* species. Nornicotine is the major alkaloid in about 30%–40% of *Nicotiana* species. Anabasine and anatabine are not usually the principal alkaloids in *Nicotiana* (17B05). Tobaccos that accumulate and have high levels of alkaloids tend to also have accumulations of minor alkaloids, e.g., cotinine, myosmine, nicotyrine, 2,3′-bipyridine, and numerous derivatives of the major alkaloids, e.g., alkyl, acyl, and nitroso derivatives of nicotine and the other major alkaloids. The starting materials for the biosynthesis of the alkaloids are all present in tobacco. The precursors for pyridine, pyrrolidine, piperidine, and the most abundant nicotine alkaloids (nicotine, anabasine, anatabine, cotinine, myosmine) are well known and have been reviewed by Bush et al. (17B05). Although great advances in our understanding of alkaloid biosynthetic processes have occurred over the last 50 years, the metabolic and degradative processes occurring in *Nicotiana* species are still being researched. The biosynthesis of some of the six-membered *N*-containing ring compounds (pyrazines, pyridazines, triazoles) is still not completely understood. As mentioned earlier, the biosynthesis of pyridine, pyrrolidine, and piperidine will be presented. The subsequent biosynthesis of the major alkaloids will then follow. It should be noted that although biosynthesis is the most important means of producing the six-membered *N*-containing ring compounds and the alkaloids found in tobacco, other processes for their production in leaf are also operative. Several tobacco processing operations such as aging, fermentation, thermal treatments of tobacco prior to use in products, tobacco expansion, blending operations, and additive applications can vary (both increase or decrease) the concentration of various six-membered *N*-containing ring compounds and alkaloids.

Pyridine and the pyridine ring of nicotine, nornicotine, anabasine, and anatabine are formed from nicotinic acid.

Yang et al. (17B62) reported that quinolinic acid was the precursor to nicotinic acid via quinolinic acid phosphoribosyltransferase. Glyceraldehyde-3-phosphate (from glycerol) and aspartic acid via a series of enzymes are converted to quinolinic acid. Jackanioz and Byerrum (17B17) showed that ^{14}C-labeled aspartate and malate incorporated into the C-2 and C-3 positions of the pyridine ring when these amino acids were fed to tobacco plants. The total biosynthetic pathway and intermediates involved have not yet been completely elucidated.

The most accepted biosynthetic pathways for piperidine is lysine via Δ′-piperidine (3973, 17B05). Piperidine can also be formed through decarboxylation and dehydrogenation of nicotinic acid (17B37).

The pyrrolidine ring and particularly the *N*-methylpyrrolidine ring of nicotine is biosynthesized through putrescine (1,4-butanediamine), *N*-methylputrescine, and 4-methylaminobutanal to the *N*-methyl-Δ′-pyrrolinium salt (17B41). Dewey et al. (17B11) and Leete (17B29) fed ^{14}C-ornithine to tobacco and found incorporation of activity in the C-2′ and C-5′carbons of the *N*-methylpyrrolidine ring. Arginine via arginine decarboxylase forms agmatine that is converted to putrescine as a second source of this intermediate for the production of the pyrrolidine ring. Again, some of the intermediates and enzymes involved in the biosynthetic production of pyrrolidine are still not completely known (2334, 17B02, 17B63, 17B64).

Dawson et al. (17B07, 17B08) showed that nicotinic acid formed the pyridine ring in nicotine. Yang et al. (17B62) showed that the pyrrolidine ring of nicotine was attached at the C-3 position of the pyridine ring of nicotine. Dawson et al. (17B07) in another publication showed that the hydrogen at the C-6 position of nicotinic acid was lost during nicotine formation. Dawson and Osdene (17B09) and Leete (2330c) showed that nicotine formation proceeds through the reduction of nicotinic acid to 3,6-dihydronicotinic acid. Friesen and Leete (1241a) proposed that dihydronicotinic acid forms a zwitterion by proton transfer that readily decarboxylates to yield 1,2-dihydropyridine. 1,2-Dihydropyridine in turn reacts with *N*-methyl-Δ′-pyrrolinium salt to yield 3,6-dihydronicotine. The 3,6-dihydronicotine is oxidized with the loss of the hydrogen originally present at the C-6 position of nicotinic acid and retention of the hydrogen added in the reduction step to 3,6-dihydronicotinic acid. This pathway adequately explains the majority of the intermediates formed during nicotine biosynthesis and the fact that all nicotine in tobacco plants is (-)-2′S-nicotine (Figure 17.3).

Although nicotine is formed and is present in large quantities in tobacco, it is important to understand that the vast majority of all nicotine in tobacco is present in the form of organic salts. Very little exists in the free base form due to the acidic nature of tobacco. The exact identities of the nicotine salts that exist in tobacco are not known, but there have been several reports by Perfetti (2918a, 2924, 2926, 3156), Seeman et al. (17B48), and Dixon et al. (989) who have speculated on the various salt forms of nicotine.

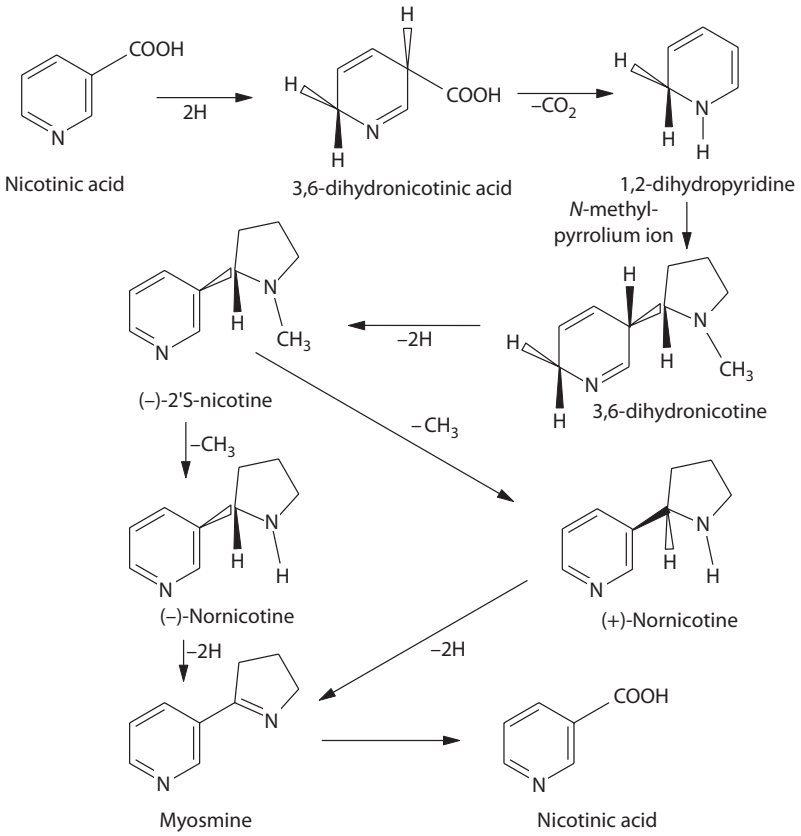


FIGURE 17.3 Proposed biosynthetic pathways for production of several pyridine alkaloids (17B05).

Both of the six-membered *N*-containing rings of anatabine (pyridine and piperidine) can be formed from the two methylene carbons and nitrogen of aspartate and two carbons from a glycerol derivative via nicotinic acid (2330c, 17B32, 17B33, 17B37). Nicotinic acid is reduced to 3,6-dihydronicotinic acid and decarboxylated to 1,2-dihydropyridine and 2,5-dihydropyridine. 1,2-Dihydropyridine reacts with 2,5-dihydropyridine via an electrophilic attack to form 3,6-dihydroanatabine which aromatizes to (-)-2′S-anatabine (17B36).

Although one might expect that anatabine and anabasine could be interconverted enzymatically in the plant, as these compounds differ by only two hydrogens, this does not appear to be true. The pyridine ring of anabasine has been shown to originate from nicotinic acid via decarboxylation (17B54). The precursor for the piperidine ring is lysine via Δ′-piperidine with the nitrogen derived from the ε-nitrogen of lysine (17B35). This was shown to occur via ^{14}C-lysine feeding studies by LEETE (17B30, 17B34). ^{14}C was incorporated into the C-2′ position of the piperidine ring of anabasine.

Nornicotine is formed from nicotine during the growth period of the tobacco plant and during senescence (17B06). Enzymatic demethylation of nicotine yields nearly equal quantities of the (+) and (−) isomers of nornicotine (17B05).

Myosmine can be formed from nornicotine by enzymatic dehydrogenation (2332, 17B24).

Cotinine and 2,3′-bipyridyl and their derivatives represent the major oxidized alkaloids in tobacco. Cotinine is synthesized from nicotine via enzymatic oxidation or auto-oxidation (1157, 17B03). 2,3′-Bipyridyl is formed by oxidation of anatabine. Frankenburg et al. (1221a, 1222–1224) were the first to identify 2,3′-bipyridyl as a fermentation product along with 3-acylpyridine. Other oxidized alkaloids identified in green and cured tobacco are nicotyrine, nicotinic acid, nicotinamide, and nicotine-*N*-oxides. Enzell et al. (1149a) found that these oxidation products of tobacco alkaloids tend to increase in yield during curing and storage of tobacco.

Pyrimidines play a central role in cellular regulation and metabolism. They are substrates for DNA/RNA biosynthesis, regulators of biosynthesis of some amino acids, and cofactors in the biosynthesis of phospholipids, glycolipids, sugars, and polysaccharides (17B45). Pyrimidine biosynthesis is very complicated and involves formic acid, glutamate, and aspartate as starting materials in a series of enzymatic reactions to eventually form orotic acid. Orotic acid, or uracil-6-carboxylic acid, is an intermediate in the metabolism of pyrimidine nucleotides. The naturally occurring derivatives of pyrimidine are components of the nucleic acids cytosine, thymidine, and uracil. Free pyrimidine and functionalized pyrimidine compounds in tobacco are believed to be formed from the catabolism of various nucleosides (17B21).

Although pyrazines, e.g., pyrazine-2-carboxylate and pyrazine-2,3-dicarboxylate, are formed biosynthetically, the vast majority of the varied pyrazine derivatives in tobacco are formed during curing via nonenzymatic reactions. Pyrazines can arise in tobaccos by a number of chemical pathways ranging from the heating or aging of proteins and amino acids to the interaction of amino acids and/or ammonia with sugars or carbonyl constituents. No single pathway is involved in the formation of pyrazine. The formation of pyrazine compounds is complex and depends on a variety of factors and chemical mechanisms (2339b). Adachi et al. (17B01) postulated that tetramethylpyrazine is derived enzymatically from 2 mol of acetoin (acetylmethylcarbinol) and 2 mol of ammonia. This finding was supported by the findings of Demain et al. (17B10) that a block in the isoleucine–valine pathway leads to the accumulation and excretion of a large amount of tetramethylpyrazine. Shu (17B51) treated acetoin with amino acids to determine whether ammonia is released, leading to the formation of tetramethylpyrazine. His results showed that all reactions between amino acids and acetoin generate not only alkylated pyrazines, e.g., tetramethylpyrazine, but also the corresponding Strecker aldehydes.

Pyridazines and triazines are not usually biosynthesized in plants. The exception is azathymine (6-methyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione) which has been identified in modified bases from DNA of tobacco mosaic virus (3973). The majority of the identified pyridazines and triazines in tobacco are believed to originate from residues of agronomic chemicals. The pyridazine structure is found in herbicides containing maleic hydrazide. The triazine structure is found in the tobacco herbicide Metribuzin® and the fungicide Anilizine®.

A variety of alkyl-, acyl-, and hydroxyacyl-substituted alkaloids exist in tobacco. These have been identified and studied by a number of research groups [Bolt (389), Warfield et al. (4133), Matsushima et al. (17B39), Severson et al. (17B49), Zador and Jones (17B65)]. The mechanisms proposed for the biosynthesis of these alkaloids are oxidation or formylation. For example, *N*′-formylnornicotine [2-(3-pyridinyl)-1-pyrrolidinecarboxaldehyde] can be formed by formylation of nornicotine or by oxidation of the *N*-methyl group of nicotine (2330c, 17B03). Additionally, Burton et al. (17B03) have proposed that many acylated alkaloids are formed via acylation of secondary amine alkaloids (994). The concentrations of these alkylated and acylated alkaloids are small in comparison to the total alkaloid concentration in tobacco. Their occurrence is mainly influenced by plant genetics and agricultural practices (17B05). It is believed that their accumulation in leaf may be significant to flavor perception (17B05).

A number of tobacco *N*-nitrosamines are listed in this chapter. Chapter 15 is devoted to *N*-nitrosamines, but a few comments must be included here. Interest in tobacco-specific *N*-nitrosamines (TSNAs) has been a result of reports that some of them have induced malignant tumors in mice, rats, and hamsters [Boyland et al. (421a, 422, 423), Hecht et al. (1557–1559, 1563–1571a, 1574–1585)]. The TSNAs of greatest interest are *N*′-nitrosonornicotine (NNN), *N*′-nitrosoanatabine (NAT), *N*′-nitrosoanabasine (NAB), and 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK). The formation of TSNAs can be biosynthetic (via mechanisms within the plant itself), produced by

bacteria on the surface of the plant, and by organic reactions of flue gas during curing practices [Peele et al. (2917); see also Figure 5 in Rodgman and Green (3300)].

17.2.3 Other Means for the Formation of the Six-Membered *N*-Containing Ring Compounds Found in Tobacco

Nitrogenous compounds in tobacco account for approximately 12%–25% of the dry weight of freshly harvested tobacco leaves (841a, 2337) (2%–6% expressed as nitrogen). As previously mentioned, the large variation in types and yields of nitrogenous compounds in tobacco is due to the great number of *Nicotiana* species, the variety of different agricultural practices, and soil types worldwide for the cultivation of different tobaccos. The major organic nitrogen constituents of tobacco leaf are nicotine and related alkaloids, proteins, and amino acids (2337). The alkaloids as discussed earlier are biosynthesized along with a portion of most of the six-membered *N*-containing ring compounds found in tobacco. But there are also other ways that these six-membered *N*-containing ring compounds can be produced.

The varied methods of curing and aging tobacco cause only a small decrease in the total nitrogen content, but significant changes occur as a result of organic transformations from one type of nitrogenous compound to another, e.g., the enzymatic hydrolysis of leaf protein produces free amino acids (1493). After curing, dynamic changes continue to occur during aging of tobacco leaf. Weybrew et al. (4226) and Tomita et al. (3923) recognized in 1965 that chemical reactions of amino acids in tobacco play an important role in the formation of tobacco flavor. Employing model systems, reactions of amino compounds with sugars or carbonyl compounds were shown to produce flavor compounds present in tobacco (2047, 2048, 2337, 3649).

During tobacco aging, tobacco undergoes a natural "sweating" process several times. This "sweating" is a mild, natural fermentation that produces some heating of the tobacco. This mild, natural fermentation releases reducing sugars, amino acids, phenolics, and flavonoids through nonenzymatic browning reactions to produce the flavor characteristic of aged tobacco. Much of the flavor that is produced is due to Maillard and Strecker reactions of amino acids with reducing sugars (or other carbonyls). The role of nonenzymatic browning reactions of amino acids and sugars is generally accepted as being one of the most important processes in which natural flavors are produced (2337).

There are at least three other ways (other than through biosynthesis) that the six-membered *N*-containing ring compounds can be formed in tobacco leaf (2337):

- Oxidative transformations
- Ambient temperature nonenzymatic transformations
- Heat-induced nonenzymatic transformations

It must be remembered that compounds formed by enzymatic processes can react subsequently in a nonenzymatic transformation. Additionally, by examining the chemical transformations involved in the production of compounds via nonenzymatic browning reactions, several routes can be involved in the production of the same compounds from different precursors (2337).

A type of Maillard reaction that occurs naturally in tobacco which requires the presence of active α-dicarbonyl components is the Strecker degradation of α-amino acids to aldehydes and ketones of one less carbon atom. Schonberg and Moubacher (17B46, 17B47) studied the mechanism of the Strecker degradation involving pyruvaldehyde and α-alanine, leading to the formation of 2,5-dimethylpyrazine and 2,5-dimethyl-3-ethylpyrazine. The fact that different amino acids can produce the same flavor compounds has been shown by a number of workers in studies on the relative formation of pyrazines under controlled reaction conditions between amino acids and glucose (2048, 2337). Similar studies have shown that thermal decompositions of various amino acids and other aminohydroxy compounds such as glucosylamine can directly form pyrazine mixtures (17B60). Because of the complexity of the chemical interactions and transformations involved, the types and ratios of active flavor products, e.g., pyrazines, formed by nonenzymatic browning are dependent on the reaction conditions which may occur during aging or during the smoking process itself.

Examples of how processing tobacco affects the production of flavorful pyrazine were provided by Mays et al. (17B40) and Green et al. (1369) of R.J. Reynolds Tobacco (RJRT) Company. Ammonia/carbon dioxide expansion was conducted on flue-cured, burley, and processed tobacco sheet. Test and control cigarettes were fabricated. The tobacco aroma of the ammonia/carbon dioxide–processed tobaccos increased in all cases after processing *vs*. the control materials. Comparison of the per cigarette mainstream smoke (MSS) yields of eight pyrazines indicated their yields in the MSS from ammonia/carbon dioxide–expanded tobacco were significantly greater than those in the control tobacco MSS [see Tables 3, 4, and 5 in (3261)].

Additionally, browning reactions can occur during the smoking process (2337). Some of the reaction products occurring during the smoking process involve six-membered *N*-containing ring compounds that can significantly contribute to tobacco smoke flavor and aroma, e.g., some pyrazine and pyridine derivatives (2339b).

17.2.4 Six-Membered *N*-Containing Ring Compounds in Tobacco and Tobacco Smoke

Knowledge of tobacco smoke composition grew rapidly each year by the application of new analytical methods. Prior to 1959, only 16 nitrogen compounds had been reported in tobacco and tobacco smoke. In 1959, Johnstone and Plimmer (1971) summarized the identification of about 50 nitrogen compounds. Ten years later, Neurath (2724) reported on the presence in tobacco and tobacco smoke of 181 nitrogen compounds, among which were 2 piperidines, 24 pyridines, 10 pyridines, and 11 alkaloids. In this report,

TABLE 17.6
Distribution of Six-Membered *N*-Containing Ring Compounds between Tobacco and Tobacco Smoke

	Number of Identified Six-Membered *N*-Containing Ring Compounds in Tobacco and Tobacco Smoke			
Component	**Total**	**Smoke**	**Tobacco**	**Smoke and Tobacco**
Piperidines	44	40	13	9
Tetrahydropyridines	7	3	5	1
Dihydropyridines	6	4	2	0
Pyridines	365	324	125	84
Piperazines	12	12	0	0
Dihydropyridazines	5	3	3	1
Pyrazines	106	90	57	41
Pyrimidines	33	14	20	1
1,2,4-Triazines	1	0	1	0
1,3,5-Triazines	2	0	2	0
Totals	581	490	228	137

we have cataloged 37 piperidines, 312 pyridines, 78 pyrazines, and over 160 alkaloids.

Table 17.6 provides the distribution of six-membered *N*-containing ring compounds in tobacco and tobacco smoke. Of the 581 identified compounds, about 84% (or 490 compounds) are found in tobacco smoke and about 39% (or 228 compounds) are found in tobacco. Of the 581 compounds, 23% (137 compounds) are found in both tobacco and smoke.

Figure 17.4 illustrates the general structures for the 10 types of six-membered *N*-containing ring compounds found in tobacco and tobacco smoke. The four major compound classes are the piperidines, pyridines, pyrazines, and the pyrimidines. A brief discussion of general information on each of these four classes of six-membered *N*-containing ring compounds follows.

17.2.4.1 Piperidine and the Tetra- and Dihydropyridines

Piperidine and Δ^3-piperideine were first identified by Neurath et al. in 1965 (2749) and 1966 (2734), respectively [see Table 3 in Neurath (2724)]. The piperidines in tobacco and tobacco smoke are found as substituted ketones, acids, and alkyl derivatives. None of the 48 nonaromatic six-membered *N*-heterocycles found in tobacco and tobacco smoke has been shown to provide positive contributions to the flavor of tobacco smoke, although piperidine is on the GRAS list as a food flavor (3215).

Pyrolysis and smoke studies of amino acids indicate that they are potential precursors of several nitrogen heterocyclic ring systems found in tobacco smoke (1351). For example, indole can be formed from tryptophan, proline has been shown to be efficiently converted to pyrrole upon pyrolysis (3219, 3726), and γ-amino acids can be pyrolyzed to form 2-pyrrolidones (1967, 3079). By a similar mechanism, γ-amino acids form 2-piperidones (1967, 3079).

17.2.4.2 Pyridines

A great variety of pyridines (currently 365) have been identified in tobacco and tobacco smoke. As a class, there are more pyridines in smoke than any other heterocycle. Vohl and Eulenberg (4064) were the first to isolate and identify pyridine in tobacco smoke in 1871. Since that time, a wide variety of substituted [methyl- (picolines), dimethyl- (lutidines), ethyl-, allyl-, butyl-, vinyl-, cyano-, formyl-, alkylamino-] pyridines have been identified. Most of the substituted groups in these pyridines occur at the 3-position, although there are some substituted pyridines with functionalities at the 2- and 4-positions (2724).

The presence of pyridine compounds in smoke is naturally associated with the tobacco alkaloids. The formation of substituted pyridines that occur during the pyrolysis of nicotine has long been known [Woodward et al. (4275a), Kaburaki et al. (2006), Jarboe and Rosene (1923a), Schmeltz et al. (3499)]. Pyridine, 3-methyl- and/or 4-methylpyridine, 3-vinylpyridine, and 3-cyanopyridine have all been identified as major pyrolysis products of nicotine. Minor pyridine pyrolysis products included 2-methylpyridine, dimethylpyridines, 3-ethylpyridine, and 2- and/or 4-cyanopyridine. All have been identified in tobacco smoke. While the formation of pyridines from nicotine might be expected to involve simple rupture of the pyridine–pyrrolidine bond, a more complex pathway is taking place. When either nicotine-*N*-methyl-^{14}C or nicotine-2′-^{14}C was pyrolyzed, several alkylated ^{14}C-labeled pyridines were among the products.

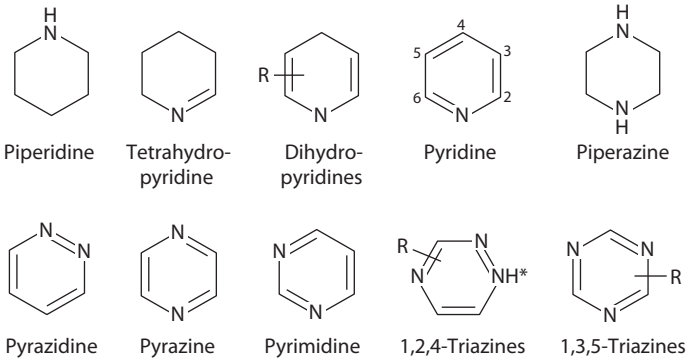


FIGURE 17.4 Structures of the six-membered *N*-containing compounds found in tobacco and tobacco smoke.

This indicated that fragments of the pyrrolidine ring can recombine and aromatize to give pyridines (1580).

The pyrolytic formation of pyridines has been observed in studies on a number of nitrogenous substances. Pyrolysis of tobacco pigment and of tobacco leaf gave a spectrum of pyridines similar to those observed in smoke [Schmeltz et al. (3499), Schlotzhauer and Schmeltz (3463)]. Pyridines were observed in the pyrolysis of proline [Higman et al. (1647)] and pyridine was a product of pyrolysis of poly-*L*-proline [Johnson et al. (1968)]. Pyrolysis of nicotinamide at 1050°C gave pyridines and 3-cyanopyridine, among other products [Bruzel and Schmeltz (515)]. Pyridines were also observed in pyrolysates of pyrrole, maleic hydrazide, and *N*,*N*-dimethyldodecylamine [Patterson et al. (2907, 2908)]. In view of the previously mentioned results on pyrolysis of nicotine-^{14}C and previous mechanistic studies [Hurd et al. (1851)], it is not surprising that pyridines should arise on pyrolysis of such diverse *N*-containing compounds. Studies on cigarettes enriched in nicotine or nornicotine indicated that nornicotine was an important precursor for pyridines [Glock and Wright (1316), Hecht et al. (1580)].

Pyridines can be formed by mechanisms other than pyrolysis. The reaction of aldehydes with amino acids has been shown to generate pyridines (50). When a glycine–propanal mixture was heated to 180°C, 3,5-dimethyl-2-ethylpyridine, 3,5-dimethyl-4-ethylpyridine, and 3,5-dimethylpyridine formed. Glycine–propanal mixtures, also heated to 180°C, gave 2,5-dimethylpyridine and 3,4-dimethylpyridine. This is an example of a nonpyrolytic method of forming pyridines. As small-chain aldehydes required for this reaction are abundant in smoke, this is a feasible route to pyridines.

Pyridines contribute to the characteristic tobacco flavor of smoke. Fujimori (1248) identified 26 pyridines as components of tobacco aroma. Leffingwell et al. have tabulated the flavor and aroma characteristics of many pyridines (2341). Pyridines as a class of compounds enhance tobacco flavor, add burley flavor, or can add flue-cured flavor. Pyridines are responsible for that characteristic note in smoke which identified the smoke as that from tobacco (1587a). Hoffmann and Wynder (1803) have made the comment that pyridines are responsible for the off-taste and irritancy of the smoke from large cigars and that pyridines reduce the inhalability of cigar smoke.

Roberts commented that two particular pyridine compounds were noteworthy, 2-acetylpyridine [1-(2-pyridinyl)-ethanone] and 2-methyl-5-isopropylpyridine [2-methyl-5-(1-methylethyl)-pyridine] (3215). The former adds some sweet, roasted, and musty notes, and the latter adds body and burley character to the tobacco blend. Additionally some pyridines may react with other smoke compounds synergistically. For example, it is believed that some pyridines reduce the sweet, burnt-sugar taste of cyclopentenones and furanones (3215).

17.2.4.3 Pyrazines

Pyrazines constitute a very small percentage by weight of smoke condensate (5–50 µg/cig), but pyrazines as a class of tobacco and tobacco smoke compounds are very important because of their positive flavoring properties. Pyrazine, methylpyrazine, and 2,6-dimethylpyrazine were first recognized in tobacco smoke in 1965 by Testa and Testa (3888). To date, 106 pyrazines have been identified in tobacco and tobacco smoke. Nearly 40% of the identified pyrazines are found in both tobacco and tobacco smoke.

In the 1968 review by Stedman (3797), he listed only three pyrazines as components of tobacco smoke: pyrazine, 2-methylpyrazine, and 2,6-dimethylpyrazine. In that same year, Neurath and Dünger (2732) identified eight additional pyrazines, including 2-methyl-5-(2′-furyl) pyrazine. Leffingwell in 1976 (3237) mentioned six new pyrazines, including three acetyl-substituted pyrazines. Green (1351), in 1977, disclosed another eight novel pyrazines including 2-methyl-5-phenylpyrazine, 3-methylpyrazinol, and pyrrolo[1,2-*a*]pyrazine. Heckman and Best (1587) have also identified a number of pyrazines including five cyclopentapyrazines. There is a great diversity of pyrazines that have been identified in tobacco smoke.

Pyrazines have also been isolated from tobacco (938). Their presence in leaf arises from biosynthesis and from browning reaction chemistry that can occur during curing and tobacco processing. At present, 58 pyrazines have been identified in tobacco. Bright et al. (431) have demonstrated that the necessary precursors for the formation of pyrazines are present in tobacco leaf. In their experiments, the levels of dimethylpyrazine in untreated tobaccos were measured, and then the same tobaccos were heated at 120°C for 4 h and the levels measured again. In each case, the level of dimethylpyrazine was found to be very low in the untreated tobacco and appreciably increased following the roasting. Their results also showed a decrease in amino acid levels during the heat treatment of the tobaccos, indicating the possible involvement of amino acids in the formation of the pyrazines. Some pyrazines have been isolated from flue-cured (965) and burley tobaccos (937). The presence of pyrazines in tobaccos may be due to reactions of leaf precursors at the temperature used in curing of these tobacco types (1351).

Amadori compounds are β-ketoamino acids that are structurally similar to β-hydroxyamino acids. Amadori compounds can yield pyrazines. Leffingwell (2337) and Green (1351) have both mentioned the presence of Amadori compounds in leaf as has Tomita (3923) who stated that Amadori compounds account for as much as 2% of the dry weight of flue-cured leaf. Thermal treatment of Amadori compounds does, in fact, give pyrazines as decomposition products [Shigematsu et al. (17B50)]. The formation of 2,5-bis-(tetrahydroxybutyl)pyrazine (fructosazine) from the reaction of fructose or glucose with alcoholic ammonia and from self-condensation of glucosamine or isoglucosamine has been known for a long time (17B57); in fact, the earliest reports date back to the beginning of the twentieth century. Deoxyfructosazine and its 2,6-isomer have been isolated from mixtures obtained by reaction of glucose and fructose with ammonia under weakly acidic conditions (1153, 1156, 17B13). The fructosazine and deoxyfructosazine isomers

can be obtained synthetically by use of such sugar–ammonia reactions. The yields and isomer ratios are somewhat contingent on the choice of sugar (glucose or fructose) and the mole ratio of sugar to ammonium formate (1153). For example, xylose and aqueous ammonium formate yielded 2,5-bis (*D*-threo trihydroxypropyl)pyrazine (xylulosazine) and the related 2,5- and 2,6-deoxyxylulosazines (1248). Several deoxyfructosazine isomers have been isolated from tobacco (1352). The tobacco-derived deoxyfructosazines were shown to improve the aroma and taste of tobacco (1351). Lynm (2420, 2421, 2423, 2424) at RJRT conducted several studies on the presence, formation, and analysis of deoxyfructosazines in tobacco and tobacco products.

Two mechanisms have been suggested for pyrazine formation during smoking: pyrolytic decomposition of leaf constituents and nonenzymatic sugar–amine reactions. Kato et al. (2048) showed that direct pyrolysis of serine yielded pyrazine, methylpyrazine, ethylpyrazine, 2-ethyl-6-methylpyrazine, 2,6-diethylpyrazine, and 2,6-diethyl-6-methylpyrazine. Pyrolysis of threonine gave 2,5-dimethylpyrazine, trimethylpyrazine, and 2,5-dimethyl-3-ethylpyrazine. Sugars condense with amino acids to form sugar–amino acid adducts which then undergo Amadori rearrangement to give Amadori compounds.

Although pyrolysis of selected leaf constituents generates pyrazines, the diversity and abundance of pyrazines in smoke cannot be adequately accounted for by this mechanism alone. Maga and Sizer (2439) and Enomoto et al. (17B12) have reviewed the occurrence of pyrazines in roasted foods and proposed pathways for pyrazine formation. Their summaries present a large array of pyrazines found in the flavor fractions of a number of roasted foods. It is striking that nearly all pyrazines commonly found in tobacco smoke have been identified in at least one roasted food. For example, 2,3-dimethylpyrazine has been found in peanuts, barley, coffee, baked potatoes, mushrooms, lamb fat, and tobacco smoke (1587a).

Of particular interest in relating leaf to smoke composition are the studies of Koehler and coworkers (17B26, 17B27) on the formation of pyrazine compounds in sugar–amino acid systems. Using model systems, Koehler and Odell (17B27) showed that pyrazines are formed when sugars and amino acids are heated between 100°C and 150°C. Glucose reacts with either an amino acid or ammonia to form a glycosylamine. The amino acid complex then undergoes a Strecker-type degradation to yield an eneaminol which can also be formed by the loss of water from glucosylamine. The eneaminol then isomerizes and undergoes reverse aldol condensation to form 1-aminoacetone which is known to self-condense to yield pyrazines (116). As shown by Schonberg and Moubacher (17B46), during the condensation of the aminoacetone, further reaction with aldehydes can take place. Similar pathways can be postulated for the generation of 1-aminoacetaldehyde, 1-aminopropionaldehyde, and 1-amino-2-butanone from sugar–amine reactions. Hypothetical reaction of these aminocarbonyl compounds either individually or in pairs can account for most of the alkylpyrazines reported in smoke (1351). Additionally, Koehler and Odell (17B27) showed that a number of smaller compounds, acetaldehyde, glycerol, glyoxal, 2,3-butanedione, and acetol, also yielded pyrazines when heated with nitrogen sources. Koehler et al. (17B26) had previously shown, using radiotracer techniques, that the sugar moiety served as the principal source of carbon atoms and that the amine furnished only nitrogen to the pyrazine molecule. These data imply that sugar decomposes to small intermediary carbonyl compounds which in turn react with the nitrogen source, e.g., amine and amino acid, to form pyrazines.

Other possible mechanisms for the formation of pyrazines during smoking are possible. For instance, leaf carbohydrates could be degraded either through pyrolysis or Maillard reactions to form α-dicarbonyl compounds, which could, in turn, react with amino acids to undergo a Strecker degradation forming the α-aminocarbonyl compounds [1671a, 2439, Velisek et al. (17B59)] which can condense to form pyrazines (1351).

Pyrazines are the most important *N*-heterocycles in characterizing the aroma and flavor of tobacco and tobacco smoke (2341, 3215, 3491, 3553). The alkylpyrazines, for example, provide the cocoa and nutty-type notes associated with tobacco smoke. 2-Acetylpyrazine [1-pyrazinylethanone], isolated and identified in burley tobacco by Roberts (3202, 3204) in 1963, contributes a nutty, popcorn-type flavor unique to tobacco smoke. Pyrazines, in general, contribute the "brown notes" associated with tobacco smoke taste (3215). It is obvious that cigarette MSS flavor and aroma may be enhanced by addition of appropriate pyrazine compounds to the tobacco blend, e.g., among the 460 pure compounds listed by Doull et al. (1053) as possible cigarette tobacco ingredients used by U.S. cigarette manufacturers are 23 (5%) pyrazine derivatives. In 1977, RJRT conducted an immense study on the Philip Morris' Merit cigarette that advertised the use of a "flavor package." One of the interesting results of that study was that the MSS from Merit contained numerous alkylpyrazines, particularly higher levels of tetramethylpyrazine and several trimethylpyrazines compared to other commercial cigarette brands of similar FTC "tar." Much of the Merit research conducted at RJRT was summarized by Lloyd (2385a).

17.2.4.4 Pyrimidines

Thirty-three pyrimidine derivatives identified in tobacco and tobacco smoke are listed in Table 17.7. The vast majority of these compounds (61%) have been identified in tobacco. Only 14 are known to exist in tobacco smoke. As previously mentioned, the naturally occurring derivatives of pyrimidine are components of nucleic acids: cytosine, thymidine, and uracil. Free pyrimidine and functionalized pyrimidine compounds in tobacco are believed to be formed from the catabolism of various nucleosides (17B21). Several of the pyrimidine-containing compounds in tobacco are agronomic chemical residues, while other compounds identified in tobacco smoke are formed from those agronomic residues.

Pyrimidine derivatives do not generally have positive flavor notes and are considered neutral to poor.

TABLE 17.7
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

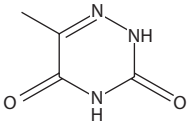
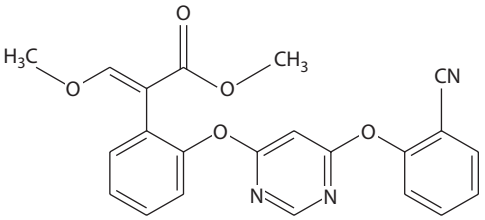
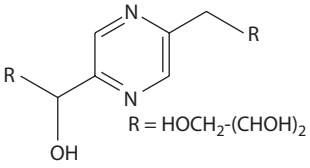
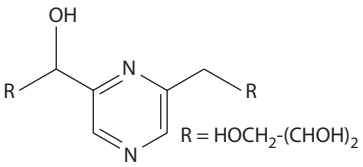
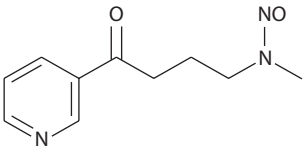
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4906	
2.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249	
3.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
4.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	
5.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
6.	932-53-6	Azathymine 		3973, 4249	
7.	131860-33-8	Benzeneacetic acid, methyl(α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)- {Azoxystrobin®} 		5568	
8.	68510-02-1	1,2,3,4-Butanetetrol, 1-[5-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,5-deoxyfructosazine} 		480, 1361, 1587a, 2339b, 2420, 2421, 2423, 2424, 4249, 4422, 4747, 5540, 17B57	
9.	68510-03-2	1,2,3,4-Butanetetrol, 1-[6-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,6-deoxyfructosazine} 		480, 1361, 1587a, 2339b, 2420, 2421, 2423, 2424, 4249, 4422, 4747, 5540, 17B57	
10.		1-Butanone, 1-(methyl-2-pyridinyl)-	4570a		
11.		1-Butanone, 1-(3-methyl-2-pyridinyl)-	4570a		
12.		1-Butanone, 1-(4-methyl-2-pyridinyl)-	4570a		
13.	61892-81-7	1-Butanone, 1-pyrazinyl-	568b, 3553, 4249		
14.	22971-32-0	1-Butanone, 1-(2-pyridinyl)-	4570a, 5811		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
15.	1701-70-8	1-Butanone, 1-(3-pyridinyl)- {propyl pyridyl ketone}	568b, 1587, 2724, 2939, 3054, 3056, 3302, 3491, 4249, 5811b	120, 568b, 1225, 1226, 2359, 2724, 2939, 3056, 3444, 3491, 3974a, 4249, 4766	
16.	78210-70-5	1-Butanone, 2-methyl-1-(3-pyridinyl)-	568b, 1587, 4249, 5811b		
17.	71278-11-0	1-Butanone, 4-amino-1-(3-pyridinyl)- {poikiline}	3302, 3742, 4207, 4213, 4248	120, 2270, 4207, 4249, 5079	
18.	59578-62-0	1-Butanone, 4-hydroxy-1-(3-pyridinyl)-	5087, 5508	4249, 5508	
19.		1-Butanone, 4-(methylamino)-1-(2,6-dihydroxy-3-pyridinyl)-		1101, 4249	
20.		1-Butanone, 4-(methylamino)-1-(6-hydroxypyridinyl)-		1101, 4249	
21.	2055-23-4	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)- {pseudooxynicotine}		553, 2221, 3974, 4236, 4249, 5079, 5222	
22.	64091-91-4 110053-55-9 121268-99-3 126165-82-0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}  {1-Butanone, 4-[(nitrosomethyl)amino]-1-(3-pyridinyl)-}	7, 23–26, 28–31, 34, 59, 70, 75, 97–99, 126, 126a, 126b, 172, 174b, 174c, 237, 239, 402, 458–460, 463, 478, 483, 484, 486, 501, 502, 508, 514, 568b, 572, 573, 595, 603, 688, 728, 772, 895, 998, 1001, 1002, 1004, 1006a, 1011, 1013–1016, 1016a, 1051, 1058, 1099, 1148, 1191–1200, 1373, 1386, 1445, 1557, 1564, 1566, 1567, 1567a, 1569–1571, 1571a, 1572, 1573a, 1580, 1584, 1674, 1679, 1685, 1692, 1696, 1702, 1710, 1725, 1727, 1728, 1730, 1731, 1736, 1741, 1746, 1750, 1751, 1768, 1769, 1781, 1842, 1870–1872, 1987, 1988, 2133, 2134a, 2142, 2168, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2879, 2949, 2991, 2992, 2993, 3007, 3094, 3178, 3179, 3180, 3181, 3182, 3184, 3190, 3255–3257, 3265, 3300, 3342, 3343, 3365, 3370, 3376, 3378, 3844, 3952, 3973, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5070, 5087, 5494, 5531, 5546, 5556, 5569, 5679, 5692, 5811, 5811a, 5811b, 5836	29, 33, 34, 64, 70, 97–99, 174c, 201, 324–326, 458, 463, 465, 468, 478, 483, 484, 486, 498, 501, 505, 508, 510, 548–550, 553, 554, 557, 568b, 595, 655, 720, 772, 895, 998, 1002, 1004, 1010, 1014, 1015, 1051, 1156, 1191–1200, 1385, 1564, 1566, 1567, 1567a, 1569–1571, 1573a, 1576, 1577, 1584, 1679, 1685, 1696, 1702, 1712, 1722, 1725, 1728, 1730, 1731, 1746, 1750, 1768, 1771, 1870–1872, 1988, 2050–2052, 2169, 2235, 2326c, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2638, 2674, 2700, 2914–2917, 2949, 2992, 2996, 2997, 3144a, 3176a, 3177, 3183, 3441a, 3491, 3773, 3774, 3816, 3943b, 3947, 3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4090, 4128, 4161, 4236, 4247, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5531, 5579, 5584, 5589, 5811, 5811a, 5811b	

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

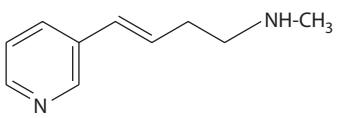
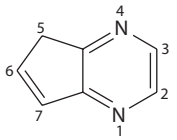
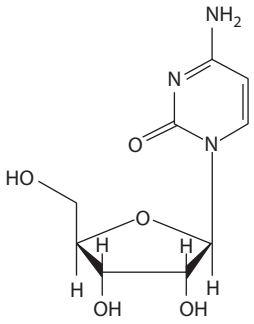
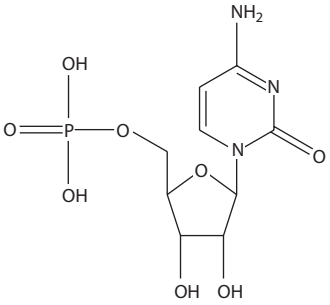
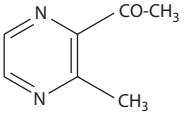
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
23.	76014-82-9	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-, *N*-oxide		4249	
24.	53872-97-2	2-Butanone, 3-methyl-1-(3-pyridinyl)-	4249		
25.	20173-36-8	3-Buten-1-amine, *N,N*-dimethyl-4-(3-pyridinyl)-	2731, 2735, 2767, 4249		
26.	538-79-4	3-Buten-1-amine, *N*-methyl-4-(3-pyridinyl)- {metanicotine} 	761, 568b, 1078, 1084, 2724, 2734, 3054, 3302, 3499, 3557, 3797, 4249	120, 568b, 1087, 2270, 2349, 2746, 4249, 5079, 5382, 5390, 5804, 5811b	
27.	80508-24-3	2-Buten-1-one, 1-(3-pyridinyl)-	4249		
28.	23103-98-2	Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester {Pirimicarb®}		3633, 4249, 4271a	
29.	25042-83-5	5*H*-Cyclopentapyrazine 	1587		
30.	23747-47-9	5*H*-Cyclopentapyrazine, 6,7-dihydro-	568b, 4249		
31.	38917-63-4	5*H*-Cyclopentapyrazine, 6,7-dihydro-2,3-dimethyl-	1587, 1587a, 4249, 5811b		
32.	38917-60-1	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-ethyl-	1587, 1587a, 1590, 4249, 5811b		
33.	52517-53-0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-ethyl-	568b, 4249		
34.	23747-46-8	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-methyl-	1587, 1587a, 4249, 4570a, 5811b	1590	
35.	23747-48-0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-methyl-	1587, 1587a, 1590, 4249, 4570a, 5811b	174b, 3266	
36.	41330-21-6	5*H*-Cyclopentapyrazine, 6,7-dihydro-5,7-dimethyl-	4570a		
37.	61891-57-4	5*H*-Cyclopentapyrazine, dimethyl-	2570, 3553, 4249, 5811b		
38.	61929-05-3	5*H*-Cyclopentapyrazine, 2,3-dimethyl-	568b, 4249		
39.	65129-00-2	5*H*-Cyclopentapyrazine, 2-ethyl-	568b, 4249		
40.	65-46-3	Cytidine {2(1*H*)-pyrimidinone, 4-amino-1-β-*D*-ribofuranosyl-} 		429b, 4249, 4477, 4554a	
41.	65-47-4	Cytidine 5′-(tetrahydrogen triphosphate)		429b, 4249, 4474, 4505	

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
42.	63-37-6	5′-Cytidylic acid 		429b, 4249, 4299, 4474	
43.	78210-69-2	Ethanone, 1-(1,2-dihydro-2-methyl-3-pyridinyl)-	568b, 1587, 4249, 5811b		
44.	78249-87-3	Ethanone, 1-(methylpyridinyl)- {Two isomers}	1587, 4249, 4570a, 5811, 5811a, 5811b		
45.	1122-62-9	Ethanone, 1-(2-pyridinyl)- {2-acetylpyridine}	1099, 1360, 1371, 1375a, 1587, 1949, 2234, 2543, 2727, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2939, 3056, 3255, 3266, 3398, 3491, 3557, 4249, 4570a, 5034, 5811b	937, 1053, 1949, 2336, 2337a, 2339a, 2359, 2724, 2917a, 2939, 3056, 3204, 3215, 3266, 3491, 3550, 3974a, 4159a, 4249	1360, 1375a
46.	23787-80-6	Ethanone, 1-(3-methylpyrazinyl)- {2-acetyl-3-methylpyrazine} 	1587a, 3491, 4249, 4570a	937, 2337, 3219, 3491, 3547, 3974a, 4249	
47.	350-03-8	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine or methyl 3-pyridyl ketone}	568b, 761, 1075, 1078, 1083, 1360, 1364, 1371, 1375a, 2224, 2234, 2270, 2493, 2543, 2724, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 2939, 3054, 3058, 3059, 3062, 3255, 3266, 3308, 3386, 3397, 3398, 3410, 3499, 3505, 3553, 3797, 4249, 5034, 5811b	120, 404, 568b, 937, 1053, 1086, 1223, 1225, 1662, 1854, 2339a, 2359, 2386, 2389, 2544, 2917a, 2939, 3266, 3430, 3547, 3905, 3973, 3974a, 3983a, 4249, 5079, 5720, 5811b	1360, 1375a
48.	25343-57-1	Ethanone, 1-[3-(1,4,5,6-tetrahydropyridinyl)]-		2917a, 4249	
49.	27300-27-2	Ethanone, 1-[3-(3,4,5,6-tetrahydropyridinyl)]-		2917a, 4249	
50.	59576-31-7	Ethanone, 1-(4,6-dimethyl-2-pyridinyl)-	568b, 1587, 4249, 5811b		
51.	59576-26-0	Ethanone, 1-(4-methyl-2-pyridinyl)-	568b, 1587, 4249, 5811b		
52.	1122-54-9	Ethanone, 1-(4-pyridinyl)- {4-acetylpyridine}	568b, 1587, 2234, 4249, 5034, 5811b	568b, 2359, 2917a, 4249	
53.	32974-92-8	Ethanone, 1-(5-ethylpyrazinyl)-		1053, 3266	
54.	42972-46-3	Ethanone, 1-(5-methyl-3-pyridinyl)-	568b, 1587, 2727, 3266, 3491, 4249, 5811b	568b, 3266, 4249	

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

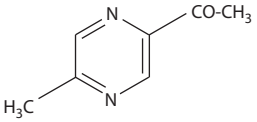
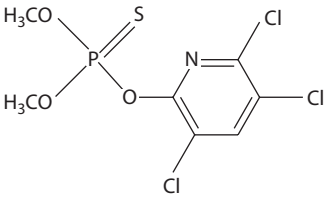
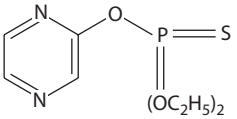
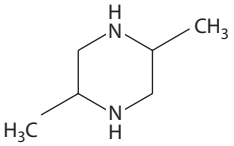
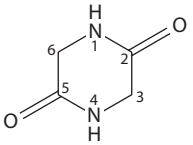
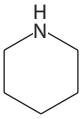
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
55.	22047-27-4	Ethanone, 1-(5-methylpyrazinyl)- {2-acetyl-5-methylpyrazine} 	1587a, 3266, 4249	937, 3215, 3491, 3547, 3974a, 4249	
56.	6940-57-4	Ethanone, 1-(6-methyl-2-pyridinyl)-	1587, 4249, 5811b		
57.	36357-38-7	Ethanone, 1-(6-methyl-3-pyridinyl)-	568b, 1371, 2731, 2735, 4249	5811b	
58.	22047-26-3	Ethanone, 1-(6-methylpyrazinyl)- {2-acetyl-6-methylpyrazine}	1587a, 937, 3491, 4249	2337, 3204, 3205, 3215, 3219, 3547, 3974a, 4249, 5811b	
59.	78249-86-2	Ethanone, 1-(dimethylpyridinyl)-	1587, 4249, 4570a, 5811b		
60.	57276-33-2	Ethanone, 1-cyclopropyl-2-(3-pyridinyl)-	568b, 1587, 4249, 5811b		
61.	22047-25-2	Ethanone, 1-pyrazinyl- {acetylpyrazine}	568b, 1587, 1587a, 2470, 3266, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1207, 2337, 3204, 3202, 3205, 3215, 3219, 3266, 3370, 3491, 3547, 3550, 4249, 5811b	
62.	56625-04-8	Formamide, *N*-(3-pyridinylmethyl)-	568b, 1587, 4249, 5811b		
63.	55484-04-3	Furan, 2-(4-pyridyl)-	4407, 4249		
64.	20971-79-3	2(3*H*)-Furanone, dihydro-5-(3-pyridinyl)-	568b, 3553, 4249, 5811b		
65.	24966-13-0	Methanone, cyclopropyl-3-pyridinyl-	568b, 1587, 4249, 5811b		
66.	15769-88-7	2*H*-1,2-Oxazine, tetrahydro-2-methyl-6-(3-pyridinyl)-, (-)-	568b, 761, 1587, 2270, 2761, 4249, 5811b	568b, 2270, 3547, 3549, 3550, 4249	
67.	71607-95-9	2*H*-1,2-Oxazine, tetrahydro-3-(1-methylethyl)-6-(3-pyridinyl)-	568b, 1587, 4249, 5811b		
68.	2921-88-2	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyrifos®; Chlorpyriphos®; Dursban®} 	717, 1333, 21A19	717, 1219a, 1219b, 1219c,1333, 2058a, 3381, 3633, 3919, 3977, 4249, 21A19	
69.	297-97-2	Phosphorothioic acid *O,O*-diethyl *O*-pyrazinyl ester {Thionazine®} 		3633, 4249, 4271a	
70.	333-41-5	Phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester {Diazinon®}	5811b	1219b, 1219c, 2058a, 2650b, 3633, 3973, 4249, 4271a	
71.	29232-93-7	Phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-dimethyl ester {Pirimiphos-methyl®}		4249	
72.	25057-77-6	Piperazine, 1,2-dimethyl-	568b, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
73.	106-58-1	Piperazine, 1,4-dimethyl-	568b, 3553, 4249		
74.	106-55-8	Piperazine, 2,5-dimethyl- 	568b, 2947a, 4249		
75.	109-01-3	Piperazine, 1-methyl-	568b, 4249		
76.	109-07-9	Piperazine, 2-methyl-	568b, 3553, 4249		
77.	106-57-0	2,5-Piperazinedione 	1351, 3553, 4249		
78.	5076-82-4	2,5-Piperazinedione, *N,N*-dimethyl-	568b, 3553, 4249		
79.	14771-77-8	2,5-Piperazinedione, 3-(1-methylethyl)-	3553, 4249, 5811b		
80.	61892-78-2	2,5-Piperazinedione, 3-(2-propenyl)-	568b, 3553, 4249		
81.	5625-46-7	2,5-Piperazinedione, 3,6-dimethyl-	568b, 3553, 4249		
82.	5625-53-6	2,5-Piperazinedione, 3-methyl-	1351, 1364, 3410, 3553, 4249, 5811b		
83.	4526-77-6	2,5-Piperazinedione, 3-methyl-, (S)-	4249		
84.	110-89-4	Piperidine {azacyclohexane} 	568b, 1078, 1084, 1140, 2001, 2088, 2724, 2734, 2749, 2889, 3059, 3302, 3308, 3491, 3505, 3797, 4249, 4319, 5034, 5811b	120, 568b, 1877, 2270, 2724, 2746, 2939, 3491, 3763, 3797, 3973, 3974a, 4249, 5079, 5811b, 17B30, 17B35, 17B56	
85.		Piperidine, C_2-alkyl-	2889, 3491, 4249		
86.		Piperidine, C_3-alkyl-	2889, 3491, 4249		
87.		Piperidine, C_4-alkyl-	2889, 3491, 4249		
88.	5347-68-2	Piperidine, 2,3-dimethyl-	568b, 4249, 5811b		
89.	23513-39-5	Piperidine, 2,3-dimethyl-, *cis*-	2889, 3491, 4249		
90.	6287-19-0	Piperidine, 2,4-dimethyl	5811, 5811a, 5811b	5811, 5811a, 5811b	
91.	19683-91-1	Piperidine, 2,4-dimethyl-, *cis*-	2889, 3491, 4249		
92.	504-03-0	Piperidine, 2,6-dimethyl-	568b, 2889, 3491, 4249, 5811b		
93.	17721-95-8	Piperidine, 2,6-dimethyl-1-nitroso-	2884, 4249		
94.	35794-11-7	Piperidine, 3,5-dimethyl-	568b, 4249		
95.	766-09-6	Piperidine, 1-ethyl-	568b, 4249		
96.	1484-80-6	Piperidine, 2-ethyl-	568b, 1371, 2889, 3491, 4249, 5811b		
97.	14300-04-0	Piperidine, 2-ethyl-1-nitroso-	2884, 4249		
98.	626-67-5	Piperidine, 1-methyl-		568b, 984, 4249	
99.	109-05-7	Piperidine, 2-methyl-	568b, 4249		
100.	626-56-2	Piperidine, 3-methyl-	568b, 2889, 3491, 4249, 5811b		
101.	13603-07-1	Piperidine, 3-methyl-1-nitroso-	2884, 4249		
102.	626-58-4	Piperidine, 4-methyl-	568b, 4249		
103.	15104-03-7	Piperidine, 4-methyl-1-nitroso-	2884, 4249		
104.	71607-72-2	Piperidine, (1-methylethyl)-	2889, 3491, 4249		

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

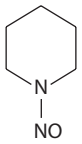
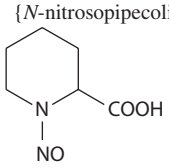
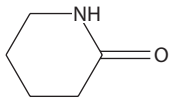
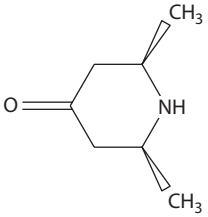
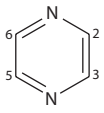
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
105.	100-75-4	Piperidine, 1-nitroso- {NPIP} 	30, 31, 203–206, 239, 457, 568b, 572, 573, 746c, 1058, 1428, 1740, 1741, 1743, 1744, 1781, 1784, 1808, 1870–1872, 1952, 2118, 2205, 2442, 2443, 2516, 2724, 2825, 2884, 3255–3257, 3265, 3300, 3302, 3308, 3491, 3595–3598, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	498, 568b, 1870–1872, 2139, 2205, 2516, 3947, 3948, 3994, 4249, 5001, 5496, 5811b	
106.	77-10-1	Piperidine, 1-(1-phenylcyclohexyl)-	4249, 17B41a	17B41a	17B41a
107.	13406-98-9	1-Piperidinecarboxylic acid		2566, 4249, 4511	
108.		2-Piperidineacetic acid, 1-nitroso- {NPIPAC}		486, 4249	
109.	535-75-1	2-Piperidinecarboxylic acid {pipecolic acid}	5048	1351, 2337, 2722, 3491, 3797, 3974a, 4249, 4398c, 4475, 5079, 5873	
110.	4515-18-8 30310-81-7	2-Piperidinecarboxylic acid, 1-nitroso- {*N*-nitrosopipecolic acid (NPIC)} 	3256, 3300, 3943a, 3944–3946, 4249, 5811, 5811a, 5811b	486, 992, 3943a, 3944–3948, 4249, 5811, 5811a, 5811b	
111.	65445-62-7	3-Piperidinecarboxylic acid, 1-nitroso-	3951	3300, 4249	
112.	6238-69-3	4-Piperidinecarboxylic acid, 1-nitroso-		3300, 4249	
113.	1121-89-7	2,6-Piperidinedione {glutarimide}	568b, 1360, 1371, 1375, 1375a, 1375b, 1586, 2543, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3553, 3557, 4249, 4407, 5811b		1360, 1375a
114.		2,6-Piperidinedione, methoxy-	1371, 1586, 4249		
115.		2,6-Piperidinedione, 3-methoxy-	568b, 4249		
116.	61892-70-4	2,6-Piperidinedione, 4-methoxy-	1365, 2773, 2775, 3553, 4249, 5811b		
117.	72692-70-7	2,6-Piperidinedione, methyl-	1586, 2767, 3557, 4249		
118.	29553-51-3	2,6-Piperidinedione, 3-methyl-	568b, 2767, 3553, 3557, 4249, 5811b		
119.	25077-26-3	2,6-Piperidinedione, 4-methyl-	568b, 3553, 3557, 3559, 4249, 5811b		
120.	27154-43-4	Piperidinone	1586, 4249		
121.	675-20-7	2-Piperidinone 	1371, 1375, 1375b, 1586, 2570, 2767, 2775, 3553, 4249, 5811b	2389, 2544, 3491, 3550, 4249, 5811b	
122.	61891-65-4	2-Piperidinone, methyl-	3553, 3557, 4249, 5811b		
123.	931-20-4	2-Piperidinone, 1-methyl-	568b, 2767, 3553, 4249, 5811b	404, 568b, 2386, 2389, 2544, 3491, 4249, 5811b	
124.	4775-98-8	2-Piperidinone, 6-methyl-	1586, 2767, 2769, 3557, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
125.	13200-35-6	4-Piperidinone, 2,6-dimethyl-, *cis*- 	1120, 3559, 4249, 5811b		
126.	69135-98-4	4-Piperidinone, 2,6-dimethyl-, *trans*-	1120, 4249, 5811b		
127.	3311-23-7	4-Piperidinone, 2,2,6-trimethyl-, (R)-	1120, 4249, 5811b		
128.		Propanamide, *N*-(2-methylpyridyl)-	568b, 4249		
129.		1-Propanone, 1-(4-methyl-2-pyridinyl)-	4570a		
130.	3238-55-9	1-Propanone, 1-(2-pyridinyl)-	4570a		
131.		1-Propanone, 1-(2-pyridinyl)-2-methyl-	4570a		
132.	1570-48-5	1-Propanone, 1-(3-pyridinyl)- {pyridyl ethyl ketone}	568b, 761, 916, 1587, 2079, 2107, 2170, 2224, 2228, 2270, 2724, 2731, 2735, 2939, 3054, 3056, 3058, 3062, 3302, 3308, 3444, 3523, 3553, 3708, 4202, 4249, 5079, 5811b	568b, 937, 2359, 2939, 3056, 3444, 3973, 4249, 5079, 5382, 5811b	
133.	1701-69-5	1-Propanone, 1-(4-pyridinyl)-	568b, 1587, 4249		
134.	80933-75-1	1-Propanone, 1-[2-(3,4,5,6-tetrahydropyridinyl)]-		2917a, 4249	
135.	6302-03-0	2-Propanone, 1-(3-pyridinyl)-	2724, 2727, 2731, 2735, 2939, 3302, 3491, 4249	937, 3491, 4249	
136.		2-Propanone, 1-(4-pyridinyl)-	1587, 4249		
137.	54356-27-3	2-Propenenitrile, 3-(3-pyridinyl)-, (*E*)-	568b, 1587, 4249, 5811b		
138.	54356-28-4	2-Propenenitrile, 3-(3-pyridinyl)-, (*Z*)-	568b, 1587, 4249, 5811b		
139.	145917-24-4	2-Propen-1-one, 1,3-di-3-pyridinyl-, (*E*)-		4249, 4786	
140.	290-37-9	Pyrazine 	172, 241, 299, 431, 568b, 775, 1063–1066, 1068–1075, 1348, 1349, 1351, 1369, 1371, 1426, 1580, 1587a, 1744, 1842, 2382, 2439, 2470, 2543, 2545, 2724, 2727, 2765–2767, 2773, 2775, 2777, 3261, 3386, 3559, 3797, 4249, 4407, 5034, 5512, 5811b	568b, 937, 1580, 2339a, 2359, 2381, 2724, 2917a, 3491, 3973, 3974a, 4249, 5811b, 17B12, 17B13, 17B26, 17B27, 17B40, 17B51, 71B60	
141.		Pyrazine, alkyl-	722, 1364, 1371, 2543, 2545, 2570, 2761, 2762, 2799a, 4249	2381, 4249	
142.	66288-42-4	Pyrazine, butenyl-	2767, 4249, 4570a		
143.	29460-93-3	Pyrazine, 2-(2-butenyl)-	568b, 4249	568b, 4249	
144.	78210-56-7	Pyrazine, 3-butenyl- = pyrazine, 2-butenyl-	1587, 2767, 2769, 4249, 4570a	937, 4249	
145.	29460-91-1	Pyrazine, 2-butyl-	568b, 1124a, 4249, 4570a, 5811b		
146.	32184-51-3	Pyrazine, 2-cyclopentyl-6-methyl-	2773, 2775, 4249		

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
147.	15707-24-1	Pyrazine, 2,3-diethyl-	1369, 1371, 1884, 2724, 2727, 2732, 2767, 3204, 3261, 3266, 3386, 4249	172a, 174b, 937, 1053, 1369, 3204, 3266, 3370, 3905, 4249	
148.	18138-04-0	Pyrazine, 2,3-diethyl-5-methyl-	568b, 4249	568b, 4249	
149.	13238-84-1	Pyrazine, 2,5-diethyl-	1351, 1587a, 1884, 2570, 2727, 2731, 2732, 2735, 2767, 3204, 3266, 3386, 3491, 4249, 5811b	1053, 1369, 2338, 3204, 3266, 3905, 4249	
150.	32736-91-7	Pyrazine, 2,5-diethyl-3-methyl-	568b, 4249		
151.	13067-27-1	Pyrazine, 2,6-diethyl-	1351, 1587a, 1590, 1884, 2724, 2727, 2731, 2732, 2735, 2767, 3204, 3266, 3386, 3491, 4249	937, 1053, 1369, 2389, 2544, 2724, 3204, 3266, 3491, 3905, 4249	
152.	18138-05-1	Pyrazine, 3,5-diethyl-2-methyl- = pyrazine, 2,6-diethyl-3-methyl-	568b, 1360, 1375a, 2761, 2762, 2765, 2766, 2777, 4249		1360, 1375a
153.	25704-73-8	Pyrazine, dimethyl-	431, 480, 1365, 2506, 2507, 2731, 2735, 3397, 3398, 4249, 5811b	3973, 4249, 5811b	2506, 2507
154.	5910-89-4	Pyrazine, 2,3-dimethyl-	568b, 775, 1063–1066, 1068–1074, 1348, 1349, 1351, 1360, 1364, 1369, 1371, 1375a, 1586, 1587a, 1884, 2142, 2337, 2439, 2470, 2543, 2545, 2724, 2727, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3261, 3266, 3491, 4249, 4407, 4570a, 5811b	172a, 174b, 404, 568b, 937, 1053, 1369, 2337, 2339a, 2339b, 2359, 2724, 3204, 3266, 3491, 4249, 5811b	1360, 1375a
155.	15707-34-3	Pyrazine, 2,3-dimethyl-5-ethyl-	568b, 4249, 5811b		
156.		Pyrazine, 2,3-dimethyl-6-propyl-	4570a		
157.	123-32-0	Pyrazine, 2,5-dimethyl-	299, 480, 568b, 1063–1066, 1068–1075, 1348, 1349, 1351, 1364, 1365, 1369, 1371, 1587a, 1884, 2337, 2439, 2470, 2493, 2543, 2545, 2570, 2724, 2727, 2731, 2732, 2735, 2767, 2773, 2775, 3190, 3255, 3261, 3266, 3398, 3491, 3559, 3992, 4249, 4407, 4570a, 5811b	172a, 174b, 568b, 1053, 1369, 2337, 2339a, 2339b, 2359, 2386, 2724, 2917a, 3186, 3188, 3266, 3370, 3491, 4249	
158.	80935-98-4	Pyrazine, 2,5-dimethyl-3-ethenyl-	568b, 4249		
159.		Pyrazine, 2,5-dimethyl-3-(1-methylethyl)- = pyrazine, 3,6-dimethyl-2(1-methylethyl)-		2359, 4249	
160.		Pyrazine, 2,5-dimethyl-6-propyl-	4570a		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
161.	108-50-9	Pyrazine, 2,6-dimethyl-	299, 568b, 775, 1063–1066, 1068–1074, 1348, 1349, 1351, 1364, 1365, 1369, 1371, 1587a, 1884, 2337, 2387, 2439, 2470, 2543, 2545, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3261, 3266, 3491, 3555, 3559, 3888, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 937, 965, 1053, 1369, 2337, 2339a, 2339b, 2386, 2389, 2544, 2611, 2724, 2917a, 3266, 3491, 3555, 4249, 5811b	2387
162.		Pyrazine, 2,6-dimethyl-3-ethenyl-	568b, 4249		
163.	71607-73-3	Pyrazine, dimethylethyl-	1587a, 2724, 2732, 2767, 3491, 4249	2724, 3491, 4249	
164.	4177-16-6	Pyrazine, 2-ethenyl-	568b, 1587, 1587a, 2773, 3255, 4249, 5811b	568b, 3547, 4249	
165.	13925-08-1	Pyrazine, 2-ethenyl-5-methyl-	568b, 1587, 1587a, 4249, 4570a, 5811b	568b, 3905, 4249	
166.	13925-09-2	Pyrazine, 2-ethenyl-6-methyl-	299, 568b, 1587, 1587a, 2543, 2773, 4249, 4570a, 5811b	568b, 937, 3491, 3547, 4249	
167.	13925-00-3	Pyrazine, ethyl- = pyrazine, 2-ethyl-	568b, 775, 1075, 1348, 1349, 1364, 1369, 1371, 1428, 1587a, 2337, 2387, 2439, 2543, 2545, 2570, 2727, 2731, 2735, 2767, 2769, 2773, 2775, 3255, 3261, 3386, 3410, 3491, 4249, 4407, 4570a, 5811b	568b, 2339a, 4249	2387
168.	33504-66-4	Pyrazine, ethylmethyl-	2731, 2735, 3398, 4249, 5811b		
169.	13360-65-1	Pyrazine, 2-ethyl-3,6-dimethyl- = pyrazine, 6-ethyl-2,5-dimethyl-	568b, 775, 1351, 1369, 1587a, 1884, 2337, 2439, 2727, 2731, 2735, 2767, 3261, 3266, 4249, 4570a	172a, 174b, 568b, 937, 1053, 2337, 3266, 3370, 3491, 4249, 5811b	
170.	13925-07-0	Pyrazine, 2-ethyl-3,5-dimethyl- = pyrazine, 3-ethyl-2,6-dimethyl-	568b, 775, 1351, 1369, 1587, 1587a, 1884, 2439, 2732, 2737, 2775, 3266, 4249, 4570a	172a, 174b, 431, 568b, 1053, 2836, 3266, 3370, 3491, 4249	
171.	15707-34-3	Pyrazine, 2-ethyl-5,6-dimethyl- = pyrazine, 5-ethyl-2,3-dimethyl-	1360, 1371, 1375a, 1587a, 2337, 2543, 2761, 2762, 2765, 2766, 2773, 2767, 4249, 4570a	965, 2337, 2389, 2544, 3491, 4249	1360, 1375a
172.		Pyrazine, 2-ethyl-5-ethylene-		3547, 4249	
173.	25680-58-4	Pyrazine, 2-ethyl-3-methoxy-		1053, 3266, 4249	
174.		Pyrazine, 2-ethyl-5-methoxy-		1053, 3266, 4249	
175.	67845-38-9	Pyrazine, 2-ethyl-6-methoxy-		1053, 3266, 4249	

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
176.	15707-23-0	Pyrazine, 2-ethyl-3-methyl-	568b, 1075, 1351, 1364, 1587, 1587a, 2387, 2439, 2545, 2724, 2731, 2735, 2767, 3266, 4249, 4570a, 5811b	172a, 174b, 568b, 937, 1053, 2359, 2386, 2724, 3266, 3905, 4249	2387
177.	13360-64-0	Pyrazine, 2-ethyl-5-methyl-	568b, 775, 1348, 1349, 1351, 1369, 1371, 1587a, 2337, 2439, 2470, 2543, 2570, 2727, 2731, 2735, 2761, 2762, 2765, 2767, 2773, 2775, 3261, 3410, 3491, 3559, 4249, 4570a, 5811b	568b, 937, 984, 2337, 3219, 3491, 4249, 5811b	
178.	13925-03-6	Pyrazine, 2-ethyl-6-methyl- = pyrazine, 6-ethyl-2-methyl-	568b, 775, 1351, 1360, 1375a, 1587a, 2337, 2387, 2543, 2724, 2727, 2731, 2732, 2735, 2765–2767, 2773, 2775, 2777, 3255, 3491, 3555, 4249, 4570a, 5811b	568b, 937, 965, 2337, 2339a, 2359, 2724, 3491, 3555, 3974a, 4249, 5811b	1360, 1375a, 2387
179.	17398-16-2	Pyrazine, 2-ethyl-3,5,6-trimethyl-		2339a, 4249	
180.	32736-95-1	Pyrazine, 2-furanyl-	568b, 1351, 1587a, 2727, 2731, 2735, 2799a, 3410, 3491, 4249, 5811b	568b, 3547, 4249	
181.	32737-01-2	Pyrazine, 2-(2-furanyl)-3-methyl-	568b, 4249		
182.	29460-98-8	Pyrazine, 3-furanyl-	1587, 2799a, 4249, 5811b		
183.	36238-34-3	Pyrazine, 5-(2-furanyl)-2,3-dimethyl- = pyrazine, 2-(2-furanyl)-5,6-dimethyl-	1351, 2731, 2735, 4249, 5811b		
184.	27610-38-4	Pyrazine, 2-(2-furanyl)-5-methyl-	568b, 1351, 1587a, 2543, 2545, 2724, 2727, 2731, 2732, 2735, 2773, 2775, 3255, 3410, 3491, 3553, 4249, 5811b	568b, 2724, 3491, 3547, 4249	
185.	32737-03-4	Pyrazine, 2-(2-furanyl)-6-methyl-	568b, 1075, 1351, 1587a, 2727, 2731, 2735, 3410, 3491, 4249, 5811b	568b, 3547, 4249	
186.	29461-10-7	Pyrazine, 2-(3-furanyl)-5-methyl-	2775, 4249		
187.	3149-28-8	Pyrazine, methoxy-		1053, 3266, 4249	
188.	2847-30-5	Pyrazine, 3-methoxy-2-methyl-		172a, 174b, 568b, 1053, 3266, 3370, 4249	
189.	2882-22-6	Pyrazine, 5-methoxy-2-methyl-		172a, 174b, 1053, 3266, 4249	
190.	2882-21-5	Pyrazine, 6-methoxy-2-methyl-		172a, 174b, 1053, 3266, 4249	
191.	24683-00-9	Pyrazine, 2-methoxy-3-methylpropyl-		568b, 1053, 3266, 4249	

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

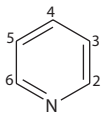
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
192.	109-08-0	Pyrazine, methyl- = pyrazine, 2-methyl-	143, 157, 159, 167, 172, 299, 431, 480, 568b, 775, 1063–1066, 1068–1075, 1348, 1349, 1351, 1360, 1364, 1365, 1369, 1371, 1375a, 1427, 1428, 1587a, 1842, 1881, 1884, 1949, 2142, 2337, 2439, 2493, 2543, 2545, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3190, 3255, 3266, 3386, 3397, 3398, 3491, 3992, 4249, 4407, 4570a, 4733, 5811b	172a, 174b, 568b, 937, 965, 984, 1053, 1369, 1852, 1949, 2337, 2339a, 2359, 2544, 2611, 2724, 2917a, 3266, 3491, 4249, 5811b	1360, 1375a
193.	38713-41-6	Pyrazine, (1-methylethenyl)-	568b, 1587a, 3255, 4249	568b, 937, 3491, 4249	
194.	29460-90-0	Pyrazine, (1-methylethyl)-	4570a	937, 2336, 4249	
195.	34514-52-8	Pyrazine, methyl(1-methylethyl)-	2727, 2735, 3491, 4249, 5811b		
196.		Pyrazine, 2-methyl-3-butyl-	4570a		
197.	15986-81-9	Pyrazine, 2-methyl-3-(1-methylethyl)-		568b, 2735, 4249	
198.		Pyrazine, 2-methyl-3-(2-methylbutyl)-	4570a		
199.	32737-06-7	Pyrazine, 2-methyl-3-(3-methylbutyl)-	568b, 4249, 4570a		
200.	13925-06-9	Pyrazine, 2-methyl-3-(2-methylpropyl)-	4570a		
201.	13925-05-8	Pyrazine, 2-methyl-5-(1-methylethyl)-	568b, 4249, 4570a		
202.	29444-53-9	Pyrazine, 2-methyl-3-phenyl-	568b, 4249		
203.	58861-90-8	Pyrazine, 2-methyl-5-phenyl-	568b, 1351, 1587a, 2543, 2773, 3553, 4249, 5811b		
204.	74233-03-7	Pyrazine, 2-methyl-6-phenyl-	568b, 4249		
205.	55138-67-5	Pyrazine, 2-methyl-6-(1-propenyl)-		2917a, 4249	
206.	36541-30-7	Pyrazine, methylpropyl-	1587a, 2727, 2735, 3491, 4249		
207.	29461-03-8	Pyrazine, 2-methyl-5-propyl-	568b, 1587, 1587a, 4249, 5811b		
208.	29444-46-0	Pyrazine, 2-methyl-6-propyl-	568b, 4249, 4570a		
209.	67952-65-2	Pyrazine, 3(5 or 6)-methyl-2-methylthio-		1053, 3266, 4249	
210.	6303-75-9	Pyrazine, 2-pentyl-	568b, 3406, 4249		
211.	29460-97-7	Pyrazine, 2-phenyl-	568b, 3410, 4249	568b, 3547, 4249	
212.	28217-95-0	Pyrazine, 2-phenylmethyl-	568b, 4249		
213.		Pyrazine, 2-(1-propenyl)-	4570a		
214.	18138-03-9	Pyrazine, 2-propyl-	568b, 1587, 1587a, 4249, 4570a		
215.	1124-11-4	Pyrazine, tetramethyl-	568b, 775, 1075, 1351, 1360, 1375a, 1587a, 1590, 1884, 2337, 2543, 2724, 2727, 2732, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 3204, 3266, 3491, 3553, 3555, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 937, 965, 1053, 1590, 2337, 2339b, 2386, 2389, 2544, 2724, 3204, 3266, 3370, 3491, 3555, 3905, 4249, 5811b, 17B01, 17B10	1360, 1375a

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
216.	14667-55-1	Pyrazine, trimethyl-	299, 568b, 775, 1063–1066, 1068–1075, 1348, 1349, 1351, 1360, 1369, 1371, 1375a, 1587a, 1881, 1884, 1949, 2337, 2387, 2470, 2506, 2507, 2543, 2545, 2570, 2724, 2727, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3204, 3255, 3261, 3266, 3386, 3491, 3555, 3559, 4249, 4407, 4570a, 5811b	172a, 174b, 404, 568b, 937, 965, 1053, 1369, 1949, 2337, 2339a, 2339b, 2359, 2386, 2389, 2544, 2611, 2724, 2917a, 3204, 3266, 3370, 3491, 3555, 3905, 3974a, 4249, 5811b	1360, 1375a, 2387, 2506, 2507
217.	61892-91-9	Pyrazinebutanol, 3-methyl-	568b, 2767, 4249		
218.	5780-66-5	Pyrazinecarboxaldehyde	1062, 4249		
219.		Pyrazinecarboxaldehyde, 5-(2-furanyl)-3-methyl-		568b, 3547, 4249	
220.	6705-31-3	Pyrazineethanol	568b, 2570, 2767, 3553, 4249, 5811b	568b, 3649, 4249	
221.	61892-92-0	Pyrazineethanol, 3-methyl-	568b, 2767, 3553, 4249	568b, 3649, 4249	
222.	61892-93-1	Pyrazineethanol, 6-methyl-	568b, 2767, 3553, 4249, 4407	568b, 3649, 4249	
223.	6705-33-5	Pyrazinemethanol	2767, 3255, 3553, 4249		
224.	61892-95-3	Pyrazinemethanol, 5-methyl-	568b, 3553, 3559, 4249	568b, 3649, 4249	
225.		Pyrazinepentanol		3553, 4249	
226.	6270-63-9	2(1*H*)-Pyrazinone = 2-pyrazinol	568b, 4249		
227.	78210-68-1	2(1*H*)-Pyrazinone, 1-methyl-3-(1-methylethyl)-	568b, 1587, 4249, 5811b		
228.	19838-07-4	2(1*H*)-Pyrazinone, 3-methyl-	568b, 1351, 1587a, 3553, 3559, 4249, 5811b	568b, 3649, 4249	
229.	20721-17-9	2(1*H*)-Pyrazinone, 5-methyl-	4249		
230.	20721-18-0	2(1*H*)-Pyrazinone, 6-methyl-	4249		
231.	289-80-5	Pyridazine	568b, 4249		
232.	123-33-1	3,6-Pyridazinedione, 1,2-dihydro- {maleic hydrazide}	715, 716, 1333, 1470, 1507, 1580, 1741, 2384, 2385, 3300, 3493, 4274, 5512, 21A19	479, 480, 691,704, 715, 716, 905, 1147, 1333, 1473, 1474, 1580, 2277, 2383, 2385, 2906, 2907, 2939, 3493, 3585c, 3633, 3723, 3725, 3728, 3767a, 3811a, 3973, 3974b, 3977, 3998, 4236, 4269, 4271a, 4274, 5016, 5553, 5568, 5586, 5605, 5642, 5667, 5686, 5687, 5717, 5774, 5811b, 21A19	
233.	5716-15-4 21422-41-3	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt		3636, 4249, 5811b	
234.	51542-52-0	3,6-Pyridazinedione, 1,2-dihydro-, potassium salt		3636, 4249	
235.		(2*H*)-Pyridazinone, 1-methyl-3-propyl-	568b, 4249		
236.	26445-05-6	Pyridinamine	3302, 4249		
237.	71607-77-7	Pyridinamine, *N*-methyl-	4249, 4866		
238.	504-29-0	2-Pyridinamine	568b, 1587, 3255, 3386, 4249, 5811b	568b, 3550, 4249	
239.	1603-40-3	2-Pyridinamine, 3-methyl-	2378a, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

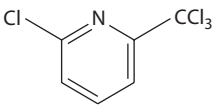
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
240.	695-34-1	2-Pyridinamine, 4-methyl- {2-amino-4-picoline}	568b, 4249		
241.	1603-41-4	2-Pyridinamine, 5-methyl-	2378a, 4249		
242.	1824-81-3	2-Pyridinamine, 6-methyl-	568b, 2378a, 3410, 4249		
243.	462-08-8	3-Pyridinamine	568b, 3255, 3386, 3967, 4249		
244.	61771-67-3	3-Pyridinamine, 6-methoxy-*N*-methyl-	3553, 4249		
245.	3430-10-2	3-Pyridinamine, 2-methyl-	3797, 4249		
246.	3430-27-1	3-Pyridinamine, 4-methyl-	4249		
247.	18364-47-1	3-Pyridinamine, *N*-methyl-	1140, 2724, 2734, 3308, 3797, 4249		
248.	504-24-5	4-Pyridinamine	568b, 1587, 3559, 4249, 5811b		
249.	110-86-1	Pyridine 	38, 107, 126b, 156, 167, 172, 173a, 174b, 195, 237, 239, 299, 376, 395, 424, 462, 480, 512, 568b, 688, 775, 920, 985–988, 1063–1075, 1078, 1084, 1099, 1100, 1137, 1140, 1225, 1263, 1314, 1338, 1348, 1349, 1360, 1364, 1365, 1369, 1371, 1375a, 1386, 1426, 1427, 1437, 1445, 1580, 1587a, 1590, 1634, 1644, 1645, 1647–1649, 1659, 1673, 1674, 1699, 1741, 1744, 1803, 1812, 1842, 1857, 1884, 1890, 1891, 1903, 1911, 1966, 2001, 2006, 2088, 2133, 2142, 2170, 2191, 2224, 2226, 2228, 2230, 2233, 2234, 2267, 2270, 2313a, 2313c, 2326, 2337, 2342, 2342a, 2343, 2349, 2382, 2470, 2493, 2506, 2507, 2524, 2543, 2545, 2628, 2629, 2634, 2636, 2710, 2724, 2734, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 2857, 2858, 2869, 2912, 2936–2938, 2939, 2973, 2986–2988, 3007, 3008, 3022, 3025, 3029, 3044, 3059, 3204, 3140, 3255, 3257, 3261, 3266, 3300, 3302, 3308, 3324, 3386, 3397, 3398, 3410, 3444, 3463, 3482, 3499, 3505, 3692, 3761, 3797, 3803,3909, 3910, 3912,	120, 568b, 984, 1020, 1053, 1263, 1580, 1590, 1852, 2001, 2079, 2337, 2339a, 2359, 2389, 2544, 2724, 2917a, 2939, 2987, 3022, 3044, 3204, 3266, 3444, 3499, 3797, 3973, 3974a, 4064, 4249, 5079, 5390a, 5173, 5382, 5720, 5811b, 17B56	1360, 1375a, 2506 (0), 2507 (0), 3393

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine (cont.)	3924, 3934, 3967, 3976, 3992, 3999, 4005–4007, 4064, 4065, 4120–4122, 4127, 4132, 4202, 4228, 4249, 4407, 5034, 5079, 5124, 5138, 5140, 5189, 5263, 5359, 5512, 5770, 5811b, 5836, 5869a		
250.		Pyridine, alkyl-	568b, 722, 2543, 2765, 2766, 2773, 4249		
251.		Pyridine, C_3-alkyl-	568b, 1586, 2761, 2762, 2765–2767, 2773, 2777, 3410, 3559, 4249		
252.		Pyridine, (C_3-alkylphenyl)- {Two isomers detected}	568b, 1587, 4249		
253.	31388-09-7	Pyridine, butyl	5811b		
254.	65375-18-0	Pyridine, butenyl {three isomers}	4570a, 5811b		
255.	27175-64-0	Pyridine, dimethyl- {lutidine}	167, 480, 512, 1644, 1645, 1649, 1803, 2079, 2170, 2342, 2342a, 2524, 3255, 3397, 3733, 3750, 3752, 3976, 4064, 4249, 5034, 5079, 5811b	2727, 3491, 3973, 4064, 4249, 5079, 5382, 5811b	
256.	29011-62-9	Pyridine, dimethylethenyl-	3733, 3750, 3752, 4249		
257.		Pyridine, dimethylethyl- {Two isomers detected}		2339a, 4249	
258.		Pyridine, dimethyl-2-(1-methylethyl)-	4570a		
259.		Pyridine, dimethylphenyl-	3733, 3750, 3752, 4249		
260.	56842-43-4	Pyridine, diphenyl-	2141, 4249, 5811b		
261.	1337-81-1	Pyridine, ethenyl-	167, 480, 512, 1075, 1215, 1427, 1649, 1842, 2951, 4249, 5034, 5811b		
262.	25638-00-0	Pyridine, ethenylmethyl-	1644, 1645, 3398, 4249, 5034, 5811b		
263.		Pyridine, ethenyltrimethyl-	3733, 3750, 3752, 4249		
264.	28631-77-8	Pyridine, ethyl-	2777, 2858, 2939, 3190, 3992, 4249, 5034		
265.	27987-10-6	Pyridine, ethylmethyl- {four isomers}	1360, 1375a, 1587, 2727, 2761, 2762, 2765, 2766, 2773, 2777, 3491, 3559, 4249, 5034, 5811, 5811a, 5811b	2339a, 3430, 4249, 5811, 5811a, 5811b	1360, 1375a
266.	64849-96-3	Pyridine, ethylphenyl-	2141, 4249, 5811b		
267.	1333-41-1	Pyridine, methyl- {picoline}	167, 480, 512, 1263, 1316, 1445, 1644, 1645, 1647, 1649, 1744, 1842, 2079, 2170, 2270, 2342, 2342a, 2506, 2507, 2570, 2710, 2777, 2799a, 3190, 3308, 3976, 3992, 4064, 4065, 5034, 5079, 5140, 5512, 5811b	120, 395, 1263, 1852, 4064, 5079, 5382	2506 (0), 2507 (0)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
268.	64828-54-2	Pyridine, methylphenyl-	3733, 3750, 3752, 4249, 5811b		
269.	65307-85-9	Pyridine, pentyl-	5811, 5811a, 5811b		
270.	64828-55-3	Pyridine, phenylpropyl-	2141, 4249, 5811b		
271.		Pyridine, phenyltrimethyl-	3733, 3750, 3752, 4249		
272.	65375-17-9	Pyridine, propenyl-	1075, 1360, 1375a, 2761, 2762, 2765, 2766, 4249, 5811b		1360, 1375a
273.	65307-84-8	Pyridine, propyl-	2777, 4249, 5811, 5811a, 5811b		
274.		Pyridine, tetramethyl-	3733, 3750, 3752, 4249		
275.	29611-84-5	Pyridine, trimethyl- {collidine}	1075, 1587a, 1971, 2079, 2142, 2170, 2326, 2342, 2342a, 2543, 2545, 2773, 2939, 3308, 3398, 3410, 3499, 3733, 3750, 3752, 4064, 4065, 4249, 5079, 5263, 5811b	4064, 5079, 5382, 5811b	
276.	6972-40-3	Pyridine, 1-ethyl-1,2,3,6-tetrahydro-	568b, 4249		
277.	694-05-3	Pyridine, 1,2,3,6-tetrahydro-	568b, 1140, 2724, 2734, 2883, 2889, 3308, 3410, 3491, 3797, 4249	568b, 1877, 2722, 2746, 3491, 3974a, 4249, 5811b	
278.		Pyridine, 2-(C_3-alkylphenyl)- {Two isomers detected}	1587, 4249		
279.	5058-19-5	Pyridine, 2-butyl-	568b, 1587, 4249, 4570a, 5811b		
280.	1929-82-4	Pyridine, 2-chloro-6-(trichloromethyl)- {Nitrapyrin®} 		3973, 4249	
281.	100-69-6	Pyridine, 2-ethenyl-	568b, 1099, 1100, 1371, 1427, 2233, 2234, 2727, 2775, 3190, 3255, 3491, 3733, 3750, 3752, 3992, 4249, 4407, 4570a, 5811b	5720	
282.	22382-94-1	Pyridine, 2-ethenyl-3-methyl-	568b, 1587, 4249, 5811b		
283.	3883-39-4	Pyridine, 2-ethenyl-5-methyl-	568b, 4249		
284.	1122-70-9	Pyridine, 2-ethenyl-6-methyl-	1371, 4249		
285.	14529-53-4	Pyridine, 2-ethoxy-	568b, 4249		
286.	100-71-0	Pyridine, 2-ethyl-	107, 299, 568b, 775, 1063–1066, 1068–1074, 1140, 1348, 1349, 1360, 1369, 1375a, 1587a, 2233, 2234, 2470, 2543, 2545, 2570, 2761, 2762, 2765, 2766, 2773, 2775, 3261, 3302, 3386, 3410, 4249, 4407, 4570a, 4921, 5811b	568b, 1157, 2339a, 3430, 3491, 3973, 3974a, 4249, 5720	1360, 1375a
287.	1123-96-2	Pyridine, 2-ethyl-3,5-dimethyl- = pyridine, 2,4-dimethyl-6-ethyl-	2545, 2761, 2762, 4249		

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
288.	1124-35-2	Pyridine, 2-ethyl-4,6-dimethyl-	1360, 1375a, 2777, 4249		1360, 1375a
289.	56986-88-0	Pyridine, 2-ethyl-3-methyl-	568b, 4249		
290.	2150-18-7	Pyridine, 2-ethyl-4-methyl-	568b, 1587, 2545, 4249, 5811b		
291.	18113-81-0	Pyridine, 2-ethyl-5-methyl-	568b, 2545, 4249		
292.	1122-69-6	Pyridine, 2-ethyl-6-methyl-	568b, 2543, 4249	568b, 2359, 4249	
293.	59239-12-2	Pyridine, 2-ethyl-6-phenyl-	568b, 4249		
294.		Pyridine, 2-(1-hydroxy-1-pentyl)-	568b, 4249		
295.	1628-89-3	Pyridine, 2-methoxy-	568b, 2775, 4249, 4570a		
296.	109-06-8	Pyridine, 2-methyl- {2-picoline}	107, 299, 395, 462, 512, 568b, 775, 1063–1066, 1068–1075, 1078, 1083, 1084, 1099, 1140, 1263, 1339, 1348, 1349, 1360, 1364, 1365, 1371, 1375a, 1587a, 1590, 1634, 1644, 1645, 1647, 1803, 2001, 2088, 2142, 2228, 2270, 2337, 2470, 2493, 2524, 2543, 2545, 2628, 2629, 2636, 2724, 2761, 2762, 2765, 2766, 2773, 2775, 2869, 2939, 3059, 3255, 3261, 3300, 3302, 3308, 3386, 3397, 3398, 3410, 3463, 3491, 3499, 3505, 3797, 3967, 4249, 4407, 4570a, 4921, 5079, 5811b, 25A84	568b, 1086, 1157, 1852, 2339a, 2359, 2611, 3491, 3974a, 4249, 5079, 5390a, 5382, 5720, 5811b	1360, 1375a
297.		Pyridine, 2-methyl-3-(1-methylethyl)-	4570a		
298.	64114-31-4	Pyridine, 2-methyl-3-(1-methyl-2-pyrrolidinyl)- {2-methylnicotine}	1687, 4249	1687, 4249	
299.	78210-48-7	Pyridine, 2-methyl-3-(1-propenyl)-	1587, 4249, 5811b		
300.	15032-21-0	Pyridine, 2-methyl-4-phenyl-	568b, 1587, 4249, 5811b		
301.	56057-93-3	Pyridine, 2-methyl-5-(1-methylethenyl)-	568b, 2727, 3491, 4249	568b, 937, 3491, 3547, 3561, 4249	
302.	20194-71-2	Pyridine, 2-methyl-5-(1-methylethyl)-	568b, 2731, 2735, 3559, 4249, 5811b	568b, 2389, 2544, 3215, 3543, 3549, 3560, 3561, 3905, 4249, 5811b	
303.	56057-96-6	Pyridine, 2-methyl-5-(1-propenyl)-	1587, 4249, 5811b		
304.		Pyridine, 2-methyl-6-(3-methylbutyl)-	4570a		
305.	2294-76-0	Pyridine, 2-pentyl-	568b, 3255, 4249, 4570a	568b, 1053, 3266, 4249	
306.	1008-89-5	Pyridine, 2-phenyl-	568b, 2327c, 2724, 2732, 3491, 3733, 3750, 3752, 4249, 5811b		
307.		Pyridine, 2-propenyl-	4570a		
308.	622-39-9	Pyridine, 2-propyl-	568b, 1371, 1587, 4249, 4407, 4570a		
309.	101-82-6	Pyridine, 2-(phenylmethyl)-	568b, 1587, 4249, 5811b		
310.	7399-50-0	Pyridine, 2-(1-ethylpropyl)-	2142, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
311.	59409-91-5	Pyridine, 2-(1-methyl-3-butenyl)-	1587, 4249, 5811b		
312.	6515-13-5	Pyridine, 2-(1-methylethenyl)-	4570a		
313.	644-98-4	Pyridine, 2-(1-methylethyl)-	4570a		
314.	17618-94-9	Pyridine, 2-(1-propenyl)-	568b, 1371, 1587, 4249, 4570a, 5811b		
315.	21606-61-1	Pyridine, 2-(2-butenyl)-	1587, 4249		
316.	114-91-0	Pyridine, 2-(2-methoxyethyl)-	568b, 4249		
317.		Pyridine, 2-(2-methylbutyl)-	4570a		
318.	6304-24-1	Pyridine, 2-(2-methylpropyl)-	568b, 1587, 4249, 4570a		
319.	583-61-9	Pyridine, 2,3-dimethyl- {2,3-lutidine}	107, 512, 568b, 775, 1075, 1078, 1099, 1100, 1140, 1348, 1349, 1360, 1364, 1369, 1371, 1375a, 1426, 1427, 1587a, 2142, 2228, 2233, 2234, 2470, 2543, 2545, 2724, 2761, 2762, 2765, 2766, 2775, 2777, 2869, 3255, 3261, 3302, 3308, 3386, 3398, 3410, 3463, 3491, 3499, 3505, 3797, 4249, 4921, 5811b	568b, 2339a, 4249, 5390a, 5811b	1360, 1375a
320.	78210-40-9	Pyridine, 2-(3-ethylphenyl)-	1587, 4249, 5811b		
321.	6973-66-6	Pyridine, 2-(3-methylbutyl)-	4570a		
322.	2233-29-6	Pyridine, 2,3,4-trimethyl- {2,3,4-collidine}	2233, 2234, 4249		
323.	695-98-7	Pyridine, 2,3,5-trimethyl- {2,3,5-collidine}	568b, 775, 4249	568b, 2359, 4249	
324.	1462-84-6	Pyridine, 2,3,6-trimethyl- {2,3,6-collidine}	5811b	568b, 1157, 2917a, 3491, 4249	
325.	533-37-9	Pyridine, 2,3,-trimethylene-	568b, 4249		
326.	108-47-4	Pyridine, 2,4-dimethyl- {2,4-lutidine}	37, 38, 107, 512, 568b, 775, 1078, 1099, 1140, 1348, 1349, 1364, 1365, 1369, 1426, 1427, 1587a, 2228, 2233, 2234, 2470, 2543, 2545, 2724, 2775, 2869, 3255, 3261, 3302, 3308, 3386, 3398, 3410, 3463, 3491, 3499, 3505, 3797, 4249, 4407, 4921, 5811b	568b, 2339a, 2917a, 3903, 3973, 4249, 5811b	
327.	1122-45-8	Pyridine, 2,4-dimethyl-, 1-oxide	568b, 4249		
328.	36238-36-5	Pyridine, 2,4-dimethyl-5-(1-methylethyl)-	2727, 2731, 2735, 3491, 4249, 5811b		
329.	1122-39-0	Pyridine, 2,4,5-trimethyl- {2,4,5-collidine}	2401a, 4249		
330.	108-75-8	Pyridine, 2,4,6-trimethyl- {2,4,6-collidine}	568b, 775, 1078, 1587a, 2142, 2170, 2235, 2724, 3255, 3302, 3398, 3463, 3491, 3505, 3797, 4249, 5079, 5811b	5811b	

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
331.	589-93-5	Pyridine, 2,5-dimethyl- {2,5-lutidine}	512, 568b, 775, 1075, 1348, 1349, 1360, 1364, 1369, 1375a, 1427, 1587a, 2142, 2228, 2233, 2234, 2470, 2493, 2545, 2724, 2761, 2762, 2765, 2766, 2777, 2869, 3255, 3261, 3302, 3308, 3386, 3398, 3410, 3463, 3499, 3505, 3797, 4249, 4407, 5811b	568b, 3903, 3973, 4249, 5811b	1360, 1375a
332.	15827-72-2	Pyridine, 2,5-diphenyl-		3219, 3491, 4249, 5811b	
333.	108-48-5	Pyridine, 2,6-dimethyl- {2,6-lutidine}	37, 107, 395, 512, 568b, 775, 1063–1066, 1068–1075, 1078, 1084, 1140, 1360, 1364, 1365, 1371, 1375a, 1426, 1427, 1587a, 2142, 2228, 2233, 2234, 2470, 2524, 2545, 2724, 2761, 2762, 2765, 2766, 2775, 2777, 2869, 2939, 3059, 3255, 3302, 3308, 3386, 3398, 3410, 3491, 3505, 3797, 4249, 4407, 4921, 5079, 5811b	568b, 1157, 2339a, 2389, 2544, 2917a, 3491, 3903, 3973, 4249, 5811b	1360, 1375a
334.	23580-52-1	Pyridine, 2,6-dimethyl-3-ethyl-		4249, 5811b	
335.	36917-36-9	Pyridine, 2,6-dimethyl-4-ethyl-	568b, 4249		
336.	1463-03-2	Pyridine, 2,6-dimethyl-3-phenyl-	3750, 4249		
337.	3558-69-8	Pyridine, 2,6-diphenyl-	568b, 1587, 4249, 5811b		
338.		Pyridine, (C_5-alkenyl)-	1587, 4249		
339.	3731-52-0	Pyridine, 3-(aminomethyl)-	5811, 5811a, 5811b	5811b	
340.	539-32-2	Pyridine, 3-butyl-	568b, 775, 1364, 1587a, 2543, 2545, 2773, 2775, 3444, 4249, 4570a, 5811b	568b, 2611, 3444, 4249	
341.	6760-12-9	Pyridine, 3-butyl-2,6-dimethyl-	568b, 1587, 4249, 5811b		
342.	1121-55-7	Pyridine, 3-ethenyl-	126a, 126b, 172, 237, 299, 462, 512, 568b, 1078, 1063–1066, 1068–1074, 1084, 1099, 1100, 1140, 1316, 1348, 1349, 1360, 1364, 1365, 1371, 1375a, 1445, 1587a, 1644, 1645, 1647, 1674, 1744, 1839, 1966, 2133, 2142, 2228, 2233, 2234, 2387, 2493, 2543, 2545, 2570, 2628, 2690–2695, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2829, 2835,	568b, 984, 2339a, 2359, 3430, 4249, 5720, 5811b	1360, 1375a, 2387

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine, 3-ethenyl- (cont.)	2839, 2857, 2869, 2912, 2951, 3059, 3133, 3255, 3300, 3302, 3308, 3386, 3397, 3398, 3410, 3463, 3491, 3499, 3505, 3559, 3733, 3750, 3752, 3797, 3826, 4159, 4249, 4407, 4570a, 4921, 5512, 5811b		
343.	51961-51-4	Pyridine, 3-ethenyl-5-methyl-	1587, 4249, 5811b		
344.	536-78-7	Pyridine, 3-ethyl-	107, 568b, 775, 1063–1066, 1068–1075, 1078, 1084, 1099, 1140, 1316, 1348, 1349, 1360, 1364, 1369, 1371, 1375a, 1587a, 1634, 2142, 2228, 2233, 2234, 2387, 2470, 2493, 2543, 2545, 2724, 2761, 2762, 2765, 2766, 2773, 2775, 2869, 2912, 3255, 3261, 3266, 3302, 3308, 3386, 3397, 3398, 3410, 3463, 3491, 3499, 3505, 3797, 3976, 4249, 4407, 4570a, 4921, 5811b	568b, 984, 1053, 1078, 1157, 1316, 3266, 3430, 3973, 3974a, 4093, 4249, 5720, 5811b	1360, 1375a, 2387
345.	529-21-5	Pyridine, 3-ethyl-4-methyl-	568b, 2142, 3255, 4249		
346.	3999-78-8	Pyridine, 3-ethyl-5-methyl-	568b, 1587, 4249, 5811b		
347.	7295-76-3	Pyridine, 3-methoxy-	568b, 1371, 1587, 4249, 5034, 5811b	568b, 2917a, 4249, 5811b	
348.	78210-42-1	Pyridine, 3-methoxy-5-methyl-	568b, 1587, 4249, 5811b		
349.	108-99-6	Pyridine, 3-methyl- {3-picoline}	107, 126a, 239, 299, 395, 462, 512, 568b, 775, 1078, 1063–1066, 1068–1074, 1083, 1084, 1140, 1314, 1348, 1349, 1360, 1364, 1365, 1369, 1371, 1375a, 1426, 1427, 1445, 1587a, 1644, 1645, 1647, 1674, 1803, 2001, 2088, 2142, 2217, 2270, 2337, 2493, 2543, 2545, 2724, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2857, 2858, 2869, 2912, 2939, 3255, 3261, 3300, 3302, 3308, 3386, 3397, 3398, 3410, 3444, 3463, 3491, 3499, 3505, 3553, 3559, 3729, 3797, 4159, 4249, 4921, 5770, 5811b	568b, 984, 1086, 1852, 2339a, 2917a, 3430, 3903, 3973, 4249, 5390a, 5720, 5811b	1360, 1375a

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
350.		Pyridine, 3-methyl-2-(2-methylbutyl)-	4570a		
351.		Pyridine, 3-methyl-2-(3-methylbutyl)-	4570a		
352.	72693-04-0	Pyridine, 3-methyl-2-(1-methylethyl)-	568b, 1587, 4249, 5811b		
353.	18368-73-5	Pyridine, 3-methyl-2-nitro-	1360, 1375a, 2761, 2762, 2765, 2766, 4249		1360, 1375a
354.	1003-73-2	Pyridine, 3-methyl-1-oxide	568b, 4249		
355.	10273-90-2	Pyridine, 3-methyl-2-phenyl-	568b, 4249		
356.	10477-94-8	Pyridine, 3-methyl-5-phenyl-	1587, 4249, 5811b		
357.	1802-20-6	Pyridine, 3-pentyl-	568b, 1587, 3255, 4249, 5811b		
358.	1008-88-4	Pyridine, 3-phenyl-	568b, 1360, 1371, 1375a, 2543, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 3255, 3386, 3398, 3410, 3491, 3557, 3733, 3750, 3752, 4249, 5811b	568b, 937, 984, 2339a, 2359, 2724, 3491, 4249, 5811b	1360, 1375a
359.	4673-31-8	Pyridine, 3-propyl-	568b, 1360, 1375a, 2731, 2735, 2761, 2762, 2765, 2766, 3386, 4249, 5811b		1360, 1375a
360.		Pyridine, 3-propenyl-	1586, 1587, 1587a, 2545, 2761, 2762, 2769, 2777, 4249	937, 3491, 4249	
361.	78210-50-1	Pyridine, 3-(tetrahydro-2-furanyl)-	1587, 4249, 5811b		
362.	4754-27-2	Pyridine, 3-(1-hydroxyethyl)-	568b, 4249		
363.		Pyridine, 3-(1-methyl-3-butenyl)-	1587, 4249		
364.	15825-89-5	Pyridine, 3-(1-methylethenyl)-	568b, 1371, 1587, 4249, 5811b		
365.	88111-63-1	Pyridine, 3-(1-methylethoxy)-	568b, 4249		
366.		Pyridine, 3-(1-methylethyl)-	4570a		
367.	15376-62-2	Pyridine, 3-(1-propenyl)-	568b, 1360, 1371, 1375a, 2543, 2765–2767, 2773, 2775, 4249, 4570a, 5811b	568b, 2389, 2544, 4249, 5811b	1360, 1375a
368.	78210-90-9	Pyridine, 3-(2-butenyl)-	568b, 1075, 1371, 1587, 4249, 5811b		
369.		Pyridine, 3-(2-ethylphenyl)-	568b, 4249		
370.	6312-09-0	Pyridine, 3-(2-phenylethyl)-	568b, 1587, 4249		
371.	7300-28-9	Pyridine, 3-(2-propenyl)-	568b, 1364, 4249		
372.	71532-24-6	Pyridine, 3-(3-butenyl)-	568b, 1371, 1587, 4249, 5811b		
373.	24950-44-5	Pyridine, 3,3′-(1,2-ethenediyl)bis-	568b, 1587, 4249, 5811b		
374.	78210-43-2	Pyridine, 3,3′-methylenebis-	568b, 1587, 4249, 5811b		
375.		Pyridine, 3,4′-methylenebis	1587, 4249		
376.	4385-67-5	Pyridine, 3-(3-methylphenyl)-	568b, 1587, 4249, 5811b		
377.		Pyridine, 3-(3-penten-2-yl)-	568b, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
378.	583-58-4	Pyridine, 3,4-dimethyl- {3,4-lutidine}	568b, 512, 1063–1066, 1068–1075, 1140, 1364, 1587a, 2142, 2233, 2234, 2470, 2543, 2545, 2724, 2775, 3255, 3302, 3386, 3410, 3463, 3491, 3499, 3505, 3797, 3976, 4249, 5811b	568b, 3903, 3973, 4249, 5811b	
379.		Pyridine, 3,4-diphenyl-	568b, 4249		
380.		Pyridine, 3-(4-butenyl)-	2545, 4249		
381.	78210-41-0	Pyridine, 3-(4-ethylphenyl)-	568b, 1587, 4249, 5811b		
382.	2057-39-8	Pyridine, 3-(4-methyl-3-pentenyl)-	568b, 1587, 4249, 5811b		
383.	72692-97-8	Pyridine, 3-(4-methylpentyl)-	568b, 1587, 4249, 5811b		
384.	591-22-0	Pyridine, 3,5-dimethyl- {3,5-lutidine}	37, 512, 568b, 1075, 1078, 1084, 1140, 1364, 1587a, 2142, 2228, 2233, 2234, 2545, 2724, 2869, 3255, 3302, 3308, 3386, 3398, 3463, 3491, 3499, 3505, 3797, 4249, 4407, 5811b	568b, 3973, 4249, 5811b	
385.	92-07-9	Pyridine, 3,5-diphenyl-	568b, 4249		
386.	78210-46-5	Pyridine, 3-[(5-methyl-2-furanyl)methyl]-	568b, 1587, 4249, 5811b		
387.	5335-75-1	Pyridine, 4-butyl-	568b, 1587, 4249, 5811b		
388.	100-43-6	Pyridine, 4-ethenyl-	568b, 2233, 2234, 4249, 4570a	568b, 2917a, 4249	
389.	536-75-4	Pyridine, 4-ethyl-	568b, 775, 1075, 1587a, 2142, 2233, 2234, 2545, 3255, 3386, 4249, 4921	568b, 3973, 4249	
390.	70199-60-9	Pyridine, 4-(methoxymethyl)-	568b, 1587, 4249, 5811b		
391.	108-89-4	Pyridine, 4-methyl- {4-picoline}	462, 512, 568b, 775, 1063–1066, 1068–1074, 1140, 1348, 1349, 1360, 1364, 1369, 1375a, 1587a, 1644, 1645, 1647, 1803, 2001, 2207, 2233, 2234, 2270, 2470, 2493, 2543, 2724, 2545, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2869, 2939, 3255, 3261, 3300, 3302, 3308, 3386, 3398, 3410, 3463, 3491, 3499, 3505, 3559, 3797, 4159, 4249, 4570a, 4921, 5811b	568b, 984, 1157, 1852, 2339a, 2917a, 3491, 3903, 3973, 4249, 5811b	1360, 1375a
392.		Pyridine, 4-methyl-2-(2-methylbutyl)-	4570a		
393.	78210-47-6	Pyridine, 4-methyl-2-(3-methylbutyl)-	568b, 1587, 4570a, 5811b		
394.		Pyridine, 4-methyl-2-(2-methylpropyl)-	4570a		
395.	84625-54-7	Pyridine, 4-methyl-2-pentyl-	4570a		
396.	30256-45-2	Pyridine, 4-methyl-2-propyl-	4570a, 5811b		
397.	75835-01-7	Pyridine, 4-methyl-2-(2-phenylethyl)-	568b, 1587, 4249, 5811b		

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
398.	3475-21-6 19352-29-5	Pyridine, 4-methyl-3-phenyl-	568b, 1587, 4249, 5811b	568b, 3549, 4249	
399.	939-23-1	Pyridine, 4-phenyl-	568b, 1587, 4249, 5811b	568b, 3430, 4249, 5811b	
400.	2116-65-6	Pyridine, 4-(phenylmethyl)-		2359, 4249	
401.	78210-91-0	Pyridine, 4-(1-butenyl)-	568b, 1587, 4249, 5811b		
402.	3978-81-2	Pyridine, 4-(1,1-dimethylethyl)- {4-*tert*-butylpyridine}	568b, 2142, 3255, 4249, 5811b	568b, 2359, 4249	
403.	696-30-0	Pyridine, 4-(1-methylethyl)-	568b, 4249		
404.	22241-38-9	Pyridine, 4-(4-methylpentyl)-	1587, 4249, 5811b		
405.	6304-16-1	Pyridine, 4-(2-phenylpropyll)-	568b, 4249		
406.	17618-95-0	Pyridine, 4-(1-propenyl)-	568b, 2775, 4249		
407.	140-76-1	Pyridine, 5-ethenyl-2-methyl-	568b, 1075, 1587, 4249, 5811b		
408.	104-90-5	Pyridine, 5-ethyl-2-methyl-	775, 1364, 1587, 1587a, 4249	2917a, 4249	
409.	55270-47-8	Pyridine, 5-methoxy-2-methyl-	568b, 1587, 4249, 5811b		
410.	6343-58-4	Pyridine, 5-methyl-2-(1-methylethyl)-	1587, 4249		
411.		Pyridine, 5-methyl-2-(2-methylbutyl)-	4570a		
412.		Pyridine, 5-methyl-2-(2-methylpropyl)-	4570a		
413.		Pyridine, 5-methyl-2-pentyl-	4570a		
414.		Pyridine, 5-methyl-2-propyl-	4570a		
415.	36541-27-2	Pyridinecarbonitrile, dimethyl-	2731, 2735, 4249, 5811, 5811a, 5811b	5811, 5811a, 5811b	
416.	36541-26-1	Pyridinecarbonitrile, methyl-	1587, 2727, 2731, 2735, 3491, 4249, 5811, 5811a		
417.	55738-21-1	Pyridinedicarbonitrile	1587, 4249		
418.	17945-79-8	2-Pyridinebutanol	3553, 4249		
419.	100-70-9	2-Pyridinecarbonitrile	568b, 1587, 3190, 3499, 3992, 4249, 4570a, 5811b		
420.	20970-75-6	2-Pyridinecarbonitrile, 3-methyl-	568b, 1587, 4249		
421.	1620-76-4	2-Pyridinecarbonitrile, 4-methyl-	568b, 1587, 4249		
422.	1121-60-4	2-Pyridinecarboxaldehyde	568b, 4249, 5811b		
423.	1452-77-3	2-Pyridinecarboxamide	568b, 3553, 3557, 4249, 5811b		
424.	72693-02-8	2-Pyridinecarboxamide, 4,6-dimethyl-	568b, 1587, 4249, 5811b		
425.	32743-35-4	2-Pyridinecarboxamide, 4-ethyl-	568b, 1587, 4249, 5811b		
426.	13509-17-6	2-Pyridinecarboxamide, 5-ethyl-	568b, 1587, 4249, 5811b		
427.	78210-61-4	2-Pyridinecarboxamide, 6-ethyl-	568b, 1587, 4249, 5811b		
428.	20970-77-8	2-Pyridinecarboxamide, 5-methyl-	568b, 1587, 2767, 3557, 4249, 5811b		
429.	63668-37-1	2-Pyridinecarboxamide, 6-methyl-	568b, 1587, 4249		
430.	1918-02-1	2-Pyridinecarboxylic acid, 4-amino-3,5,6-trichloro- {Picloram®}		3973, 4249	

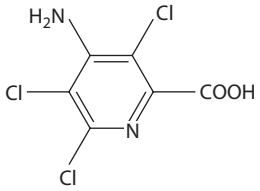
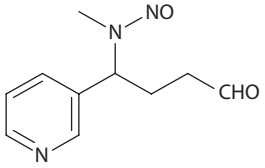
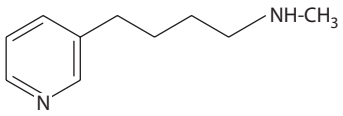
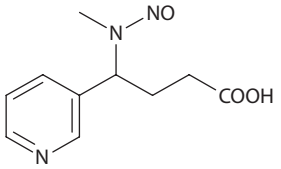
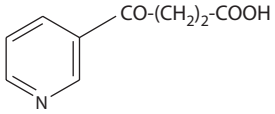
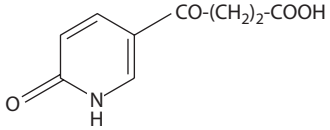
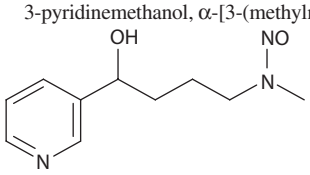


TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
431.	103-74-2	2-Pyridinemethanol	568b, 4249		
432.	35549-47-4	2-Pyridinepropanenitrile	568b, 1587, 4249, 5811b		
433.	42545-63-1	3-Pyridineacetaldehyde	568b, 1371, 4249		
434.	70898-37-2	3-Pyridinebutanal, γ-(methylamino)-		553, 2226, 4249	
435.	64091-90-3	3-Pyridinebutanal, γ-(methylnitrosoamino)- {NNA}	772, 1568, 1584, 4249	554, 772, 1565, 1584, 3973, 3974b, 4249, 5577, 5811b	
436.	64142-45-6	3-Pyridinebutanal, γ-(methylnitrosoamino)-, (*Z*)- 	1012, 1563–1565, 1567a, 1569, 1702, 1751, 3256, 4249	466, 992, 1012, 1563–1565, 1567a, 1569, 1576, 1577, 1567a, 1702, 3491, 4249	
437.	76014-80-7	3-Pyridinebutanal, γ-oxo-		4249	
438.		3-Pyridinebutanamide, *N*-methyl-	1371, 2775, 4249		
439.	6021-23-4	3-Pyridinebutanamine		5338, 5777, 5811	
440.	3000-74-6	3-Pyridinebutanamine, *N*-methyl- {dihydrometanicotine} 	568b, 761, 1078, 2228, 2724, 2730, 2734, 3054, 3302, 3308, 3505, 4249, 5811b	120, 349, 568b, 2746, 3444, 4249, 5811b	
441.	17270-48-3	3-Pyridinebutanoic acid, γ-(methylamino)-, (±)-		4249, 4770	
442.	152720-16-6	3-Pyridinebutanoic acid, γ-(methylnitroamino)-		3444, 4249	
443.	123743-84-0 133201-36-2	3-Pyridinebutanoic acid, γ-(methylnitrosamino)- {iso-NNAC} 	59, 486, 1008, 1009, 1012, 1013, 1584, 1702, 1751, 3256, 3300, 4249, 5811, 5811a, 5811b	465, 486, 992, 993, 995, 1008, 1009, 1012, 1013, 1584, 1702, 1750, 3973, 4236, 4249, 5811, 5811a, 5811b	
444.	4192-31-8	3-Pyridinebutanoic acid, γ-oxo- 		1101, 2226, 3444, 4236, 4249, 5508	
445.	15873-27-5	3-Pyridinebutanoic acid, 1,6-dihydro-γ,6-dioxo- 	4249	1110, 4249, 4709	
446.	59578-66-4 76014-81-8	3-Pyridinebutanol, δ-(methylnitrosoamino)- {NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-; 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-} 	24, 25, 59, 486, 991, 1565, 1571a, 1573a, 1584, 1702, 1751, 3184, 3256, 3300, 5565	469, 486, 507a, 728, 995, 1562a, 1565, 1571a, 1573a, 1584, 1702, 1771, 3943b, 3973, 4236, 4249, 5577, 5811b	

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

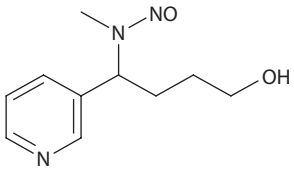
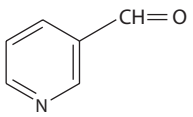
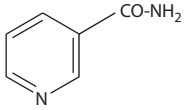
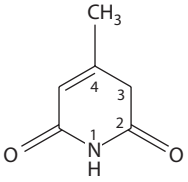
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
447.	133201-37-3	3-Pyridinebutanol, δ-(methylnitrosoamino)- {iso-NNAL} {1-butanol, 4-(*N*-methylnitrosamino)-4-(3-pyridinyl)-} 	59, 486, 508, 1584, 1702, 1751, 3256, 3943a, 3944–3946, 4249	486, 1562a, 1584, 1679, 1702, 3943a, 3944–3946, 3947, 3948, 3973, 4236, 4249, 5577	
448.	70898-36-1	3-Pyridinebutanol, δ-amino-		4249	
449.	100-54-9	3-Pyridinecarbonitrile {nicotinonitrile}	107, 299, 299, 480, 568b, 1078, 1099, 1140, 1371, 1426, 1427, 1568, 1587a, 2228, 2387, 2470, 2493, 2543, 2545, 2570, 2724, 2727, 2731, 2732, 2735, 2765, 2775, 3255, 3302, 3308, 3386, 3398, 3410, 3463, 3468, 3470, 3491, 3499, 3505, 4249, 4570a, 5034, 5079, 5811b, 25A84	568b, 937, 2339a, 3491, 4249, 5811b, 17B61	2387
450.	38076-78-7	3-Pyridinecarbonitrile, 2-amino-5-methyl-	1587, 4249, 5811b		
451.	71607-63-1	3-Pyridinecarbonitrile, dimethyl-	2727, 3491, 4249		
452.	61391-07-9	3-Pyridinecarbonitrile, 5-ethyl-	1587, 4249		
453.	3222-52-4	3-Pyridinecarbonitrile, 6-ethyl- = 5-pyridinecarbonitrile, 2-ethyl-	568b, 1587, 4249, 5811b		
454.	5444-01-9	3-Pyridinecarbonitrile, 4-methyl-	568b, 1587, 4249, 5811b		
455.	42885-14-3	3-Pyridinecarbonitrile, 5-methyl-	568b, 1371, 1587, 3729, 4249, 5811b		
456.	500-22-1	3-Pyridinecarboxaldehyde {nicotinaldehyde; 3-formylpyridine} 	568b, 1078, 1364, 1371, 2228, 2545, 2724, 2775, 2939, 3302, 3308, 3491, 3499, 3505, 3967, 4249, 5034, 5811b	568b, 937, 2359, 2389, 2544, 2917a, 3491, 4249, 5811b, 17B07, 17B08, 17B33, 17B34, 17B37, 17B48	
457.	98-92-0	3-Pyridinecarboxamide {nicotinamide} 	442, 515, 562, 563, 568b, 1224, 1360, 1371, 1375a, 1586, 1668, 1890, 1891, 1966, 2079, 2224, 2228, 2724, 2761, 2762, 2765, 2766, 2939, 3059, 3302, 3308, 3309, 3386, 3410, 3444, 3491, 3505, 3553, 3559, 3967, 4080, 4249, 5811b	120, 563, 568b, 1224–1226, 2724, 2939, 3444, 3491, 3797, 3973, 3974a, 3983a, 4249, 5079	1360, 1375a
458.	72692-96-7	3-Pyridinecarboxamide, 2,4-dimethyl-	568b, 1587, 4249, 5811b		
459.	10131-48-3	3-Pyridinecarboxamide, 2,6-dimethyl-	568b, 1587, 4249, 5811b		
460.	58539-65-4	3-Pyridinecarboxamide, 2-methyl-	568b, 1587, 2761, 2762, 2765, 3410, 4249, 5811b	568b, 3549, 4249	
461.	78210-59-0	3-Pyridinecarboxamide, 4-ethyl-	568b, 1587, 4249, 5811b		
462.	78210-60-3	3-Pyridinecarboxamide, 6-ethyl-	568b, 1587, 4249, 5811b		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
463.	6960-22-1	3-Pyridinecarboxamide, 6-methyl-	568b, 1586, 2761, 2762, 2767, 4249		
464.	4314-66-3	3-Pyridinecarboxamide, *N*-ethyl-	3559, 4249		
465.	114-33-0	3-Pyridinecarboxamide, *N*-methyl-	568b, 1371, 1568, 1586, 2776, 2775, 3054, 3056, 3255, 3302, 3386, 3410, 3444, 3553, 3559, 3742, 4249, 5811b	120, 404, 568b, 927, 1226, 1568, 2939, 3056, 3444, 3491, 3550, 3797, 3973, 3974a, 4093, 4249, 5811b	
466.	59-67-6	3-Pyridinecarboxylic acid {nicotinic acid}	43, 562, 563, 1224, 1668, 1568, 1890, 1891, 2079, 2224, 2349, 2724, 2767, 2939, 3059, 3302, 3309, 3444, 3491, 3505, 4080, 4249, 5079, 5811b, 25A84	120, 555a, 555b, 1222, 1224, 1225, 1226, 1568, 2270, 2283, 2724, 2794, 2914, 2939, 3444, 3491, 3797, 3974, 3973, 3974a, 3983a, 4249, 5079, 5390a, 5145, 5445, 5804, 5811b, 17B07, 17B08, 17B33, 17B34, 17B37, 17B48	
467.	5006-66-6	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-		4249	
468.	614-18-6	3-Pyridinecarboxylic acid, ethyl ester	5811	5811	
469.	93-60-7	3-Pyridinecarboxylic acid, methyl ester {methyl nicotinate}	278, 1568, 3266, 4249, 5811b	1053, 1254, 1256, 1568, 2338, 2339a, 2611, 3266, 3491, 4249	
470.	55557-02-3	3-Pyridinecarboxylic acid, 1,2,5,6-tetrahydro-1-nitroso-, methyl ester		5811, 5811b	
471.	89-00-9	2,3-Pyridinedicarboxylic acid {quinolinic acid}		555b, 4249, 5531	
472.	58-56-0	3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride		429b, 4249, 4789	
473.	13121-99-8	4-Pyridineacetonitrile	568b, 1568, 1587, 4249, 5811b		
474.	5264-15-3	4-Pyridinebutanol	568b, 4249, 5811b		
475.	100-48-1	4-Pyridinecarbonitrile	568b, 3255, 3499, 3729, 4249, 5811b		
476.	1453-82-3	4-Pyridinecarboxamide {isonicotinamide}		3973, 4249	
477.	70898-25-8	2,6(1*H*,3*H*)-Pyridinedione, 3,5-dimethyl-	2767, 3553, 4249	2389, 4249	
478.	72692-95-6	2,6(1*H*,3*H*)-Pyridinedione, 4-methyl- 	2767, 3553, 3557, 4249		
479.	72692-94-5	2,6(1*H*,3*H*)-Pyridinedione, 5-methyl-	2767, 3553, 4249		
480.		3-Pyridinemethanamine, ethyl-	1371, 4249		
481.	3000-75-7	3-Pyridinemethanamine, *N*-ethyl-	4249		
482.	100-55-0	3-Pyridinemethanol		2917a, 4249	
483.	76014-81-8	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-		4249	
484.	85352-99-4	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-, 1-oxide		4249	

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

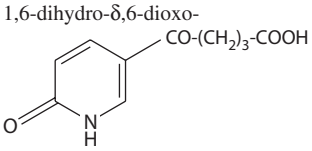
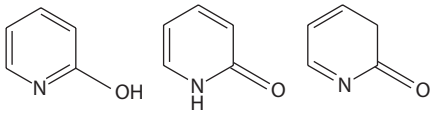
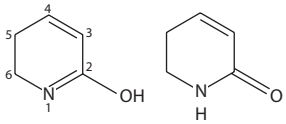
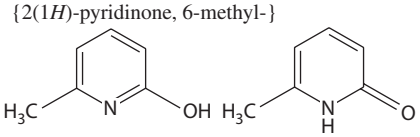
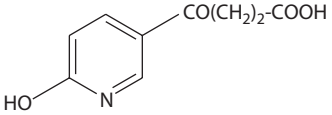
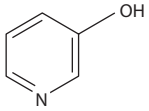
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
485.	71608-01-0	3-Pyridinepentanoic acid, 1,6-dihydro-δ,6-dioxo- 		1101, 4249, 4945	
486.	60655-87-0	Pyridinium, 1-α-*L*-arabinopyranosyl-3-carboxy-		4249, 4738	
487.	35323-45-6	Pyridinium, 3-carboxy-1-β-*D*-glucopyranosyl-, hydroxide {trigonelline}		1858a, 4249	
488.	535-83-1	Pyridinium, 3-carboxy-1-methyl-, hydroxide, inner salt		3973, 4249	
489.	27341-45-3	Pyridinol	167, 1586, 1963, 4249, 5034		
490.		Pyridinol, methyl-	1371, 1375, 1375b, 2543, 2773, 2775, 2777, 3410, 3557, 4249	3550, 4249	
491.	51025-25-3	Pyridinol, dimethyl-	1586, 2767, 4249		
492.	142-08-5 72762-00-6	2-Pyridinol {2(1*H*)-pyridinone} 	568b, 1124a, 1375, 1375b, 1586, 2724, 2767, 2773, 3553, 3557, 4249, 5811b		
493.	61892-76-0	2-Pyridinol, 5-acetyl-3,4-dihydro- {2(1*H*)-pyridinone, 5-acetyl-3,4-dihydro-}	568b, 3553, 4249		
494.	57147-25-8	2-Pyridinol, 3,4-dihydro- {2(1*H*)-pyridinone, 3,4-dihydro-}	2543, 2775, 3553, 3559, 4249		
495.	61892-77-1	2-Pyridinol, 3,6-dihydro- {2(1*H*)-pyridinone, 3,6-dihydro-}	568b, 2570, 3553, 4249		
496.	6052-73-9	2-Pyridinol, 5,6-dihydro- {2(1*H*)-pyridinone, 5,6-dihydro-; 2-piperidone, 3,4-dehydro-} 	568b, 1371, 1371, 1375, 1375b, 1586, 2387, 2545, 2570, 2761, 2762, 2765–2767, 2775, 3255, 3397, 3398, 3410, 3553, 3557, 3559, 4249, 5811b	568b, 2386, 2389, 2544, 3491, 3550, 4249	2387
497.		2-Pyridinol, 5,6-dihydro-3,6,6-trimethyl- {2(1*H*)-pyridinone, 5,6-dihydro-3,6,6-trimethyl-}		939, 4249	
498.	72692-83-2	2-Pyridinol, dimethyl- {2(1*H*)-pyridinone, dimethyl-}	3553, 4249		
499.	6456-92-4	2-Pyridinol, 1,3-dimethyl- {2(1*H*)-pyridinone, 1,3-dimethyl-}	3559, 4249		
500.	36330-90-2 95907-02-1	2-Pyridinol, 3,4-dimethyl- {2(1*H*)-pyridinone, 3,4-dimethyl-}	568b, 3553, 4249		
501.	3718-67-0	2-Pyridinol, 3,5-dimethyl- {2(1*H*)-pyridinone, 3,5-dimethyl-}	568b, 1371, 3553, 4249, 5811b		
502.	53428-02-7	2-Pyridinol, 3,6-dimethyl- {2(1*H*)-pyridinone, 3,6-dimethyl-}	568b, 3553, 4249, 5811b		
503.	16115-08-5	2-Pyridinol, 4,6-dimethyl- {2(1*H*)-pyridinone, 4,6-dimethyl-}	568b, 3553, 4249, 5811b		
504.	27992-31-0	2-Pyridinol, 5,6-dimethyl-	5811, 5811a, 5811b		
505.		2-Pyridinol, 3-ethyl- {2(1*H*)-pyridinone, 3-ethyl-}	568b, 4249		
506.	62003-48-9	2-Pyridinol, 5-ethyl- {2(1*H*)-pyridinone, 5-ethyl-}	568b, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
507.	61892-99-7	2-Pyridinol, 6-ethyl- {2(1*H*)-pyridinone, 6-ethyl-}	568b, 2767, 4249		
508.	1003-56-1 91914-04-4	2-Pyridinol, 3-methyl- {2(1*H*)-pyridinone, 3-methyl-}	568b, 3553, 3559, 4249, 5811b		
509.	91914-05-5	2-Pyridinol, 4-methyl- {2(1*H*)-pyridinone, 4-methyl-}	568b, 4249		
510.	1003-68-5 91914-06-6	2-Pyridinol, 5-methyl- {2(1*H*)-pyridinone, 5-methyl-}	568b, 2543, 3553, 4249, 5811b		
511.	3279-76-3	2-Pyridinol, 6-methyl- {2(1*H*)-pyridinone, 6-methyl-} 	568b, 1360, 1371, 1375a, 1586, 2761, 2762, 2765–2767, 2773, 2775, 3410, 3553, 4249, 5811b		1360, 1375a
512.	19006-81-6	2-Pyridinol, 4-phenyl- {2(1*H*)-pyridinone, 4-phenyl-}	642, 4249	642, 4249	
513.		2-Pyridinol-5-butanoic acid, γ-oxo- {2(1*H*)-pyridinone-5-butanoic acid, γ-oxo-} 		1101, 4249	
514.		2-Pyridinol-5-pentanoic acid, δ-oxo- {2(1*H*)-pyridinone-5-pentanoic acid, δ-oxo-}		1101, 4249	
515.	109-00-2 52536-09-1 58064-43-0	3-Pyridinol 	568b, 1099, 1360, 1371, 1375, 1375a, 1375b, 1445, 1582, 1586, 1882, 2091a, 2133, 2228, 2493, 2543, 2570, 2601a, 2724, 2761, 2762, 2765–2767, 2773–2775, 2777, 2857, 2876, 2939, 3255, 3302, 3308, 3397, 3398, 3488, 3491, 3501, 3553, 3557, 3797, 4249, 5811b	5811b	1360, 1375a
516.	17747-43-2	3-Pyridinol, acetate (ester)	568b, 3553, 4249, 4407, 5811b		
517.		3-Pyridinol, alkyl-	568b, 1582, 1583, 3491, 3559, 4249		
518.	27296-76-0	3-Pyridinol, 2,4-dimethyl-	568b, 3553, 4249, 5811b		
519.	1122-43-6	3-Pyridinol, 2,6-dimethyl-	568b, 1371, 2767, 3410, 3553, 4249, 5811b		
520.	27296-77-1	3-Pyridinol, 4,6-dimethyl-	568b, 3553, 4249, 5811b		
521.	61893-00-3	3-Pyridinol, 5,6-dimethyl-	3553, 4249		
522.	61893-02-5	3-Pyridinol, 2-ethyl-	568b, 1364, 1371, 1586, 2543, 2767, 2773, 2775, 3410, 3553, 4249	568b, 3561, 4249	
523.	62003-48-9	3-Pyridinol, 5-ethyl-	568b, 3553, 4249		
524.	51834-96-9	3-Pyridinol, 6-ethyl-	568b, 3255, 4249		
525.	42451-07-0	3-Pyridinol, 6-ethyl-2-methyl-	568b, 3410, 3553, 4249, 5811b		
526.	61893-01-4	3-Pyridinol, 6-ethyl-4-methyl-	568b, 3553, 4249		

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

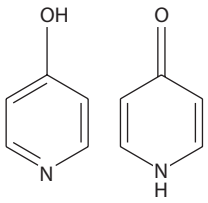
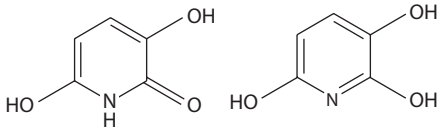
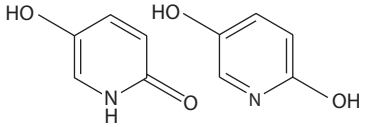
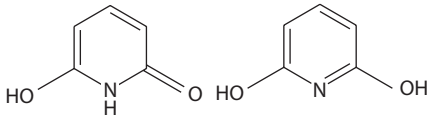
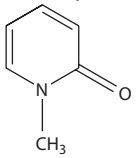
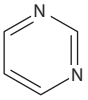
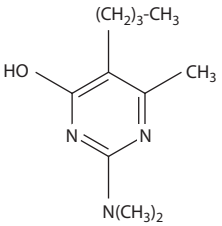
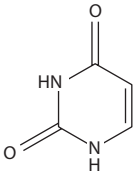
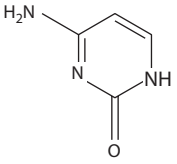
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
527.	40222-77-3	3-Pyridinol, 6-hydroxymethyl- {2-pyridinemethanol, 5-hydroxy-}	568b, 3553, 4249, 5811b		
528.	91491-14-4	3-Pyridinol, methyl-	1375, 1375b, 2570, 2775, 3410, 4249, 5811b		
529.	1121-25-1	3-Pyridinol, 2-methyl-	568b, 1586, 2570, 2767, 3410, 3553, 4249, 5811b	568b, 3561, 4249	
530.	1121-19-3	3-Pyridinol, 4-methyl-	568b, 1586, 3255, 3553, 3557, 4249, 5811b		
531.	42732-49-0	3-Pyridinol, 5-methyl-	568b, 1586, 2767, 3553, 4249, 5811b		
532.	1121-78-4	3-Pyridinol, 6-methyl-	568b, 1371, 1375, 1375b, 1582, 1583, 2570, 2767, 2775, 3410, 3491, 3553, 4249, 4407, 5811b		
533.	14159-68-3	3-Pyridinol, 2-propyl-	568b, 3553, 4249		
534.	61893-03-6	3-Pyridinol, 4-propyl-	3553, 4249		
535.	61893-04-7	3-Pyridinol, 5-propyl-	3553, 4249		
536.	108-96-3 626-64-2	4-Pyridinol {4(1*H*)-pyridinone} 	568b, 2387, 4249, 4407		2387
537.	39954-19-3	2(1*H*)-Pyridinone, 3,6-dihydroxy- {2,3,6-pyridinetriol} 		1101, 4249	
538.	5154-01-8	2(1*H*)-Pyridinone, 5-hydroxy- {2,5-pyridinediol} 		1101, 4249, 4918	
539.	626-06-2	2(1*H*)-Pyridinone, 6-hydroxy- {2,6-pyridinediol} 		1101, 4249, 4918	
540.	694-85-9	2(1*H*)-Pyridinone, 1-methyl- 	568b, 2767, 3553, 4249, 4570a, 5811b	404, 568b, 984, 2389, 2544, 4249	
541.	1445-73-4	4(1*H*)-Pyridinone, 1-methyl-	568b, 4249		

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
542.	289-95-2	Pyrimidine {1,3-diazine} 		568b, 2939, 4249, 5079, 5413, 5738, 5811b, 17B21, 17B45	
543.	5221-53-4	Pyrimidine, 5-butyl-2-dimethylamino-4-hydroxy-6-methyl- {Dimetherimol®} 		3633, 4249	
544.	72692-81-0	Pyrimidine, dimethyl-	638, 4249		
545.	14331-54-5	Pyrimidine, 2,4-dimethyl-	568b, 4249, 4570a		
546.	22868-76-4	Pyrimidine, 2,5-dimethyl-	568b, 4249		
547.		Pyrimidine, 2,5-dimethyl-6-hydroxy-	3553, 4249		
548.	694-81-5	Pyrimidine, 4,5-dimethyl-	568b, 4249		
549.	1558-17-4	Pyrimidine, 4,6-dimethyl-	568b, 4249, 4570a		
550.	88070-43-3	Pyrimidine, 5-hydroxy-4-phenyl-	2601a, 4249		
551.	3438-46-8	Pyrimidine, 4-methyl-	568b, 4249		
552.		Pyrimidine, methylethyl- {two isomers}	4570a		
553.	66-22-8	2,4(1*H*,3*H*)-Pyrimidinedione {uracil} 		568b, 3973, 4249	
554.	4160-77-4	2,4(1*H*,3*H*)-Pyrimidinedione, 3,5-dimethyl-	568b, 3553, 4249, 5811b		
555.	61893-13-8	2,4(1*H*,3*H*)-Pyrimidinedione, 3-ethyldihydro-5-methyl-	568b, 3553, 4249		
556.	608-34-4	2,4(1*H*,3*H*)-Pyrimidinedione, 3-methyl-	568b, 4249		
557.	65-71-4	2,4(1*H*,3*H*)-Pyrimidinedione, 5-methyl- {thymine}	1580, 4249	1580, 3491, 3797, 3974a, 4249	
558.	50-06-6	2,4,6(1*H*,3*H*, 5*H*)-Pyrimidinetrione, 5-ethyl-5-phenyl- {phenobarbital}		5003, 5021	
559.	71-30-7	2(1*H*)-Pyrimidinone, 4-amino- {cytosine} 	2539, 4249	120, 2270, 4249	
560.	34939-17-8	2(1*H*)-Pyrimidinone, 4,5-dimethyl- = 2-pyrimidinol, 4,5-dimethyl-	3553, 4249		
561.		4(1*H*)-Pyrimidinone, 2,3-dimethyl-6-phenyl-3,4,5,6-tetrahydro-	568b, 4249		

(*continued*)

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

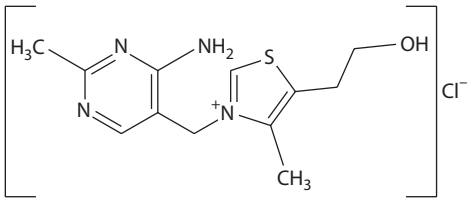
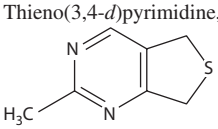
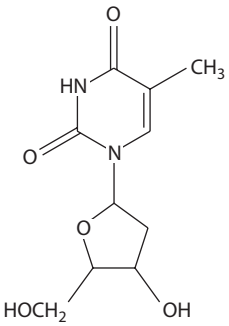
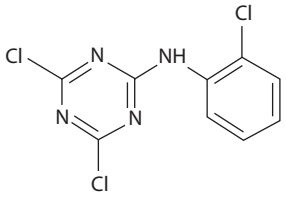
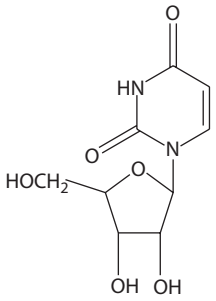
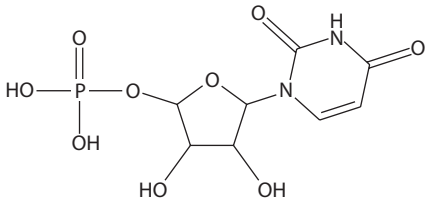
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
562.	3059-71-0 67383-34-0	4(1*H*)-Pyrimidinone, 2,5-dimethyl- = 4-pyrimidinol, 2,5-dimethyl-	3553, 4249, 5811, 5811a, 5811b		
563.	6622-92-0	4(1*H*)-Pyrimidinone, 2,6-dimethyl- = 6-pyrimidinol, 2,5-dimethyl-	3553, 4249		
564.	34916-78-4	4(1*H*)-Pyrimidinone, 5,6-dimethyl- = 6-pyrimidinol, 4,5-dimethyl-	3553, 4249		
565.	16858-16-5	4(1*H*)-Pyrimidinone, 6-methyl-2-propyl- = 6-pyrimidinol, 4-methyl-2-propyl-	3559, 4249		
566.	6294-65-1	Quinoline, 2-(3-pyridyl)-	568b, 4249		
567.	34413-35-9	Quinoxaline, 5,6,7,8-tetrahydro-	4570a	172a, 174b, 1053, 3266	
568.	38917-65-6	Quinoxaline, 2-methyl-5,6,7,8-tetrahydro-	1587, 1590, 2761, 2762, 2765, 2766, 2769, 2773, 2775, 2777, 4249, 5811b		
569.	154-87-0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-4-methyl-5-(4,6,6-trihydroxy-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, P,P′-dioxide		4051a, 4249, 4798	
570.	59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-5-(2-hydroxyethyl)-4-methyl-chloride {thiamine} 		120, 1941, 2270, 4249, 5079, 17B10	
571.	67-03-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-5-(2-hydroxyethyl)-4-methyl-chloride, monohydrochloride {thiamine hydrochloride}		1053, 3266, 4249	
572.	36267-71-7	Thieno(3,4-*d*)pyrimidine, 5,7-dihydro-2-methyl- 		1053, 3266, 17B22	
573.	50-89-5	Thymidine 		3973, 4249	

TABLE 17.7 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
574.	101-05-3	1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-(2-chlorophenyl)- {Anilazine®} 	1884	3633, 3661a, 3797, 4249, 4271a	
575.		1,3,5-Triazine, 1.4-dihydro-1,2-dimethyl-	568b, 4249		
576.	21087-64-9	1,2,4-Triazin-5(4*H*)-one, 4-amino-6-*tert*-butyl-3-(methylthio)- {Metribuzin®}		2913a, 4249	
577.	58-96-8	Uridine 		3973, 4249	
578.	133-89-1	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-glucopyranosyl ester		4249, 4489, 4580	
579.	3616-06-6	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester		429b, 4249	
580.	19253-25-9	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester		4249, 4459	
581.	58-97-9	5′-Uridylic acid 		429b, 4249, 4474	

Some pyrimidine-derived flavors (although not found in tobacco or tobacco smoke) have meaty notes. There are also some pyrimidine flavorants that do possess good flavor potential for tobacco products, e.g., 2-methyl-5,7-dihydrothieno[3,4-*d*]pyrimidine. This compound contains a bicyclic ring structure and has been identified in tobacco. 2-Methyl-5,7-dihydrothieno[3,4-*d*]pyrimidine is said to have a fresh roasted, sweet nut flavor with a popcorn character (17B22). It is a compound listed by Doull et al. as an ingredient in flavor formulations used by one or more members of the U.S. tobacco industry (1053).

17.2.5 Compounds in Tobacco and Tobacco Smoke Containing a Five- and Six-Membered *N*-Containing Ring

The origin of all the work that has been done on the isolation and identification of the tobacco and tobacco smoke began with this relatively small group of compounds. The initial tobacco and tobacco smoke compound that was of so much interest was nicotine. Literally thousands of scientific articles, reviews, and books have been published on various aspects of nicotine, e.g., pharmacological and metabolic properties, chemical and

structural properties, occurrence, biogenesis, and pyrolysis. The scope of all the work on nicotine alkaloids is so broad that a comprehensive review is beyond the scope of this chapter. The several hundred references listed in Table 17.7 testify to the enormous amount of research that has been conducted on the nicotine alkaloids. Instead, a brief history of the initial work on the isolation and identification of nicotine follows.

17.2.5.1 Nicotine and Tobacco Alkaloids with a Six-Membered *N*-Containing Ring and a Second Five-Membered *N*-Containing Ring

Nicotine is the unique component of tobacco. The history associated with the discovery of nicotine and use of the "oil" derived from tobacco dates to about 1571 (17B16). This "oil" prepared by the French chemist Gohory undoubtedly contained some level of nicotine and was used as a remedy for diseases of the skin. In 1660, another French chemist, Lefevre, described means to steam distill tobacco to obtain oil that had medicinal uses (3477). In 1807, Cerioli discovered what he called the *olio essenziale* of tobacco (17B15). In 1809, Vauquelin apparently made the same discovery. Both researchers described the oil as a volatile and colorless substance. Vauquelin recognized the basic nature of the material but failed to recognize its alkaloidal properties. He attributed the basicity of the material to the presence of ammonia (410).

In 1822, Hermbstädt confirmed Vauquelin's results of the presence of the oil described in 16 different species of what is now known as *Nicotiana* (17B15). It was not until 1828 that Posselt and Reimann (2981) succeeded in isolating a pure sample of the oil and recognized it as an alkaloid. They characterized it as a water-clear liquid, boiling at 246°C under atmospheric pressure, and miscible with water, alcohol, and ether. They named the pure compound nicotine after Jean Nicot who introduced tobacco into the French court in about 1560 (17B42). In 1826, Unverdorben isolated a water-soluble base from a dry distillate of tobacco (282). The base contained nicotine. Melsens (2528), in 1843, succeeded in isolating nicotine from the smoke of pipe tobacco and assigned the empirical formula, $C_{12}H_{14}N_2$ (2724). In 1893, Pinner (17B44) reported on the final clarification of the constitution of nicotine, determined via degradation studies. Pinner's structural formula for nicotine was confirmed by the classical synthesis of nicotine by Pictet and Rotschy (17B43) in 1895. For many years, nicotine was believed to be the only alkaloid in tobacco (17B18). It was not until 1928 that Ehrenstein reported the identification of nornicotine in tobacco [see Markwood (17B38)]. Anabasine was isolated in tobacco by Smith (17B53) in 1935. Späth and Kesztler (17B55) isolated anatabine in tobacco in 1934 (Markwood 1942). Gautier and LeBon in 1892 were the first chemists to clearly recognize that additional alkaloids accompanied nicotine in tobacco smoke. These additional alkaloids were the secondary alkaloids and decomposition products of alkaloids. Unfortunately, Gautier and LeBon did not report further on their observations (2223, 2224). Wenusch and Schöller (4210, 4211) in the early 1930s worked diligently to separate the secondary alkaloids in tobacco smoke. Though they were not wholly successful, they did discover and determine the formula for myosmine in cigar smoke in 1936 with the collaboration of Späth (2224). By 1936, Wenusch and Schöller (4213) had distinguished a large number of tobacco smoke bases in cigar and cigarette smoke by their behavior during steam distillation and extraction. Several of the alkaloid-related components (α-, β-, and γ-socratine, obelin, lohitam, anodmin, lathraein, poikiline, and gudham) first reported by Wenusch and Schöller (4210, 4211) were subsequently demonstrated to be mixtures or mislabeled components of previously known alkaloids. Until the study by Kuffner, Schick, and Bühn in 1959, there was much confusion concerning the correct identity of the secondary alkaloids of tobacco smoke. Kuffner et al. (2224) demonstrated that obelin was a salt of ammonia, α- and β-socratine were mixtures of nicotyrine and 2,3′-bipyridine, and γ-socratine was l-nornicotine. Poikiline was characterized as 4-amino-1-(3-pyridyl)-butanone. Many of these characterization corrections are described in Johnstone and Plimmer (1971) and Borgerding et al. (410).

To date, 111 components with both five- and six-membered *N*-containing rings have been identified in tobacco and tobacco smoke. In all cases, the six-membered ring is pyridine; the attached five-membered ring may be a pyrrolidine, pyrroline, pyrrole, or an imidazole ring. The vast majority of these tobacco alkaloids contain a pyrrolidine ring that is substituted at the 3-position of the pyridine ring. Table 17.8 shows the distribution of the tobacco alkaloids that occur in tobacco, tobacco smoke, and in both.

Over 60 nicotine-related alkaloids have been identified in tobacco. Many of them have been identified in tobacco smoke, and 22 of the nicotine alkaloids are found in both tobacco and tobacco smoke. The vast majority of the nicotine alkaloids contain a pyrrolidine ring connected to a pyridine ring. The most common functionalities associated with the pyrrolidine-containing nicotine alkaloids are alkyl, nitroso, carboxyl, amino, and acyl groups.

TABLE 17.8
Distribution of Components with a Six-Membered *N*-Containing Ring and a Second Five-Membered *N*-Containing Ring between Tobacco and Tobacco Smoke

	Number of Identified Compounds in Tobacco and Tobacco Smoke with a Six- and Five-Membered Ring			
Component	**Total**	**Smoke**	**Tobacco**	**Smoke and Tobacco**
Pyridine ring with a second *N*-containing ring (type)				
Pyrrolidine (nicotinoids)	79	41	60	22
Pyrroline	2	1	2	1
Pyrrole	28	27	8	7
Imidazole	2	1	2	1
Totals	111	70	72	31

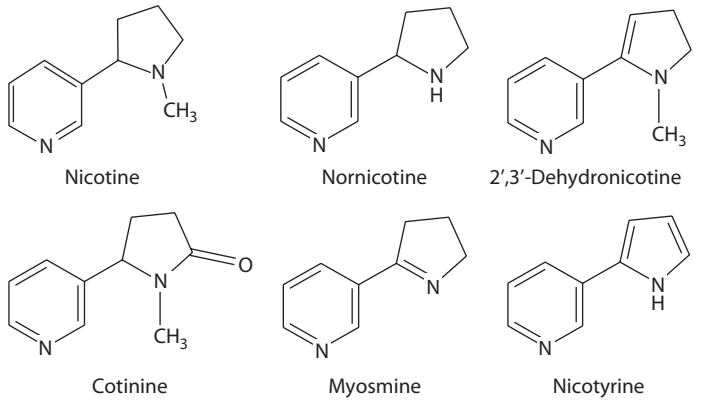


FIGURE 17.5 Common tobacco alkaloids found in tobacco and tobacco smoke.

The structures of some of the most common tobacco alkaloids found in smoke are shown in Figure 17.5. The transfer rate for nicotine is generally about 10%–12%, but a number of factors including the cutting width of the tobacco, the shape of the cigarette, the moisture content of the tobacco, and various tobacco additives can significantly affect nicotine delivery to MSS [Kuhn and Klus (2231), Hecht et al. (1580)]. Many of the alkaloids of tobacco smoke consist of components originally in the tobacco, which transfer unchanged, and various pyrolysis products of the nicotine alkaloids.

Nicotine is a major precursor of a large number of volatile bases in tobacco smoke. On heating nicotine at temperatures greater than 400°C, various patterns of fragmentation occur depending on the gaseous atmosphere and other experimental conditions. Myosmine (4275a) and 3-cyanopyridine [Woodward et al. (17B61)] are two of many pyrolysis products of nicotine at 500°C–730°C. The yields and type of pyrolysis products depend on the substrate used to hold the alkaloid, the particular alkaloid tested, e.g., nicotine or nornicotine, the temperature ramping regime, the final temperature attained, the holding time at maximum temperature, and reactor type employed for the pyrolysis experiment. The major identified pyrolytic products of nicotine at temperatures 400°C and 900°C (in a nitrogen or helium atmosphere) include all of the compounds shown in Figure 17.5. In addition to these compounds, ammonia, methylamine, and a number of smaller fragments are formed from heterolytic cleavage of nicotine. Nicotine is not fragmented significantly at temperatures below 600°C in reactors without packing. At reactor temperatures of 600°C (with samples in an inert atmosphere), about two-thirds of the nicotine is split mainly into myosmine (1′,2′-dehydronornicotine) and 3-vinylpyridine. At 700°C, nicotine is completely decomposed, with the major products being 3-vinylpyridine, 3-methylpyridine, and pyridine. At 800°C and 900°C, extensive cleavage and recombination of fragments occur to yield such products as quinoline, naphthalene, and benzonitrile. From examination of the pyrolysis products produced, dehydrogenation, demethylation, and scission of the pyrrolidine ring are initial steps in the pyrolysis of nicotine. In a C_1–C_2 fragmentation of this ring, dehydrogenation of the resulting *N*-methylaminoalkyl chain would give metanicotine which, on further elimination, produces the observed 3-(1,3-butadienyl)pyridine and subsequently 3-vinylpyridine by appropriate cleavage. Fragmentation of the pyrrolidine ring in the 2,3- or 1,5-positions might ultimately give 3-cyanopyridine after dealkylation of the side chain (3797).

The mechanism of thermal degradation of nornicotine is generally similar to nicotine, although differences in thermostability exist (175, 17B25). Nornicotine is less stable than nicotine and the pyrrolidine ring fragments at temperatures below 400°C. At 400°C (in an inert atmosphere), myosmine and 3-methylpyridine are major pyrolytic products, but at 500°C, only a small amount of myosmine is formed. Since myosmine is relatively stable (44% unchanged) on pyrolysis at 500°C, this compound may not be an intermediate of nornicotine pyrolysis at higher temperatures (175). An alternative explanation is that myosmine formed from nornicotine may react with other pyrolytic products which are not produced when myosmine is pyrolyzed alone. Although the available evidence is sparse, it appears that the pyrolytic mechanism of myosmine is different from that of nicotine and nornicotine (175). At 500°C (in an inert atmosphere), myosmine gives lower yields of 3-methylpyridine and 3-ethylpyridine and higher yields of 3-cyanopyridine than nornicotine. This pattern may indicate that a C_3–C_4 split is favored in the five-membered ring; scission of this bond might be preferred over a C_2–C_3 fragmentation adjacent to the relatively stable C═N bond (3797).

Studies with cigarettes treated with ^{14}C-nicotine have been valuable in determining the delivery of nicotine and its pyrolysis products to MSS and sidestream smoke (SSS). These experiments were reviewed in 1975 by Jenkins et al. (1933a). In a typical study with nicotine-2′-^{14}C, the total ^{14}C-activity in mainstream total particulate matter (TPM) was 15.4% of the original activity in the tobacco burned, while the contribution of the alkaloids to mainstream TPM was 14.9% (1836). Thus, 96.8% of the ^{14}C-activity of the mainstream TPM was due to transfer of alkaloids, and 3.2% was due to products formed from nicotine during smoking; mainstream gas phase (4.1%) contained only pyrolysis products. In the sidestream TPM, 41.1% of the original ^{14}C was detected, i.e., 10% of this material was decomposition products. Sidestream gas phase (16.3%) exclusively comprised pyrolysis products. Most of the remaining ^{14}C-activity (20.2%) was found in

the butt. Thus, approximately 30% of nicotine in a cigarette is converted to products which appear in the SSS and MSS. Pyrolysis studies on nicotine, discussed in the previous section, indicate that pyridines would comprise a significant portion of the particulate-phase products. However, nicotine can undergo other transformations during smoking, including reactions with nitrogen oxides (1580). These will be discussed in the chapter on nitrosamines.

Several studies have been conducted on the fate of nicotine during smoking. Jenkins and Comes (17B20) and Perfetti (2920–2922, 2924) have examined the fate of exogenous *vs*. endogenous transfer of nicotine during smoking. These authors concluded that the transfer into smoke of exogenous nicotine (regardless of its form [free base or salt, *d*- or *l*-conformation]) was similar to that of endogenous material, in contrast to observations with tobacco sterols. Thus, use of ^{14}C-nicotine in tracer studies on cigarette smoke is justified. A comparison of the fate of ^{14}C-nicotine in a pyrolysis study *vs*. its fate during the smoking of a cigarette resolved a long-standing disagreement between those investigators who maintained that the fate of compound on pyrolysis at a temperature similar to that in a burning cigarette was the same as the fate of that compound in a smoked cigarette and those who maintained that the fates would definitely be different. Schmeltz et al. (3512) with ^{14}C-nicotine in a pyrolysis *vs*. a cigarette smoking study reported that the fates were quite different. On the basis of their findings, they stated that these results suggest to us that pyrolysis experiments may be of limited value for establishing the fate of nicotine and possibly other tobacco components in a burning cigarette.

The transfer rate of nornicotine during smoking is significantly lower than that of nicotine, with typical values ranging from 5% to 8% [Glock and Wright (1316), Haag and Larson (17B14)]. When high nornicotine tobaccos were smoked, significant increases in the levels of myosmine were observed compared to conventional burley cigarettes. Similar results were obtained when cigarettes were enriched with nornicotine (1316). Thus, nornicotine is not only an efficient precursor for pyridines but also for myosmine as previously mentioned. This is thought to contribute to the unfavorable taste of smoke from nornicotine-rich (so-called cherry-red) tobacco. The ease of formation of myosmine from nornicotine is likely to be an important factor in its relatively low transfer rate.

The nicotine alkaloids contribute substantially to the unique flavor of tobacco smoke, mainly due to their rather large concentration in tobacco and their rather substantial transfer to tobacco smoke. The nicotine alkaloids as a class are not considered positive flavorants as they contribute a harsh, irritating flavor to the smoke. Nicotine and its contribution to smoking satisfaction are a subject unto itself that is fraught with numerous social and scientific controversies and will not be discussed here. It is well known that tobacco products that contain no or very low levels of nicotine (for numerous reasons) have never found consumer acceptance or commercial success.

17.2.5.2 Compounds in Tobacco and Tobacco Smoke with Two or More Six-Membered *N*-Containing Rings

In tobacco and tobacco smoke, the 76 identified compounds with two or more six-membered *N*-containing rings (Table 17.10) include 2,2′-bipiperidine, several bipyridines, anatabine-type compounds, anabasine-type compounds, anatalline, and nicotelline-type compounds. They are distributed as follows:

1. Over 50 bipyridines, the majority of which are derivatives of 2,3′-bipyridine plus several 2,2′-, 2,4′-, 3,3′-, and 4,4′-bipyridine derivatives.
2. Anatabine and anabasine derivatives which number 16 and 15, respectively.
3. Three compounds with two pyridine rings and a piperidine ring [anatalline [2,4-di(3-pyridinyl) piperidine] and anabasamine [5-(2-piperidinyl)-2,3′-bipyridine] plus its methyl derivative].
4. Two compounds with three pyridines, the so-called terpyridines, one of which is nicotelline (3,2′:4′,3″-terpyridine).
5. One bipiperidine compound has been identified in both tobacco and tobacco smoke (2,2′-bipiperidine).

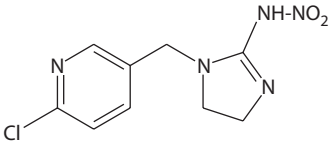
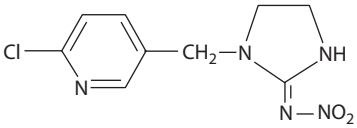
Of the 76 compounds in this class, 66 have been identified in tobacco smoke, 33 in tobacco, and 23 in tobacco and tobacco smoke.

Figure 17.6 illustrates the structures of some of the common tobacco alkaloids found in tobacco and tobacco smoke with two or more six-membered *N*-containing rings.

Although nicotine is the principal alkaloid in commercial tobaccos (*Nicotiana tabacum* and *Nicotiana rustica*), nornicotine is the main alkaloid in most other species of *Nicotiana*. Anabasine is the third most abundant tobacco alkaloid. Anabasine is found in the stem of the (*Nicotiana glauca*) plant. Anatabine has been reported as a minor alkaloid in the roots of these plants, although it is present also in the leaf and stem (3491). All of the alkaloids in Figure 17.6, including bipiperidine, the bipyridines, anatabine, anabasine, anatalline, and nicotelline, can be biosynthesized from lysine and nicotinic acid in *Nicotiana* species to some extent depending on the species (429b, see KEGG, Alkaloid biosynthesis II - Reference pathway, EC-Number 1.1.1.206, Pathway 00960, see http://www.genome.jp/kegg/pathway/map/map00960.html).

Nicotelline (3,2′:4′,3″-terpyridine) is another minor alkaloid of tobacco initially isolated from tobacco by Kuffner and Kaiser (17B28). It was originally believed to be formed by the condensation of two molecules of nicotinoylacetic acid (17B31), although this compound could also result from the degradation of nicotine. However, feeding experiments of [2′-^{14}C]-nicotine or ethyl [carbonyl-^{14}C]-nicotinoyl acetate to tobacco (17B58) failed to yield labeled nicotelline. Currently, nicotelline and anatalline [2,4-di(3-pyridinyl)-piperidine] are considered to be formed by the trimerization of dihydropyridines from nicotinic acid (17B23). A similar reaction is proposed for the formation of the terpyridines.

TABLE 17.9
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	71385-82-5	β-*D*-Fructofuranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2155, 4249	
2.	79886-47-8	β-*D*-Fructopyranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		3667, 3668, 4249	
3.	70906-15-9	*D*-Fructose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		4159, 4249	
4.	105827-78-9	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl) methyl)-4,5-dihydro-*N*-nitro- {Admire®} 		2892a, 4249	
5.	138261-41-3	Imidazolidinimine, 1-((6-chloro-3-pyridinyl) methyl)-*N*-nitro- {Imidacloprid®} 	568b, 4249, 21A19	568b, 4249, 5064, 5568, 21A19	
6.		1*H*-Indole, 2,3-dihydro-3-(3-pyridinyl)-	1587, 4249		
7.	78210-52-3	1*H*-Indole, 2,3-dihydro-3-(3-pyridinylmethyl)-	568b, 1587, 4249, 5811b		
8.	30315-34-5	2-Pyridinamine, 5-(1-methyl-2-pyrrolidinyl)-,(S)-		4249, 4572	
9.	64811-57-0	Pyridine, dihydro-3-(1-methyl-l*H*-pyrrol-2-yl)-	5811, 5811b		
10.	64114-31-4	Pyridine, 2-methyl-3-(1-methyl-2-pyrrolidinyl)- {2-methylnicotine}	1687, 4249	1687, 4249	
11.	64389-08-8	Pyridine, 2-(1,5-dimethyl-1*H*-pyrrol-2-yl)-	3559, 4249		
12.	525-75-7	Pyridine, 2-(1-methyl-1*H*-pyrrol-2-yl)- {α-nicotyrine}	1587, 2570, 4249, 5811b	5685, 5735, 5905	
13.	78210-51-2	Pyridine, 2-(1*H*-pyrrol-1-ylmethyl)-	568b, 1587, 4249, 5811b		
14.		Pyridine, 3-(1-butyl-2-pyrrolidinyl)-,	568b, 4249		
15.	73952-98-4	Pyridine, 3-(dimethyl-1*H*-pyrrolyl)-	5811, 5811a, 5811b		
16.	78210-38-5	Pyridine, 3-(1,3-dimethyl-1*H*-pyrrol-2-yl)-	568b, 1587, 2493, 4249, 5811b	568b, 3550, 4249	
17.	27293-93-2	Pyridine, 3-(1,3-dimethyl-2-pyrrolidinyl)-		4249, 4863	
18.	65734-44-3	Pyridine, 3-(1,5-dimethyl-1*H*-pyrrol-2-yl)-	568b, 1587, 4249, 5811, 5811a, 5811b		
19.	78210-88-5	Pyridine, 3-[1-(5-ethyl-2-furanyl)-1*H*-pyrrol-2-yl]-	568b, 1587, 4249, 5811b		
20.	91429-66-2	Pyridine, 3-(1-ethyl-2-pyrrolidinyl)-	568b, 4249		
21.	5979-92-0	Pyridine, 3-(1-ethyl-2-pyrrolidinyl)-, (S)-	568b, 1371, 2543, 2773, 2775, 3410, 3553, 3559, 4249, 5811b	5811b	
22.	78210-87-4	Pyridine, 3-[1-[2-(2-furanyl)ethyl]-2-pyrrolidinyl]-, (S)-	568b, 1587, 4249, 5811b		
23.	78210-85-2	Pyridine, 3-[1-(2-furanylmethyl)-2-pyrrolidinyl]-,(S)-	568b, 1371, 1587, 2773, 2775, 3410, 4249, 5811b		
24.	123676-95-9	Pyridine, 3-[1-[(hydroxy-1-oxooctyl)oxy]-2-pyrrolidinyl]-		2567, 4249, 5811b	
25.	72461-69-9	Pyridine, 3-[1-(1-methylethyl)-2-pyrrolidinyl]-, (S)-		2565, 4249	
26.	78210-86-3	Pyridine, 3-[1-[(5-methyl-2-furanyl)methyl]-2-pyrrolidinyl]-, (S)-	568b, 1587, 4249, 5811b		

(*continued*)

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

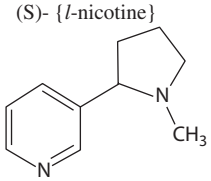
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
27.	78210-84-1	Pyridine, 3-[1-methyl-2-(1-methylethyl)-1*H*-imidazol-5-yl]-	568b, 1587, 4249, 5811b		
28.	22083-74-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (±)-		2099a, 4249	
29.	25162-00-9	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (R)- {*d*-nicotine}	2921, 2922, 2924, 2974, 4249	4249, 17B55	
30.	54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} 	14, 29–31, 41–43, 50, 83, 85a, 86–89, 95, 96, 106, 107, 117, 119, 123, 126, 126a, 126b, 126c, 160, 171, 172, 173a, 174b, 174c, 175, 178, 187, 188, 196–198, 207, 209, 211, 218, 222–224, 237, 239, 270, 274–276, 282, 288, 292b, 293, 294, 302, 306, 308, 337–339, 352, 353, 355, 357a, 357b, 362–365, 375, 376, 378, 382, 388, 395, 409, 410, 413, 424, 427–429, 429e, 437, 438, 441, 442, 445, 446, 456, 462, 469a, 473, 480, 488, 489, 491, 492, 499, 521, 527, 559, 568b, 575, 576, 578, 590, 603, 636, 638, 677b, 678, 679, 681, 686, 688, 723, 761, 765, 767, 768, 804, 824, 830a, 849, 850, 852, 866, 887, 888, 916, 918a, 919, 921, 953, 959, 962, 966, 973, 975, 988a, 989, 998, 999, 1006a, 1007, 1011, 1016, 1022, 1031, 1051, 1063–1075, 1078, 1083, 1084, 1088, 1089a, 1097, 1099, 1100, 1107, 1112, 1118, 1128b, 1129, 1134, 1137, 1138, 1162, 1166–1170, 1177b, 1187, 1188, 1199, 1203, 1215, 1225, 1232, 1263, 1271, 1275, 1283, 1284, 1293, 1301, 1314, 1317–1319, 1320, 1323, 1329–1334, 1334a, 1336, 1338, 1339, 1341, 1348–1350, 1354, 1360–1363, 1366, 1368, 1371–1375, 1375a, 1375b, 1376, 1377, 1378, 1380, 1384–1386, 1388–1390, 1423, 1427, 1437, 1442–1445, 1449, 1450, 1464, 1466, 1469, 1483, 1484, 1491, 1492, 1497, 1502, 1519, 1523, 1536, 1542, 1546, 1567a, 1568, 1580, 1584, 1586, 1589, 1606, 1607, 1614, 1615, 1637, 1639, 1642,1673, 1674, 1686, 1687, 1692, 1695, 1696, 1700, 1702, 1709, 1719, 1725, 1730, 1736,	29, 64, 69, 120, 174c, 207, 212, 256, 261, 262, 306, 308, 324, 337, 339, 374, 404, 410, 427–429, 429e, 468, 480, 499, 504, 506–508, 515, 548–550, 555, 555a, 557, 559, 568b, 647, 654, 660, 667, 677b, 678, 679, 685, 687, 689, 722, 792, 830a, 856, 866, 867, 888, 910, 914, 915a, 915b, 959, 963, 984–986, 989, 995, 997, 998, 1003, 1004, 1007, 1015, 1020, 1033, 1035, 1036, 1063–1066, 1068–1074, 1086, 1088, 1090, 1101, 1107, 1113, 1114, 1118, 1176, 1189, 1193–1199, 1203, 1220–1226, 1276, 1324, 1327, 1329, 1330, 1332, 1333, 1361, 1384, 1385, 1388–1390, 1393, 1464, 1492, 1546, 1549, 1550, 1564, 1567a, 1568, 1575, 1577, 1580, 1584, 1606, 1608–1613, 1615, 1624, 1676,1686, 1702, 1709, 1712, 1719, 1725, 1730, 1746, 1749, 1774, 1811, 1812, 1814, 1836, 1837, 1848, 1853b, 1860a, 1927, 1933a, 1962a, 1990, 2006, 2079, 2104–2111, 2118, 2139, 2146–2150, 2152, 2153, 2164, 2166, 2167, 2191,	50 (0), 1330 (0), 1332 (0), 1354, 1360, 1375a (0), 1377 (0), 1378 (0), 2387, 2506 (0), 2507 (0)

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

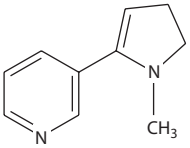
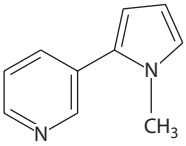
		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	1738, 1741, 1743, 1749, 1760, 1761, 1764, 1766, 1797, 1807a, 1810–1812, 1814, 1818, 1827, 1836, 1837, 1842, 1848, 1860a, 1878, 1882, 1887a, 1890, 1891, 1901, 1908, 1909, 1912, 1913, 1921, 1928, 1933, 1942, 1950, 1966, 1984–1996, 1989, 1990, 2006, 2007, 2012, 2055, 2061, 2062, 2079, 2088, 2097, 2100, 2103, 2110, 2111, 2133, 2134a, 2142, 2144, 2146–2153, 2164, 2166, 2167, 2170, 2171, 2181, 2191, 2211, 2212, 2223, 2225–2229, 2231, 2247, 2254, 2261, 2263, 2267, 2269, 2270–2272, 2294, 2303, 2313, 2313b, 2324, 2327c, 2337, 2338, 2349, 2353a, 2371, 2372, 2374–2378, 2400d, 2401, 2408, 2410, 2412, 2416, 2417, 2446, 2451, 2458, 2459, 2482, 2488, 2493, 2503, 2504, 2506, 2507, 2517, 2523, 2524, 2524a, 2528, 2535, 2543, 2545, 2546, 2549, 2557a, 2570, 2601a, 2603, 2606, 2610, 2612, 2613, 2622, 2628, 2632, 2635, 2652, 2653, 2658, 2668–2673, 2683, 2688, 2690–2695, 2696, 2717, 2719, 2724, 2737, 2739, 2740, 2744, 2761, 2762, 2767, 2774, 2777, 2792, 2793, 2799a, 2800, 2827–2829, 2831, 2832, 2835–2837, 2839, 2840, 2842–2845, 2848, 2857, 2863, 2869, 2874, 2877, 2878a, 2879, 2880, 2899, 2912, 2919, 2920, 2921, 2924–2927, 2936–2939, 2947, 2951, 2958, 2959, 2966, 2967a, 2969, 2970, 2973–2976, 2980, 2982, 2984–2986, 2998, 3008–3016, 3019, 3021, 3022, 3024, 3025, 3027–3029, 3035, 3040, 3041, 3044, 3045, 3054, 3056, 3057, 3059, 3072b, 3078, 3087–3089, 3116, 3121a, 3133, 3137, 3139, 3140, 3142, 3143, 3148a, 3156, 3190, 3214, 3227, 3228, 3254, 3255, 3257, 3258, 3265, 3274, 3300, 3302, 3308,	2212, 2226, 2263, 2270, 2272, 2273, 2282, 2283, 2290, 2294, 2331a, 2332, 2334, 2337, 2338, 2339a, 2349, 2359, 2372, 2374, 2389, 2417, 2446, 2488, 2503, 2504, 2528, 2529, 2532, 2534, 2543–2545, 2557a, 2606, 2611, 2682, 2688, 2689, 2724, 2761, 2762, 2765, 2766, 2786, 2792, 2841, 2844, 2913, 2914, 2917a, 2919, 2920, 2921, 2924–2926, 2938, 2939, 2954 2979–2982, 2989, 3016, 3019, 3022, 3024, 3027, 3028, 3034, 3035, 3041, 3044, 3056, 3059, 3063, 3073, 3074, 3087, 3155, 3188, 3214, 3219, 3254, 3329, 3333, 3375, 3420, 3430, 3444, 3459, 3460, 3476, 3477, 3482, 3491, 3499, 3511, 3512, 3517, 3543, 3549, 3560, 3561, 3570, 3571, 3608a, 3614, 3633, 3634, 3670a, 3705, 3707, 3767a, 3797, 3816, 3905, 3925, 3926, 3928, 3942, 3943b, 3950, 3961, 3972–3974, 3974a, 3974b, 3976, 3980, 3983a, 3999, 4009–4011, 4016, 4017, 4043, 4045, 4047, 4051, 4071, 4073, 4103, 4127, 4159, 4169, 4173, 4213, 4218, 4236, 4249, 4266a, 4267,	

(*continued*)

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	3333, 3370, 3373, 3375, 3378, 3386, 3397, 3398, 3406, 3407, 3410, 3415, 3443–3446, 3457, 3461, 3454, 3477, 3482, 3491, 3493, 3499, 3505, 3516, 3517, 3521, 3548, 3553, 3557, 3559, 3562, 3563, 3570–3572, 3576, 3577, 3585, 3623, 3640, 3658, 3659, 3662, 3670–3672, 3682, 3722, 3731, 3739–3742, 3782–3784, 3790, 3796, 3797, 3803, 3822, 3826, 3833, 3844, 3876, 3884, 3896, 3909, 3910, 3921, 3926, 3928, 3930, 3934, 3936–3939, 3942, 3943, 3952, 3955–3959, 3961, 3972, 3980, 3984, 3990, 3992, 3999, 4009–4011, 4016, 4017, 4039, 4045, 4064, 4065, 4072, 4075, 4076, 4078, 4082, 4103, 4116, 4119–4122, 4127, 4132,4134, 4137, 4138, 4140–4143, 4162, 4167–4176, 4178–4183, 4189–4191, 4194, 4197, 4198, 4202–4207, 4210, 4211, 4213, 4240, 4248, 4249, 4259, 4264, 4267, 4268, 4273, 4275a, 4285, 4291, 4309, 4310, 4319, 4330, 4363, 4366, 4370, 4385, 4398, 4418, 4529, 4570a, 4636, 4745, 4921, 4994, 5000, 5008, 5013, 5017, 5034, 5035, 5041, 5045, 5047, 5052., 5065, 5068, 5069, 5071, 5079, 5082, 5084, 5099, 5100, 5104, 5112, 5118, 5124, 5129, 5130, 5140, 5159, 5163, 5166, 5175, 5179, 5183, 5189, 5207, 5210, 5211, 5219, 5225, 5226, 5236, 5258, 5259, 5263, 5325, 5343, 5346, 5351, 5390, 5401, 5412, 5414, 5427, 5431, 5443, 5452, 5458–5461, 5470–5472, 5473, 5475, 5476, 5480, 5489, 5507, 5508, 5512, 5520, 5529, 5531, 5532, 5544–5546, 5554, 5558, 5563, 5565, 5643a, 5679, 5706, 5770, 5811b, 5836, 25A84, 25A85	4370, 4418, 4420, 4529, 4744, 4745, 4817, 4885, 4921, 5000, 5001, 5005, 5018, 5020, 5024, 5033, 5040, 5053, 5079, 5083,, 5106, 5107, 5112, 5121, 5122, 5126, 5131, 5133, 5140, 5144, 5146, 5150, 5159, 5161, 5162, 5165, 5171, 5172, 5174, 5189, 5198, 5209, 5213, 5214, 5223, 5229, 5244, 5247, 5258, 5259, 5263, 5267, 5294, 5324, 5331, 5335, 5336, 5339, 5349, 5351, 5366, 5382, 5389, 5390, 5390a, 5391, 5404, 5405, 5416, 5419, 5427, 5430, 5439a, 5444, 5445, 5451–5453, 5463, 5469, 5474, 5477, 5481, 5482, 5487, 5488, 5498, 5499, 5508, 5512, 5528, 5535, 5536, 5542, 5561, 5573, 5582, 5622, 5623, 5634, 5652, 5654–5656, 5663, 5664, 5667, 5676, 5681, 5685, 5701, 5702, 5712, 5725, 5726, 5734, 5735, 5765, 5771, 5772, 5774, 5775, 5790, 5803, 5811b, 5824, 5828, 5848, 5853, 5884, 5886, 5895, 5896, 5901, 5905, 17B05, 17B06, 17B08, 17B11, 17B14, 17B18, 17B20, 17B29, 17B42, 17B43, 17B44, 17B48, 17B61, 17B62, 17B64, 21A07, 21A08, 21A40–21A42	

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	65-30-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate (2:1) {Black Leaf 40}		3633, 3634, 3874c, 4249	
32.	6505-86-8	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate {Black Leaf 40}		3633, 3634, 3874c, 4249	
33.	2820-55-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, 1-oxide, (S)- {nicotine-*N*-oxide}	353, 830a, 1702, 1890, 1891, 2128, 2224, 2228, 2349, 2482, 2724, 2939, 3031, 3302, 3308, 3386, 3444, 3491, 3505, 4249, 5079, 5348	120, 1114, 1223–1225, 1702, 1712, 2270, 2339a, 2349, 2724, 2914, 2917a, 2939, 3444, 3491, 3797, 3973, 3974, 3974a, 3983a, 4098a, 4249, 5079, 5390a, 5334, 5348, 5685, 5703, 5727, 5735, 5804, 5811b, 5828	
34.	2820-51-1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, hydrochloride, (S)-		4249, 4849	
35.	16586-18-8	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, labeled with ^{14}C, (S)-		167, 1836, 1933a, 4249	
36.	25429-24-7	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, monohydroxy derivative, (S)-	568b, 3553, 3559, 4249	554, 568b, 3444, 4249	
37.	2055-29-0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, *N*,1-dioxide, (S)-		568b, 4249, 4453, 5811b	
38.	491-26-9	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, *N*-oxide, (2S)-	568b, 1846b, 4249, 5811b	5811b	
39.	6912-85-2	Pyridine, 3-(1-methyl-2-pyrrolinyl)- {2,3-dehydronicotine} 	1195, 1316, 1567a, 1580, 1971, 2228, 2724, 3302, 3308, 3491, 3797, 3967, 4249	1221, 1567a, 4249	
40.	101540-79-8	Pyridine, 3-(1-methyl-2-pyrrolinyl)-6-methyl-		3547, 4249	
41.	487-19-4	Pyridine, 3-(1-methyl-1*H*-pyrrol-2-yl)- {nicotyrine} 	43, 172, 395, 438, 441, 442, 568b, 761, 922, 1225, 1375, 1375b, 1427, 1567a, 1580, 1586, 1702, 1890, 1891, 2079, 2170, 2224, 2228, 2327c, 2470, 2493, 2543, 2570, 2601a, 2724, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2939, 3056, 3059, 3255, 3302, 3308, 3386, 3397, 3398, 3410, 3444, 3491, 3553, 3557, 3559, 3739–3742, 3797, 3967, 3972, 4202, 4210, 4249, 4407, 5079, 5811b	120, 404, 504, 543a, 568b, 689, 937, 984, 1063–1066, 1068–1074, 1113, 1114, 1221, 1567a, 1580, 1590a, 1702, 1854, 2079, 2224, 2270, 2338, 2339a, 2349, 2359, 2386, 2724, 2917a, 2939, 3056, 3059, 3444, 3491, 3511, 3549, 3550, 3797, 3905, 3972, 3974, 4098a, 4249, 5079, 5390a, 5330, 5407, 5454, 5464, 5465, 5582. 5685, 5735, 5811b, 5905	

(*continued*)

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

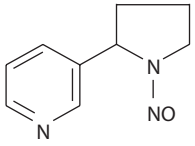
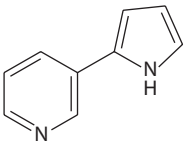
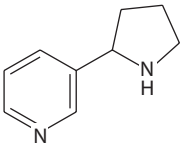
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
42.	16543-55-8	Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-, (S)- {NNN} 	126a, 126b, 167, 172, 174b, 174c, 203, 226, 237, 239, 313, 368, 402, 422, 423, 458–460, 463, 471, 478, 483, 484, 486, 488, 489, 499, 501, 568b, 572, 573, 575, 576, 595, 603, 632, 651, 684, 688, 772, 895, 1011, 1015, 1016, 1051, 1057, 1058, 1099, 1148, 1191–1200, 1216, 1217, 1304, 1373, 1386, 1437, 1442, 1445, 1559, 1564, 1567a, 1568–1571, 1580, 1569, 1574, 1578, 1584, 1585, 1653, 1672, 1674, 1692, 1696, 1702, 1710, 1712, 1717, 1725, 1727, 1722, 1730–1732, 1734, 1736, 1740, 1741, 1743, 1744, 1746, 1750, 1751, 1753, 1761, 1769, 1773, 1781, 1808, 1842, 1870–1872, 1987, 1988, 2128, 2133 2134a, 2136, 2138, 2142, 2168, 2169, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2730, 2799a, 2825, 2879, 2949, 2991, 3007, 3050, 3080, 3094, 3190, 3255–3257, 3265, 3300, 3302, 3308, 3313, 3342, 3343, 3364, 3370, 3491, 3493, 3654, 3714, 3844, 3943a, 3944–3946, 3952, 3976, 3992, 4009–4011, 4059, 4078, 4128, 4249, 4547, 4570a, 4683, 4885, 5008, 5049, 5071, 5494, 5508, 5512, 5518, 5531, 5569, 5679, 5692, 5811b, 5836, 5869a	29, 33, 64, 97–99, 174c, 201, 313, 322, 324, 326, 368, 458, 468, 478, 483, 484, 486, 498, 501, 503, 505, 507, 548–550, 557, 568b, 595, 650, 653–657, 660, 667, 677b, 685, 720, 772, 895, 951, 988a, 994, 995, 997, 1003, 1010, 1015, 1051, 1175a, 1191–1200, 1206a, 1216, 1385, 1564, 1567a, 1568–1571, 1576, 1577, 1579, 1569, 1575, 1577, 1579, 1580, 1584, 1585, 1679, 1696 1702, 1704, 1712, 1725, 1727, 1731–1734, 1742–1744, 1750, 1753, 1771, 1870–1872, 1916a, 1988, 2050–2052, 2138, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2637, 2638, 2660, 2674, 2700, 2914–2917, 2949, 2996, 2997, 3144a, 3176a, 3177, 3491, 3654, 3670a, 3773, 3774, 3816, 3943a, 3943b, 3944–3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4247, 4249, 4410b, 4413, 4547, 4683, 4885, 5001, 5005, 5007, 5008, 5018, 5023, 5033, 5038, 5053, 5063, 5531, 5561, 5579, 5584, 5811b	
43.	53844-45-4	Pyridine, 3-(1-nitroso-2-pyrrolidinyl-2-^{14}C)-, (S)-	683b, 4249	683b, 4249	
44.		Pyridine, 3-(1-pentyl-2-pyrrolidinyl)-	568b, 4249		
45.	78210-89-6	Pyridine, 3-[1-(5-propyl-2-furanyl)-1*H*-pyrrol-2-yl]-	568b, 1587, 4249, 5811b		

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
46.	69698-09-5	Pyridine, 3-(1-pyrrolidinyl)-	5811, 5811a, 5811b	5811, 5811a, 5811b	
47.	5746-86-1	Pyridine, 3-(2-pyrrolidinyl)-	5811a		
48.	72692-99-0 50966-74-0	Pyridine, 3-(1*H*-pyrrol-1-yl)-	568b, 1587, 4249		
49.	80866-95-1	Pyridine, 3-(1*H*-pyrrol-1-ylmethyl)-	568b, 4249		
50.	36127-43-2	Pyridine, 3-(1,3,3-trimethyl-2-pyrrolidinyl)-	568b, 4249		
51.	494-98-4	Pyridine, 3-(1*H*-pyrrol-2-yl)- {nornicotyrine} 	761, 1225, 1360, 1375a, 1580, 2224, 2228, 2724, 2939, 3056, 3059, 3302, 3308, 3444, 3491, 3797, 3967, 4249, 5079	120, 1221, 2079, 2270, 2724, 3056, 3059, 3444, 3491, 3974a, 4249, 5079, 5905	1360, 1375a
52.	78210-49-8	Pyridine, 3-(2-methyl-1*H*-pyrrol-1-yl)-	568b, 1587, 4249, 5811b		
53.	7076-23-5	Pyridine, 3-(2-pyrrolidinyl)-, (R)- {*d*-nornicotine}	2921, 2922, 4249	5038	
54.	494-97-3	Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine} 	126, 174b, 237, 239, 429e, 480, 568b, 761, 830a, 1078, 1084, 1222, 1315–1317, 1373, 1375, 1375b, 1437, 1567a, 1568, 1584, 1696, 1702, 1751, 1842, 2079, 2228, 2482, 2647, 2724, 2734, 2767, 2844, 2845, 2921, 2922, 2939, 3044, 3056, 3057, 3059, 3126c, 3265, 3302, 3308, 3444, 3477, 3491, 3499, 3553, 3557, 3559, 3742, 3797, 3972, 3999, 4103, 4249, 4350, 5008, 5079, 5258, 5259, 5531, 5811b	64, 120, 174b, 324, 429e, 480, 504, 548–550, 555a, 557, 568b, 654, 660, 667, 687, 792, 830a, 856, 915b, 995, 1005, 1010, 1015, 1087, 689, 867, 1101, 1114, 1221, 1311, 1315–1317, 1324, 1327, 1564, 1567a, 1568, 1584, 1696, 1702, 1712, 1916a, 1927, 1962a, 2079, 2139, 2224, 2283, 2331a, 2334, 2349, 2359, 2532, 2543, 2647, 2724, 2746, 2761, 2762, 2765, 2766, 2844, 2914, 2921, 2922, 2939, 3044, 3050, 3056, 3059, 3063, 3126c, 3444, 3459, 3460, 3477, 3482, 3491, 3499, 3260a, 3511, 3608a, 3670a, 3767a, 3797, 3943b, 3972–3974, 3974a, 3974b, 3983a, 3999 4073, 4103,	

(*continued*)

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

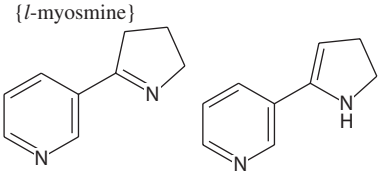
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine} (cont.)		4161, 4218, 4236, 4249, 4683, 4885, 4974, 5005, 5008, 5023, 5033, 5038, 5079, 5189, 5258, 5259, 5382, 5390, 5406, 5408, 5409, 5416, 5455, 5463, 5477, 5488, 5497, 5561, 5573, 5582, 5620, 5676, 5685, 5701, 5702, 5727, 5771, 5804, 5811b, 5820, 5853, 5864, 5884, 5895, 5896, 5901, 5905, 17B06, 17B18, 17B38, 17B55	
55.	53844-44-3	Pyridine, 3-(2-pyrrolidinyl-2-^{14}C)-, (S)-	683b, 4249	683b, 4249	
56.		Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)- {*d*-myosmine}	2327c, 2921, 4249		
57.	532-12-7	Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)- {*l*-myosmine} 	167, 172, 174b, 395, 438, 441, 442, 480, 568b, 761, 830a, 916, 1063–1066, 1068–1074, 1099, 1100, 1360, 1365, 1371, 1375a, 1427, 1567a, 1568, 1580, 1702, 2079, 2172, 2224, 2226, 2493, 2543, 2601a, 2647, 2710, 2724, 2734, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2869, 2921, 2939, 3054, 3056, 3057, 3059, 3255, 3308, 3386, 3397, 3398, 3410, 3444, 3491, 3499, 3505, 3553, 3559, 3739–3742, 3762, 3826, 3972, 3999, 4208, 4209, 4249, 4319, 4407, 5034, 5079, 5811b	120, 174b, 395, 480, 504, 548–550, 568b, 778, 685, 687, 984, 1087, 1221, 1223, 1324, 1327, 1567a, 1568, 1702, 1712, 1980, 2079, 2270, 2331a, 2338, 2359, 2389, 2544, 2647, 2724, 2917a, 2920, 2921, 2939, 2995, 3056, 3059, 3430, 3444, 3491, 3499, 3511, 3549, 3550, 3608a, 3260a, 3905, 3972–3974, 3974a, 3983a, 3999, 4249, 4921, 5011, 5079, 5573, 5582, 5720, 5727, 5811b	1360, 1375a
58.	525-74-6	Pyridine, 3-(4,5-dihydro-1-methyl-2*H*-pyrrol-5-yl)- {*N*-methylmyosmine}	5811b	120, 568b, 1101, 1221, 1854, 2079, 2270, 2349, 2939, 3973, 4249, 5079, 5312, 5390a, 5811b, 5905	
59.	65719-03-1	Pyridine, 3-(3,4-dihydro-2-methyl-2*H*-pyrrol-5-yl)-	568b, 4249		
60.	78249-81-7	Pyridine, 3-(3,4-dihydro-3-methyl-2*H*-pyrrol-5-yl)-	568b, 1587, 4249, 5811b	5811b	
61.	78210-37-4	Pyridine, 3-(3,4-dihydro-4-methyl-2*H*-pyrrol-5-yl)-	568b, 1587, 4249, 5811b		
62.	78210-39-6	Pyridine, 3-(3-ethyl-3,4-dihydro-2*H*-pyrrol-5-yl)-	568b, 1587, 4249, 5811b		

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
63.	78210-45-4	Pyridine, 3-[2,5-dihydro-1-[(5-methyl-2-furanyl)methyl]-1*H*-pyrrol-2-yl]-	568b, 1587, 4249, 5811b		
64.	34137-26-3	Pyridine, 5-fluoro-3-(1-methyl-2-pyrrolidinyl)-, (S)-		4249, 4736	
65.		Pyridine, 6-methyl-3-(1-methyl-2-pyrrolinyl)-	568b, 4249		
66.	70969-38-9	2(1*H*)-Pyridinone, 5-(3,4-dihydro-2*H*-pyrrol-5-yl)-		2226, 4249	
67.	40316-88-9	2(1*H*)-Pyridinone, 3-(1-methyl-2-pyrrolidinyl)-, (*S*)- {2-Pyridinol, 3-(1-methyl-2-pyrrolidinyl)-}- {nicotone}	2224, 2228, 2724, 3308, 4249	2226, 4249, 4572	
68.	10516-09-3	2(1*H*)-Pyridinone, 5-(1-methyl-2-pyrrolidinyl)-, (S)- {2-Pyridinol, 5-(1-methyl-2-pyrrolidinyl)-}		554, 1101, 2226, 4249	
69.	5979-94-2	Pyrrolidine, 1-acetyl-2-(3-pyridinyl)-, (S)- {*N*′-acetylnornicotine}	568b, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 2761, 2762, 2765–2767, 2777, 3410, 3553, 3739–3741, 4249, 5811b	64, 568b, 993, 2359, 3550, 3260a, 3973, 4133, 4236, 4249, 5811b	1360, 1375a
70.	86900-39-2	Pyrrolidine, 1-ethyl-2-(3-pyridinyl)- {*N*′-ethylnornicotine}		2917a, 4249	
71.	91907-45-8	Pyrrolidine, 1-propyl-2-(3-pyridinyl)- {*N*′-propylnornicotine}		2917a	
72.	117642-93-0	Pyrrolidine, 1-(10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		4249	
73.	120376-92-3	Pyrrolidine, 1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		4249	
74.	117642-94-1	Pyrrolidine, 1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-, (S)-		4249	
75.	120042-36-6	Pyrrolidine, 1-(11-methyl-1-oxododecyl)-2-(3-pyridinyl)-, (S)-		4249	
76.	120376-93-4	Pyrrolidine, 1-(12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
77.	69730-91-2	Pyrrolidine, 1-(1-oxobutyl)-2-(3-pyridinyl)-, (S)-	568b, 1587, 2775, 3410, 3742, 4249, 5811b	64, 568b, 994, 1248, 2497, 2498, 3742, 4236, 4249, 5811b	
78.	115849-75-7	Pyrrolidine, 1-(1-oxododecyl)-2-(3-pyridinyl)-, (S)-		4249	
79.	74173-71-0	Pyrrolidine, 1-(1-oxoheptyl)-2-(3-pyridinyl)-, (S)-	3742, 4249, 5811b		
80.	38854-09-0	Pyrrolidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-	1587, 3742, 4249, 5811b	64, 389, 994, 3491, 3742, 4236, 4249, 5811b	
81.		Pyrrolidine, 1-(1-oxo-?-octenyl)-2-(3-pyridinyl)-,(S)-	3742, 4249		
82.		Pyrrolidine, 1-(1-oxo-5-octenyl)-2-(3-pyridinyl)-	3742, 4249		
83.		Pyrrolidine, 1-(1-oxo-6-octenyl)-2-(3-pyridinyl)-	3742, 4249		
84.		Pyrrolidine, 1-(1-oxo-7-octenyl)-2-(3-pyridinyl)-	3742, 4249		
85.	38854-10-3	Pyrrolidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-	568b, 1587, 2885a, 3742, 4249, 5811b	64, 389, 404, 568b, 994, 2389, 2544, 2865a, 3491, 3742, 4236, 4249, 5811b	
86.	120042-35-5	Pyrrolidine, 1-(1-oxotridecyl)-2-(3-pyridinyl)-, (S)-		4249	

(*continued*)

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
87.	115849-82-6	Pyrrolidine,1-(3-hydroxy-10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		4249	
88.	115849-79-1	Pyrrolidine,1-(3-hydroxy-10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		4249	
89.	116353-95-8	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotetradecyl)-2-(3-pyridinyl)-		4249	
90.	115849-84-8	Pyrrolidine,1-(3-hydroxy-12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
91.	120042-33-3	Pyrrolidine, 1-(3-hydroxy-14-methyl-1-oxopentadecyl)-2-(3-pyridinyl)-		4249	
92.	115849-80-4	Pyrrolidine, 1-(3-hydroxy-1-oxododecyl)-2-(3-pyridinyl)-		4249	
93.	120042-32-2	Pyrrolidine, 1-(3-hydroxy-1-oxohexadecyl)-2-(3-pyridinyl)-		4249	
94.	120042-34-4	Pyrrolidine, 1-(3-hydroxy-1-oxopentadecyl)-2-(3-pyridinyl)-		4249	
95.	115849-85-9	Pyrrolidine, 1-(3-hydroxy-1-oxotetradecyl)-2-(3-pyridinyl)-		4249	
96.	115849-83-7	Pyrrolidine, 1-(3-hydroxy-1-oxotridecyl)-2-(3-pyridinyl)-		4249	
97.		Pyrrolidine, 1-(3-pyridinemethyl)-2-cyano-	4570a		
98.	96552-73-7	Pyrrolidine, 1-(4-methyl-1-oxohexyl)-2-(3-pyridinyl)-	3742, 4249, 5811b		
99.	77829-17-5	Pyrrolidine, 1-(6-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		994, 2566, 2567, 3973, 4236, 4249, 5811b	
100.	96574-02-6	Pyrrolidine, 1-(6-methyl-1-oxoheptyl)-2-(3-pyridinyl)-, (S)-	3742, 4249, 5811b		
101.	77829-18-6	Pyrrolidine, 1-(7-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		994, 2566, 2567, 3973, 4236, 4249, 5811b	
102.	69730-92-3	Pyrrolidine, 1-[4-(dimethylamino)-1-oxobutyl]-2-(3-pyridinyl)-, (S)-		2497, 2498, 4236, 4249	
103.	38840-03-8 3000-81-5	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)- {*N*′-formylnornicotine}	568b, 830a, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 1586, 2601a, 2761, 2762, 2765–2767, 2777, 3255, 3410, 3553, 3739–3742, 4249, 4407, 5811b	64, 568b, 689, 994, 2359, 2952, 3491, 3549, 3550, 3742, 3973, 4133, 4249, 5811b	1360, 1375a
104.	69730-90-1	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, ethyl ester, (S)-		1156, 2497, 2498, 3742, 4090, 4249	
105.	56078-08-1	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)-	1578, 3491, 3742, 4249, 5811b	1578, 2497, 2498, 3742, 4249	
106.	25110-79-6	2-Pyrrolidinol, 1-methyl-5-(3-pyridinyl)-	568b, 3553, 4249, 5811b		
107.	75202-09-4	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-	3553, 4249	3797, 4249, 5811b	

TABLE 17.9 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with a Six- and Five-Membered *N*-Containing Ring

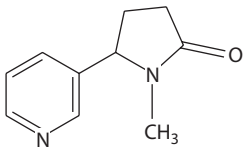
	CAS No.	Name (per CA Collective Index)	References		
			Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
108.	486-56-6	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, (S)- {cotinine} 	353, 437, 469a, 568b, 761, 830a, 1078, 1063–1066, 1068–1074, 1084, 1099, 1100, 1360, 1365, 1375a, 1567a, 1568, 1580, 1586, 1673, 1695, 1700, 1702, 1719, 1751, 2228, 2482, 2543, 2601a, 2724, 2761, 2762, 2765, 2767, 2773, 2775, 2799a, 2839, 2939, 3054, 3056, 3057, 3059, 3190, 3255, 3257, 3265, 3302, 3308, 3386, 3398, 3410, 3491, 3553, 3559, 3739–3742, 3972, 3992, 4249, 4407, 5035, 5508, 5565, 5811b	64, 120, 504, 553, 568b, 689, 830a, 984, 995, 998, 1012, 1226a, 1385, 1567a, 1568, 1702, 1712, 2338, 2359, 2724, 2917a, 2939, 2995, 3056, 3059, 3444, 3477, 3491, 3549, 3550, 3797, 3972–3974, 3974a, 4236, 4249, 4921, 5011, 5508, 5685, 5735, 5811b	1360, 1375a
109.	15569-85-4 36508-80-2	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, 1-oxide {cotinine 1-oxide}	2482, 4249		
110.	5980-06-3	2-Pyrrolidinone, 5-(3-pyridinyl)-, (S)- {norcotinine}	568b, 2767, 3553, 4249, 5811b	568b, 3797, 4249, 4666, 5811b	
111.	62003-47-8	2*H*-Pyrrol-2-one, 1,3-dihydro-5-(3-pyridinyl)-	568b, 2767, 4249		

TABLE 17.10
Distribution of Components with Two or More Six-Membered *N*-Containing Rings between Tobacco and Tobacco Smoke

Component	Number of Identified Compounds in Tobacco and Tobacco Smoke with Two Six-Membered *N*-Containing Rings			
	Total	Smoke	Tobacco	Smoke and Tobacco
Compounds with two or more six-membered *N*-containing rings (type)				
Piperidine + piperidine	1	0	1	0
Pyridine + piperidine (anabasine type)	15	11	8	4
Pyridine + pyridine (bipyridines)	39	38	8	7
Pyridine + di- or tetrahydropyridine (anatabine type)	16	12	9	5
Two pyridines + piperidine	3	1	3	1
Three pyridines	2	2	2	2
Totals	76	64	31	19

These alkaloids are possibly artifacts produced by nonenzymatic reactions which could occur during the harvesting and curing of tobacco. The lack of optical activity in the isolated anatalline supports this hypothesis (17B31).

Various bipyridines are also formed during tobacco fermentation [Frankenburg and Gottscho (1223)]. As much as 3% of the nicotine originally present in cigar tobacco was converted to 2,3′-bipyidine and other oxidative compounds (3973).

One study by Dubinin and Chelintsev (1075a) reported on the pyrolytic products of anabasine heated at 580°C–650°C in a charcoal-filled reactor. Exclusive of gases, the major products were reported to be pyridine, 2-methylpyridine, 2-ethylpyridine, 5-methylisoquinoline, and 2,3′-bipyridine. The preponderance of the 2-alkylpyridines might indicate preferential cleavage of the pyridine ring which would be unexpected; evaluation of these findings is difficult since the use of charcoal in the reactor may have produced a catalytic effect and altered the pyrolytic reactions markedly (3797).

In terms of the flavor potential of this class of compounds, very little is known. A minor tobacco alkaloid, 2,3′-bipyridine, has been reported (17B19) to exhibit a sensitizing effect on tobacco flavor and to suppress astringency (3215, 17B52).

Table 17.11 lists the compounds containing two or more six-membered *N*-containing rings identified in tobacco and tobacco smoke.

Detailed examination of the lists presented in this chapter on monocyclic nitrogen heterocycles indicates many such compounds have been identified to date in tobacco and tobacco smoke. Some of the data are summarized in Table 17.12.

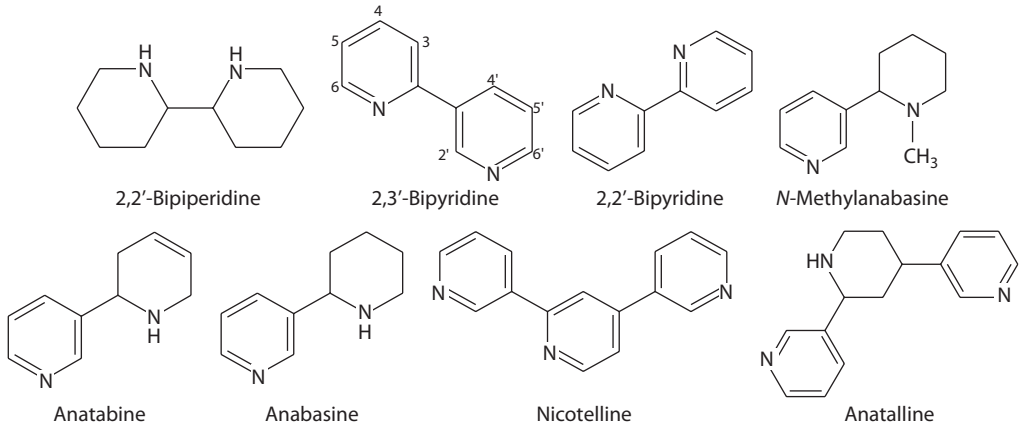


FIGURE 17.6 Common tobacco alkaloids found in tobacco and tobacco smoke with two or more six-membered *N*-containing rings.

It is obvious from the tabulation that the six-membered *N*-containing ring compounds with one or more nitrogens represent nearly 75% of the compounds identified to date.

17.3 LACTAMS

Kosak (2170) listed no lactam identified in tobacco smoke prior to 1954. In 1959, Johnstone and Plimmer (1971) listed cotinine as an alkaloid in tobacco and smoke. They did not categorize it or any other tobacco or smoke component as a lactam.

In its 1963 monograph on tobacco and smoke components, Philip Morris (2939) listed cotinine as a tobacco and smoke component. Ishiguro and Sugawara (1884) in their 1980 monograph on tobacco smoke components listed a total of 72 amides, imides, and lactams; a total of 16 lactams was listed [see Table I-15 in (1884)]. The reference for all of the 16 lactams listed was that of Schumacher et al. (3553).

The International Agency for Research on Cancer (IARC) working group met in 1985 to assess the carcinogenic risk from tobacco smoking. Its monograph summarizing the IARC findings was published in 1986. In it, the IARC stated that there was a large spectrum of amides, imides, and lactams in tobacco smoke (including some 50 aliphatic amides) [see p. 109 in (1870)]. The IARC view on these three compound classes was based on the 1977 review by Schmeltz and Hoffmann (3491) and publications in 1977 and 1981 by Schumacher et al. (3553) and Heckman and Best (1587), respectively.

Of the 35 lactams reported in tobacco smoke by Schumacher et al. (3553) at the 1975 *Tobacco Chemists' Research Conference (TCRC)* and published in 1977, 21 were new to the tobacco smoke literature. As noted in Chapters 13 and 14, used in this study was a recently developed analytical technology that permitted fractionation and identification of the water-soluble components of cigarette smoke condensate (CSC). Similarly in their 1978 TCRC presentation and 1981 publication, Heckman and Best (1587) reported the identification of two additional new lactams in tobacco smoke, 3-ethyl-5-methylene-3-pyrrolid-2-one and *N*-methyl-5-(1-methylethylidene)-3-pyrrolid-2-one. They also confirmed the presence in tobacco smoke of many of the lactams previously reported (3553). In his earlier study of the mainstream smoke from an all-burley tobacco cigarette, Heckman (1986) identified eight lactams.

Lactams frequently reported in both tobacco and its smoke but seldom classified as lactams are 1-methyl-5-(3-pyridinyl)-2-pyrrolidinone (cotinine) and several of its derivatives such as norcotinine. Ishiguro and Sugawara (1884) listed them as alkaloids [see Table I-12 in (1884)] not lactams.

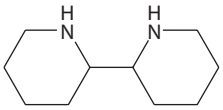
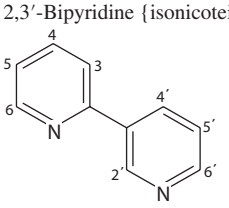
Examination of the structures of several of the CSC components indicates that the decision of their categorization is somewhat difficult. In Figure 17.7, representative structures for an imide and a lactam are presented. To which of these categories—imide or lactam—should the smoke component 1,7-dihydro-6*H*-purine-2,6-dione (xanthene) {I} be assigned? Its structure {I} is depicted in Figure 17.8. In structure {II} in Figure 17.8, its imide configuration is accentuated. Structure {III} illustrates that two lactam configurations exist in the xanthene molecule. This same situation is present with the other purine-derived smoke components. While there may be some disagreement of the preciseness of our selection, for completeness sake, such components are listed in each chapter in its major catalog table. As a result, the total number of components in each of the major catalog tables may be slightly inflated.

Table 17.13 lists a total of 138 lactams identified in tobacco and/or tobacco smoke. Of the 138, 58 were identified in tobacco, 116 were identified in tobacco smoke, and 36 were identified in both tobacco and tobacco smoke.

17.4 OXAZOLES AND OXAZINES

Several oxazoles and oxazines have been identified in tobacco and tobacco smoke. Oxazoles are generally known as 1,3-azoles or five-membered-ring aromatic heterocyclic compounds with an oxygen and a nitrogen separated by one carbon. Oxazole is the parent compound. Isoxazoles are in this same family of compounds and are generally known as 1,2-azoles. These five-membered-ring aromatic heterocyclic compounds contain adjacent oxygen and nitrogen atoms. Oxazole is an analog of imidazole where the nitrogen atom in position 1 is replaced by oxygen. Isoxazole is an analog

TABLE 17.11
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Two or More Six-Membered *N*-Containing Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	531-67-9	2,2′-Bipiperidine 	441, 4249	2917a, 4249	
2.	37275-48-2	Bipyridine	167, 568b, 1360, 1371, 1375a, 1444, 1586, 1587, 2570, 2761, 2762, 2767, 2773, 3397, 3398, 4249, 5034, 5811b		1360, 1375a
3.	78310-61-9	Bipyridine, dimethyl- {two isomers detected}	1587, 2543, 2773, 4249, 5811b		
4.		Bipyridine, diphenyl-	1587, 4249		
5.	64859-48-9	Bipyridine, ethyl-	2141, 4249, 5811b		
6.	64859-47-8	Bipyridine, methyl- {four isomers in all}	1360, 1371, 1375a, 2141, 2543, 2761, 2762, 2765, 2766, 2773, 4249		1360, 1375a
7.	78310-62-0	Bipyridine, phenyl-	1587, 4249, 5811b		
8.	366-18-7	2,2′-Bipyridine {nicotine}	441, 442, 568b, 1371, 2079, 3491, 4159, 4249, 5811b	568b, 2079, 2283, 3549, 4159a, 4249, 5079, 5332, 5382, 5811b	
9.		2,2′-Bipyridine, amino-	442, 4249		
10.	78210-73-8	2,2′-Bipyridine, 4,5-dimethyl-	1587, 4249, 5811b		
11.	56100-19-7	2,2′-Bipyridine, 4-methyl-	568b, 1587, 4249, 5811b		
12.	581-50-0	2,3′-Bipyridine {isonicoteine} 	43, 172, 480, 761, 830a, 1099, 1223, 1063–1066, 1068–1074, 1360, 1364, 1371, 1375, 1375a, 1375b, 1567a, 1580, 1584, 1586, 1744, 1842, 2224, 2228, 2270, 2327c, 2387, 2493, 2543, 2601a, 732, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2769, 2939, 3054, 3057, 3059, 3255, 3302, 3308, 3386, 3397, 3398, 3410, 3444, 3491, 3499, 3505, 3553, 3557, 3559, 3739, 3740, 3742, 3972, 4249, 4407, 4570a, 5512, 5811b	64, 120, 172, 404, 480, 689, 984, 1063–1066, 1068–1074, 1221, 1223, 1567a, 1584, 1590a, 1712, 1854, 2079, 2224, 2270, 2283, 2286, 2333, 2339a, 2359, 2389, 2544, 2724, 2917a, 2939, 3056, 3059, 3215, 3444, 3491, 3543, 3550, 3560, 3561, 3608a, 3763, 3973, 3974a, 3983a, 4133, 4236, 4249, 5079, 5382, 5403, 5582, 5703, 5727, 5811b, 17B19, 17B37	1360, 1375a, 2387
13.		2,3′-Bipyridine, dimethyl-	3742, 4249		
14.		2,3′-Bipyridine, methyl-	1371, 2777, 3255, 3410, 3739, 3740, 3742, 4249		

(*continued*)

TABLE 17.11 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Two or More Six-Membered *N*-Containing Rings

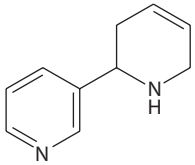
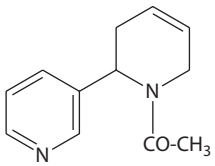
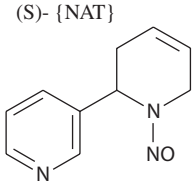
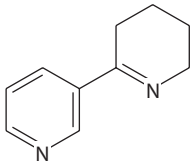
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
15.		2,3′-Bipyridine, 1,2,3,4-tetrahydro-1-methyl-	2767, 3553, 4249		
16.	2743-90-0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (±)-		4249	
17.	126454-22-6	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (R)- {*d*-anatabine}	568b, 2921, 2922, 4249	568b, 4249, 17B32, 17B33, 17B36, 17B37, 17B55	
18.	581-49-7	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (S)- {*l*-anatabine} 	126b, 172, 174b, 237, 568b, 1015, 1063–1066, 1068–1074, 1360, 1364, 1375a, 1445, 1567a, 1580, 1584, 1674, 1696, 1744, 1751, 1842, 2224, 2228, 2270, 2543, 2724, 2734, 2761, 2762, 2765–2767, 2775, 2777, 2921, 2922, 2939, 3054, 3056, 3057, 3059, 3255, 3302, 3308,3398, 3441a, 3444, 3491, 3559, 3739, 3740, 3742, 3797, 3972, 4249, 4407, 5512, 5811b	64, 120, 174b, 504, 548–550, 555a, 568b, 687, 689, 830a, 1002, 1193–1196, 1199, 1221, 1324, 1327, 1567a, 1584, 1696, 1712, 1916a, 2079, 2139, 2270, 2333, 2724, 2914, 2920, 2921, 2939, 3056, 3059, 3444, 3459, 3460, 3491, 3550, 3608a, 3260a, 3797, 3972–3974, 3974a, 3983a, 4236, 4249, 5079, 5573, 5582, 5727, 5811b, 5853, 17B32, 17B33, 17B36, 17B37, 17B55	1360, 1375a
19.		2,3′-Bipyridine, 1,2,3,6-tetrahydro-ethyl-	2767, 3410, 4249		
20.		2,3′-Bipyridine, 1,2,3,6-tetrahydro-methyl-	1371, 3410, 4249		
21.	61892-64-6	2,3′-Bipyridine, 1-acetyl-1,2,3,6-tetrahydro-, (S)- {*N*′-acetylanatabine} 	568b, 3553, 3739, 3740, 4249, 5811b	64, 568b, 3973, 4236, 4249, 5811b	
22.	5953-51-5	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-methyl-, (S)- {*N*-methylanabasine}	568b, 2224, 2767, 2773, 2775, 3302, 3444, 3553, 3559, 4249, 5811b	120, 568b, 1221, 2079, 2270, 2939, 3444, 3491, 3550, 3797, 3974a, 4098a, 4249, 5079, 5407, 5811b	
23.	96552-71-5	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxohexyl)-, (S)- {*N*′-hexanoylanatabine}	3739, 3740, 4249, 5811b		
24.	96552-72-6	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxooctyl)-, (S)- {*N*′-octanoylanatabine}	3739, 3740, 4249, 5811b		

TABLE 17.11 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Two or More Six-Membered *N*-Containing Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
25.	71267-22-6	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-nitroso-, (S)- {NAT} 	24, 28–31, 34, 59, 174b, 174c, 239, 402, 459, 463, 478, 483, 484, 486, 501, 502, 514, 568b, 572, 573, 603, 688, 895, 1002, 1015, 1051, 1192–1196, 1198, 1199, 1217, 1304, 1386, 1437, 1445, 1569–1571, 1584, 1672, 1685, 1692, 1694, 1696, 1702, 1725, 1736, 1751, 1769, 1870, 1871, 1987, 1988, 2142, 2235, 2354, 2407, 2516 2588, 2617, 2618, 2879, 2949, 2991, 3007, 3080, 3094, 3190, 3255, 3265, 3300, 3342, 3343, 3370, 3844, 3943a, 3944–3946, 3952, 3976, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5494, 5531, 5569, 5679, 5811b, 5692, 5836	29, 33, 34, 64, 174c, 201, 324, 404, 468, 478, 483, 484, 486, 501, 502, 505, 514, 548–550, 557, 568b, 655, 720, 895, 951, 995, 998, 1002, 1010, 1015, 1175a, 1192–1196, 1198, 1199, 1206a, 1385, 1569–1571, 1576, 1679, 1685, 1694, 1696, 1702, 1712, 1725, 1733, 1916a, 1988, 2050–2052, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2637, 2638, 2674, 2700, 2914, 2949, 3144a, 3176a, 3177, 3661, 3773, 3774, 3816, 3943a, 3944–3948, 3973, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5063, 5518, 5531, 5579, 5584, 5811b	
26.	3471-05-4	2,3′-Bipyridine, 3,4,5,6-tetrahydro- {anabaseine} 		5079, 5222	
27.	61892-98-6	2,3′-Bipyridine, 1-ethyl-1,2,3,6-tetrahydro-, (S)-	568b, 3553, 4249, 5811b		
28.	26636-59-9	2,3′-Bipyridine, 2′(or 3)-methyl-	1587, 4249		
29.	78210-76-1	2,3′-Bipyridine, 3-ethyl-	568b, 1587, 4249, 5811b		
30.		2,3′-Bipyridine, 3-methyl-	568b, 4249		
31.	78210-75-0	2,3′-Bipyridine, 4-(2-butenyl)-	568b, 1587, 4249, 5811b		
32.	78210-74-9	2,3′-Bipyridine, 4-(2-propenyl)-	568b, 1587, 4249, 5811b		
33.		2,3′-Bipyridine, 4-propyl-	568b, 4249		
34.	38840-05-0	2,3′-Bipyridine, 4-methyl-	1360, 1371, 1375a, 2761, 2762, 2765–2767, 2775, 2777, 4249	4133, 4249	1360, 1375a
35.	20410-87-1	2,3′-Bipyridine 7, 5-(1-methyl-2-piperidinyl)-, (+)- {anabasamine}		4133, 4249	
36.	78210-79-4	2,3′-Bipyridine, 5-(1-propenyl)-	568b,1587, 4249, 5811b		
37.	78210-81-8	2,3′-Bipyridine, 5-ethenyl-	568b,1587, 4249, 5811b		
38.	34671-89-1	2,3′-Bipyridine, 5-ethyl-	568b,1371, 1587, 4249, 5811b		
39.	26844-80-4	2,3′-Bipyridine, 5-methyl-	568b,2493, 2570, 3255, 3386, 3398, 3553, 4249, 5811b	568b,3491, 4133, 4249, 5811b	

(*continued*)

TABLE 17.11 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Two or More Six-Membered *N*-Containing Rings

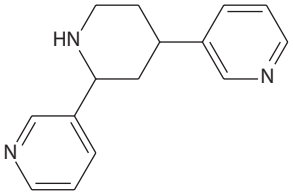
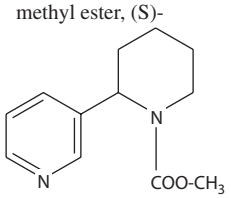
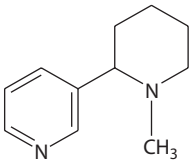
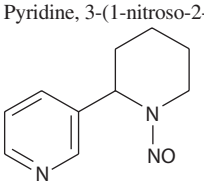
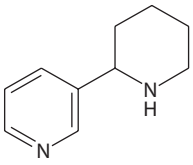
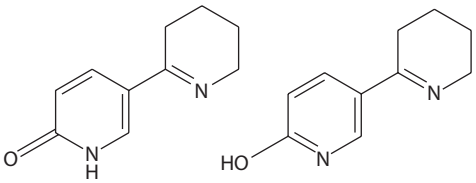
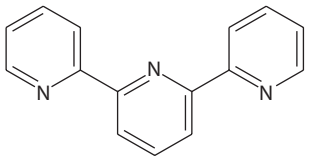
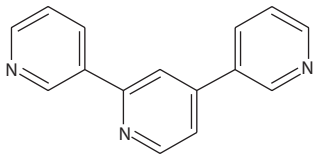
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
40.	78210-80-7	2,3′-Bipyridine, 5-propyl-	1587, 4249, 5811b		
41.	78210-77-2	2,3′-Bipyridine, 6-ethyl-	568b,1587, 4249, 5811b		
42.		2,3′-Bipyridine, 6-hydroxy-3,4,5,6-tetrahydro-	568b, 4249		
43.	78210-78-3	2,3′-Bipyridine, 6-methyl-	568b, 1587, 2767, 4249, 5811b		
44.	61892-65-7	[2,3′-Bipyridine]-1(2*H*)-carboxaldehyde, 3,6-dihydro-, (S)- {*N*′-formylanatabine}	568b, 3553, 3739, 3740, 4249, 5811b	64, 568b, 3550, 3973, 4236, 4249, 5811b	
45.	96552-70-4	[2,3′-Bipyridine]-1(2*H*)-carboxylic acid, 3,6-dihydro-, methyl ester, (S)-	4249, 5811b		
46.	70898-21-4	[2,3′-Bipyridine]-6′(1′*H*)-one, 3,4,5,6-tetrahydro-		4249, 4945	
47.	581-47-5	2,4′-Bipyridine	568b, 3255, 4249	568b, 3973, 4249, 5811b	
48.	581-46-4	3,3′-Bipyridine	442, 568b, 3255, 3553, 4249, 5811b	568b, 3430, 4249, 5811b	
49.	38840-06-1	3,3′-Bipyridine, 4-methyl-		4133, 4249	
50.	78210-82-9	3,3′-Bipyridine, 5-methyl-	568b, 1587, 4249		
51.	78210-83-0	3,3′-Bipyridine, 6-methyl-	568b, 1587, 4249, 5811b		
52.	553-26-4	4,4′-Bipyridine	441, 568b, 3386, 4249, 5811b	568b, 3973, 4249, 5811b	
53.	3350-86-5	Piperidine, 1-acetyl-2-(3-pyridinyl)-, (S)-	5811b	4249	
54.	18793-19-6	Piperidine, 2,4-di(3-pyridinyl)- {pyridine, 3,3′-(2,4-piperidinediyl)bis-; anatalline} 	2726, 3491, 4249	3491, 3973, 4249	
55.	62784-01-4	Piperidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-	5811, 5811a, 5811b		
56.	96552-69-1	Piperidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-	3742, 4249, 5811b		
57.	62783-95-3	Piperidine, 1-(1-oxopentyl)-2-(3-pyridinyl)-, (S)-	568b, 1587, 4249		
58.		Piperidine, 1-(3-pyridinemethyl)-2-cyano-	4570a		
59.		Piperidine, 1-(3-pyridinemethyl)-2-cyano-4,5-didehydro-	4570a		
60.	71635-28-4	1-Piperidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)-		568b, 1156, 2497, 2566, 2567, 4090, 4249, 5811b	
61.	56078-09-2	1-Piperidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)- 	1578, 2220, 3491, 4249, 5811b	1578, 4249, 5811b	
62.	1202-34-2	2-Pyridinamine, *N*-2-pyridinyl-	441, 568b, 4249		
63.		Pyridine, 1-methyl-6-(2-pyridinyl)-1,2,5,6-tetrahydro-		2917a, 4249	
64.	68258-35-5	Pyridine-2-^{13}C-3-^{14}C, 3-fluoro-5-(2-piperidinyl)-, (±)-		2331, 4249	

TABLE 17.11 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Two or More Six-Membered *N*-Containing Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
65.	68245-76-1	Pyridine, 3-(1-ethyl-2-piperidinyl)-, (S)-	2767, 3553, 4249	4249, 4786a	
66.	24380-92-5 19730-04-2	Pyridine, 3-(1-methyl-2-piperidinyl)-, (S)- {*N*-methylanabasine} 	441, 568b, 761, 1371, 1580, 1702, 1734, 2224, 2767, 2775, 3255, 3398, 3410, 3444, 3491, 3553, 3557, 3559, 4249, 5811b	120, 568b, 1221, 1702, 1734, 2079, 2270, 2389, 2544, 2917a, 2939, 3444, 3491, 3260a, 3797, 3974a, 4098a, 4249, 5079, 5811b	
67.	1133-64-8 37620-20-5	Pyridine, 3-(1-nitroso-2-piperidinyl)-, (S)- {NAB} 	28–31, 174b, 174c, 239, 422, 423, 460, 478, 483, 484, 486, 568b, 572, 573, 576, 603, 688, 890, 895, 1148, 1193–1196, 1199–1200, 1216, 1217, 1304, 1373, 1386, 1445, 1559, 1566, 1567, 1567a, 1569–1571, 1576, 1578, 1584, 1653, 1672, 1696, 1702, 1725, 1727, 1732, 1736, 1740, 1741, 1751, 1753, 1773, 1808, 1842, 1870–1872, 1987, 1988, 2235, 2354, 2407, 2442, 2443, 2516, 2588, 2617, 2618, 2730, 2879, 3007, 3080, 3094, 3190, 3255–3257, 3265, 3300, 3302, 3308, 3313, 3342, 3343, 3370, 3943a, 3944–3946, 3992, 4010, 4011, 4059, 4078, 4128, 4249, 4319, 4547, 5008, 5049, 5494, 5531, 5569, 5679, 5692, 5811b, 5836	29, 33, 174c, 201, 324, 468, 478, 483, 484, 486, 505, 510, 557, 568b, 655, 720, 890, 895, 922, 995, 998, 1002, 1192, 1206a, 1216, 1566, 1567, 1567a, 1569–1571, 1575, 1578, 1579, 1584, 1679, 1696, 1702, 1725, 1727, 1732, 1870–1872, 1988, 2050–2052, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2637, 2638, 2700, 2724, 2822a, 2914, 3144a, 3176a, 3661, 3773, 3774, 3816, 3943a, 3943b, 3944–3948, 3973, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5063, 5531, 5584, 5811b	
68.		Pyridine, 3-(1-pentyl-2-piperidinyl)-,	1587, 4249		
69.	13078-04-1	Pyridine, 3-(2-piperidinyl)-	568b, 768b, 4249		
70.	34366-21-7	Pyridine, 3-(2-piperidinyl)-, (R)- {*d*-anabasine}	2921, 2922, 4249, 5811a		
71.	494-52-0	Pyridine, 3-(2-piperidinyl)-, (S)- {*l*-anabasine} 	174b, 397, 488, 489, 492, 493, 761, 830a, 1360, 1373, 1375a, 1567a, 1584, 1696, 1702, 1734, 1744, 1751, 1842, 1890, 1891, 2079, 2224, 2228, 2349, 2724, 2734, 2761, 2762, 2765, 2766, 2773, 2777, 2920–2922, 2939, 3054, 3056, 3057, 3059, 3302, 3308, 3444, 3477, 3491, 3499, 3505, 3559, 3742, 3797, 3972, 3999, 4249, 4319, 4407, 5034, 5079, 5205, 5512, 5811b	64, 120, 174b, 504, 548–550, 555a, 689, 830a, 984, 1013, 1015, 1075a, 1101, 1116, 1193–1196, 1199, 1221, 1324, 1327, 1567a, 1584, 1696, 1702, 1712, 1734, 1927, 1971, 2079, 2139, 2270, 2349, 2409a, 2724, 2746, 2914, 2917a, 2920, 2921, 2939, 3056, 3059, 3441a, 3444, 3459, 3460, 3477, 3491, 3499, 3511, 3608a, 3797, 3972–3974, 3974a, 3983a, 3999, 4236,	1360, 1375a

(*continued*)

TABLE 17.11 (continued)
Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke with Two or More Six-Membered *N*-Containing Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine, 3-(2-piperidinyl)-, (S)- {*l*-anabasine} (cont.)		4249, 5001, 5079, 5189, 5276, 5321, 5339, 5366, 5391, 5397–5399, 5406, 5573, 5582, 5685, 5727, 5804, 5811, 5811b, 5853, 5901, 5905, 17B32, 17B53, 17B54, 17B55	
72.		Pyridine, 3-(2-piperidinyl)-6-oxo- {6-oxoanabasine}		5079, 5222	
73.	78210-44-3	Pyridine, 3-(4-pyridinylmethyl)-	568b, 4249, 5811b		
74.		2(1*H*)-Pyridinone, 5-(2,3,4,5-tetrahydropyridinyl)- {2-pyridinol, 5-(2,3,4,5-tetrahydropyridinyl)-} 		1101, 4249	
75.	1148-79-4	2,2′:6′,2″-Terpyridine 	2217, 2220, 2224, 2228, 2601a, 3302, 3308, 3797, 4249	3797, 4249	
76.	494-04-2	3,2′:4′,3″-Terpyridine {nicotelline} 	568b, 1587, 2079, 2217, 2220, 2270, 2939, 3444, 4249, 5811b	120, 568b, 1971, 2079, 2217, 2220, 2224, 2283, 2939, 3444, 3491, 3974, 3983a, 4249, 5079, 5390a, 5312, 5332, 5382, 5811b, 17B23, 17B28	

of pyrazole, i.e., the nitrogen atom at position 1 is replaced by oxygen [Gilchrist (17D01)]. Oxazolidine and isoxazolidine are the reduced forms of oxazole and isoxazole, respectively. Several oxazolidine and isoxazolidine derivatives, e.g., oxazolidinediones and isoxazolidinones, have also been identified in tobacco and tobacco smoke. One other component identified in tobacco is related to the oxazoles and isoxazole. It is an oxadiazole derivative, *N*-(4-bromophenyl)-5-(1-naphthalenylmethyl)-1,3,4-oxadiazol-2-amine.

Benzoxazole is a heterocyclic aromatic organic compound with a fused benzene–oxazole ring structure. Benzoxazole (1-oxa-3-azaindene) and several alkylated benzoxazoles have been identified in tobacco smoke. Benzoxazoles found in tobacco smoke are believed to arise by the mutual condensation of the oxazole and benzene rings during the combustion/pyrolysis of tobacco (1884). The only substituted benzoxazole known in tobacco is residue from the organophosphate insecticide Phosalone®.

Oxazines are six-membered-ring analogs of piperazine where the nitrogen atom in position 4 is replaced by an oxygen atom. The oxazines in tobacco and tobacco smoke are morpholine and several morpholine derivatives. The most discussed morpholine recently is *N*-nitrosomorpholine (NMOR). This volatile *N*-nitrosamine (NMOR) has been identified in both tobacco and in tobacco smoke. Morpholine is an organic heterocycle that features both amine and ether functional groups. Morpholine is also called tetrahydro-1,4-oxazine. Figure 17.9 illustrates the parent structures of the oxazoles and oxazines identified in tobacco and tobacco smoke.

Numerous reviews have been written on the compounds identified in tobacco and/or tobacco smoke over the last five

TABLE 17.12
Tobacco and Tobacco Smoke Compounds with Six-Membered Rings, with a Five- and Six-Membered Ring, or with Two or More Six-Membered *N*-Containing Rings

Ring Type					
Six-Membered Ring with One or More Nitrogens	**No. of Compounds (No. of Agronomic Chemicals)**	**Pyridine Ring with a Second *N*-Containing Ring (Type)**	**No. of Compounds (No. of Agronomic Chemicals)**	**Compounds with Two or More Six-Membered *N*-Containing Rings (Type)**	**No. of Compounds (No. of Agronomic Chemicals)**
Piperidines	37	Pyrrolidine (nicotinoids)	72 (2)[a]	Piperidine + piperidine	1
Tetrahydropyridines	5	Pyrroline	2	Pyridine + piperidine (anabasine type)	15
Dihydropyridines	6	Pyrrole	19	Pyridine + pyridine (bipyridines)	39
Pyridines	341 (4)[b]	Imidazole	2 (1)[c]	Pyridine + di- or tetrahydropyridine (anatabine type)	16
Piperazines	10			2 Pyridines + piperidine	3
Dihydropyridazine	3 (3)[d]			3 Pyridines	2
Pyrazines	100 (1)[e]				
Pyrimidines	33 (4)[f]				
1,2,4-Triazines	2 (1)[g]				
1,3,5-Triazines	1 (1)[h]				
Totals	538		95		76

[a] Black Leaf 40 (insecticide).
[b] Chlorpyrifos® (insecticide), Chlorpyriphos® (insecticide), Nitrapyrin® (bactericide), Picloram® (herbicide).
[c] Admire® (insecticide).
[d] Maleic hydrazide and salts (herbicide).
[e] Thionazine® (insecticide).
[f] Pirimicarb® (insecticide), Pirimiphos-methyl® (insecticide), Dimetherimol® (fungicide), Diazinon® (insecticide).
[g] Metribuzin® (herbicide).
[h] Anilazine® (fungicide).

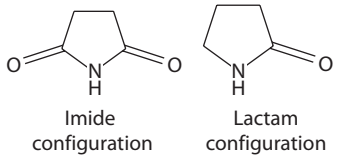


FIGURE 17.7 The imide and lactam configurations.

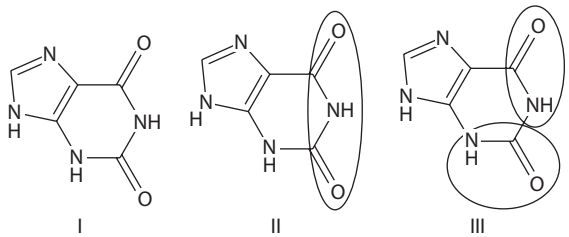


FIGURE 17.8 The imide {II} and lactam {III} configurations in 1,7-dihydro-6*H*-purine-2,6-dione (xanthine) {I}.

decades (1884, 1900, 1971, 2170, 2270, 2939, 3224, 3797). Few have listed the oxazole- and oxazine-related compounds identified in tobacco and tobacco smoke. Latimer (2270) in 1955 listed 231 compounds identified from tobacco and tobacco smoke. In his review, he listed tetrahydro-2-methyl-6-(3-pyridyl)-1,2-oxazine, a tobacco alkaloid, as the first oxazine identified in tobacco smoke. Roberts et al. in 1975 (3224) listed 2783 compounds identified in tobacco and tobacco smoke. In their report, five oxazole-related compounds identified in tobacco smoke were listed (2,4-dimethylbenzoxazole, 2-methylbenzoxazole, oxazolidinedione, 5-ethyl-*N*-methyl-2,4-oxazolidinedione, and 5-methyl-2,4-oxazolidinedione). Roberts et al. did not report any oxazole- or oxazine-related compounds found in tobacco. In 1980, Ishiguro and Sugawara (1884) listed 1889 identified tobacco smoke components in their monograph; only six oxazole-related compounds were listed (dimethyloxazole, 5-methyl-2,4-oxazolidinedione, 2,4-oxazolidinedione, 3,4,5-trimethylisoxazole, 2-methylbenzoxazole, and 2,5-dimethylbenzoxazole). The citations by Ishiguro and Sugawara for all but the dimethyloxazole were to the Schumacher et al. (3553) and Newell et al. (2769) reports on tobacco smoke composition. Roberts in 1988

TABLE 17.13
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

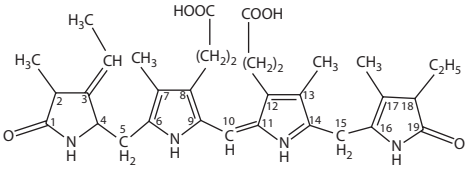
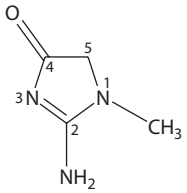
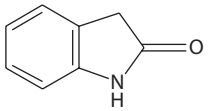
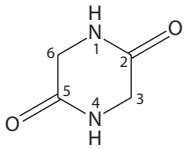
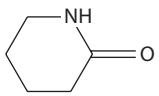
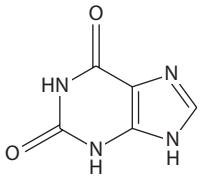
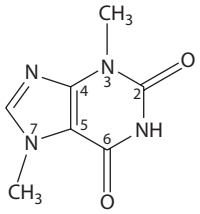
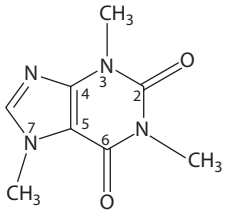
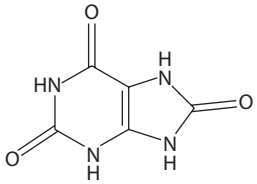
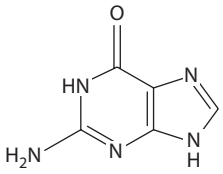
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	20298-86-6	21*H*-Biline-8,12-dipropanoic acid, 18-ethyl-3-ethylidene-1,2,3,19,22,24-hexahydro-2,7,13,17-tetramethyl-1,19-dioxo-, (2R,3E)- 		4249	
2.	70898-21-4	[2,3′-Bipyridin]-6′(1′*H*)-one, 3,4,5,6-tetrahydro-		4249, 4945	
3.	61892-75-9	4*H*-Imidazol-4-one, 1,5-dihydro-1-methyl-	568b, 3553, 4249, 5811b		
4.	60-27-5	4*H*-Imidazol-4-one, 2-amino-1,5-dihydro-1-methyl- {creatinine} 		751, 755, 756, 4249	
5.	59-48-3	2*H*-Indol-2-one, 1,3-dihydro- {phthalimidine; oxindole} 	568b, 1063–1066, 1068–1074, 1365, 1367, 2769, 3553, 4249, 4407		
6.	15379-45-0	2*H*-Indol-2-one, 1,3-dihydro-3-ethyl-	568b, 2766a, 4249		
7.	1504-06-9	2*H*-Indol-2-one, 1,3-dihydro-3-methyl-	3553		
8.	20200-86-6	2*H*-Indol-2-one, 1,3-dihydro-1,3,3-trimethyl-		2359, 2917a	
9.	40000-89-3	1,8-Naphthyridin-2(1*H*)-one, 3-methyl-	3553, 4249		
10.	106-57-0	2,5-Piperazinedione 	1351, 3553, 4249		
11.	5076-82-4	2,5-Piperazinedione, *N,N*-dimethyl-	568b, 3553, 4249		
12.	14771-77-8	2,5-Piperazinedione, 3-(1-methylethyl)-	3553, 4249, 5811b		
13.	61892-78-2	2,5-Piperazinedione, 3-(2-propenyl)-	568b, 3553, 4249, 5811b		
14.	5625-46-7	2,5-Piperazinedione, 3,6-dimethyl-	568b, 3553, 4249		
15.	5625-53-6	2,5-Piperazinedione, 3-methyl-	1351, 1364, 3410, 3553, 4249, 5811b		
16.	4526-77-6	2,5-Piperazinedione, 3-methyl-, (S)-	4249		
17.	27154-43-4	Piperidinone	1586		
18.	675-20-7	2-Piperidinone {5-pentanelactam} 	1371, 1375, 1375b, 1586, 1587, 2570, 2767, 2775, 3553, 4249, 5811b	2389, 2544, 3491, 3550, 4249, 5811b	
19.	61891-65-4	2-Piperidinone, methyl-	3553, 3557, 4249, 5811b		
20.	931-20-4	2-Piperidinone, 1-methyl-	568b, 2767, 3553, 4249, 5811b	404, 568b, 2386, 2389, 2544, 3491, 4249, 5811b	

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
21.	4775-98-8	2-Piperidinone, 6-methyl-	1586, 2767, 2769, 3557, 4249		
22.	69-89-6	1*H*-Purine-2,6-dione, 3,7-dihydro- {xanthine} 	5811b	429b, 2539, 2939, 4249	
23.	58-55-9	1*H*-Purine-2,6-dione, 3,7-dihydro-1,7-dimethyl-		568b, 4249	
24.	83-67-0	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- {theobromine} 	568b, 1375, 1375b, 2601a, 3255, 3257, 3265, 3553, 4249, 5811b	568b, 1204, 2313a, 4249	
25.	33073-01-7	1*H*-Purine-2,6-dione, 3,9-dihydro-1,9-dimethyl-	1587, 4249, 5811b		
26.	58-08-2	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine} 	568b, 1365, 1842, 3255, 3257, 3265, 3266, 3553, 4249, 5811b	568b, 1053, 3266, 4249, 4880	
27.		6*H*-Purine-2,6-dione, 1,7-dihydro-, C_3-alkyl-	1587, 4249		
28.	69-93-2	1*H*-Purine-2,6,8-trione, 7,9-dihydro- {uric acid} 	2170, 5079, 5456		
29.	73-40-5	6*H*-Purin-6-one, 2-amino-1,7-dihydro- {guanine} 	3797	120, 2270, 2539, 2939, 3491, 3797, 3973, 3974a, 4249, 5079, 5189, 5311, 5435	

(*continued*)

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

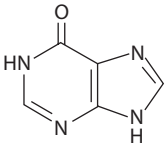
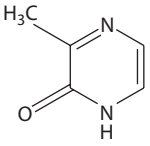
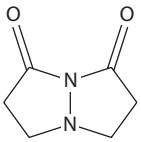
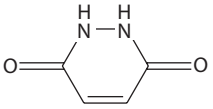
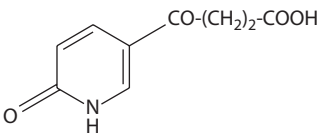
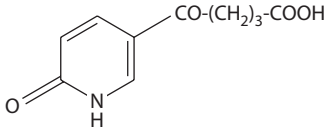
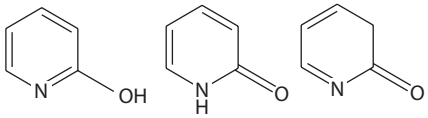
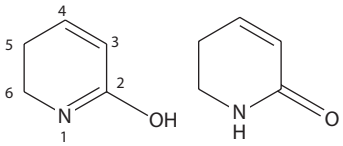
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
30.	68-94-0	6*H*-Purin-6-one, 1,7-dihydro- {hypoxanthine} 		2539, 2939	
31.	6270-63-9	2(1*H*)-Pyrazinone = 2-pyrazinol	568b, 4249		
32.	78210-68-1	2(1*H*)-Pyrazinone, 1-methyl-3-(1-methylethyl)-	568b, 1587, 4249, 5811b		
33.	19838-07-4	2(1*H*)-Pyrazinone, 3-methyl- 	568b, 1351, 1587a, 3553, 3559, 4249, 5811b	568b, 3649, 4249	
34.	20721-17-9	2(1*H*)-Pyrazinone, 5-methyl-	4249		
35.	20721-18-0	2(1*H*)-Pyrazinone, 6-methyl-	4249		
36.	61892-79-3	1*H*,7*H*-Pyrazolo[1,2-*a*]pyrazole-1,7-dione, tetrahydro- 	3553, 4249		
37.	123-33-1	3,6-Pyridazinedione, 1,2-dihydro- {maleic hydrazide; MH; MH-30} 	715, 716, 1333, 1470, 1507, 1580, 1741, 1744, 2384, 2385, 3300, 3493, 4249, 4274, 5512, 21A19	479, 480, 691,704, 715, 716, 905, 1147, 1333, 1473, 1474, 1580, 2277, 2383, 2385, 2906, 2907, 2939, 3493, 3585c, 3633, 3723, 3725, 3728, 3767a, 3811a, 3973, 3974b, 3977, 3998, 4236, 4249, 4269, 4271a, 4274, 5016, 5553, 5568, 5586, 5605, 5642, 5667, 5686, 5687, 5717, 5774, 5811b, 21A19	
38.	5716-15-4 21422-41-3	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt		3636, 4249, 5811b	
39.	51542-52-0	3,6-Pyridazinedione, 1,2-dihydro-, potassium salt		3636, 4249	
40.	15873-27-5	3-Pyridinebutanoic acid, 1,6-dihydro-γ,6-dioxo- 	4249	1110, 4249, 4709	

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
41.	71608-01-0	3-Pyridinepentanoic acid, 1,6-dihydro-δ,6-dioxo- 		1101, 4249, 4945	
42.	142-08-5 72762-00-6	2-Pyridinol {2(1*H*)-pyridinone} 	568b, 1124a, 1375, 1375b, 1586, 2724, 2767, 2773, 3553, 3557, 4249, 5811b	3974a, 4249	
43.	61892-76-0	2-Pyridinol, 5-acetyl-3,4-dihydro- {2(1*H*)-pyridinone, 5-acetyl-3,4-dihydro-}	568b, 3553, 4249		
44.	57147-25-8	2-Pyridinol, 3,4-dihydro- {2(1*H*)-pyridinone, 3,4-dihydro-}	2543, 2775, 3553, 3559, 4249		
45.	61892-77-1	2-Pyridinol, 3,6-dihydro- {2(1*H*)-pyridinone, 3,6-dihydro-}	568b, 2570, 3553, 4249		
46.	6052-73-9	2-Pyridinol, 5,6-dihydro- {2(1*H*)-pyridinone, 5,6-dihydro-; 2-piperidone, 3,4-dehydro-} 	568b, 1371, 1371, 1375, 1375b, 1586, 2387, 2545, 2570, 2761, 2762, 2765–2767, 2775, 3255, 3397, 3398, 3410, 3553, 3557, 3559, 4249, 5811b	568b, 2386, 2389, 2544, 3491, 3550, 4249	2387
47.		2-Pyridinol, 5,6-dihydro-3,6,6-trimethyl- {2(1*H*)-pyridinone, 5,6-dihydro-3,6,6-trimethyl-}		939, 4249	
48.	72692-83-2	2-Pyridinol, dimethyl- {2(1*H*)-pyridinone, dimethyl-}	3553, 4249		
49.	6456-92-4	2-Pyridinol, 1,3-dimethyl- {2(1*H*)-pyridinone, 1,3-dimethyl-}	3559, 4249		
50.	36330-90-2 95907-02-1	2-Pyridinol, 3,4-dimethyl- {2(1*H*)-pyridinone, 3,4-dimethyl-}	568b, 3553, 4249		
51.	3718-67-0	2-Pyridinol, 3,5-dimethyl- {2(1*H*)-pyridinone, 3,5-dimethyl-}	568b, 1371, 3553, 4249, 5811b		
52.	53428-02-7	2-Pyridinol, 3,6-dimethyl- {2(1*H*)-pyridinone, 3,6-dimethyl-}	568b, 3553, 4249, 5811b		
53.	16115-08-5	2-Pyridinol, 4,6-dimethyl- {2(1*H*)-pyridinone, 4,6-dimethyl-}	568b, 3553, 4249, 5811b		
54.	27992-31-0	2-Pyridinol, 5,6-dimethyl-	5811, 5811a, 5811b		
55.		2-Pyridinol, 3-ethyl- {2(1*H*)-pyridinone, 3-ethyl-}	568b, 4249		
56.	62003-48-9	2-Pyridinol, 5-ethyl- {2(1*H*)-pyridinone, 5-ethyl-}	568b, 4249		
57.	61892-99-7	2-Pyridinol, 6-ethyl- {2(1*H*)-pyridinone, 6-ethyl-}	568b, 2767, 4249		
58.	1003-56-1 91914-04-4	2-Pyridinol, 3-methyl- {2(1*H*)-pyridinone, 3-methyl-}	568b, 3553, 3559, 4249, 5811b		
59.	91914-05-5	2-Pyridinol, 4-methyl- {2(1*H*)-pyridinone, 4-methyl-}	568b, 4249		
60.	1003-68-5 91914-06-6	2-Pyridinol, 5-methyl- {2(1*H*)-pyridinone, 5-methyl-}	568b, 2543, 3553, 4249, 4407, 5811b		

(*continued*)

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

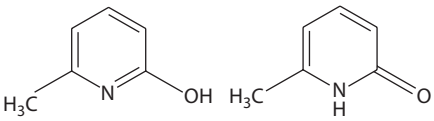
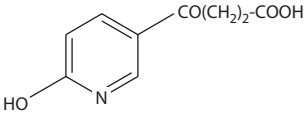
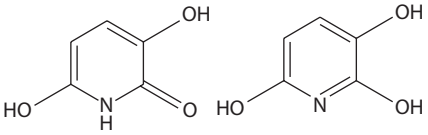
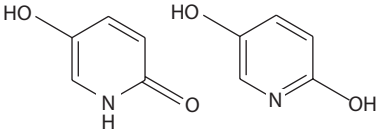
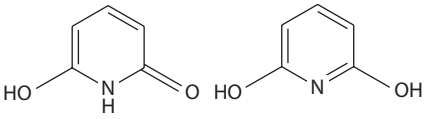
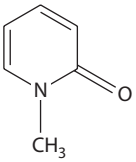
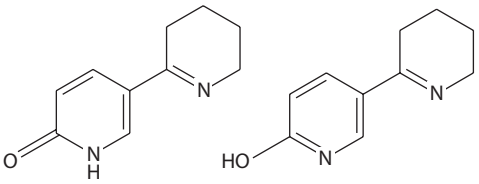
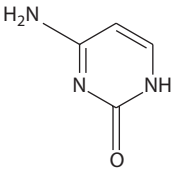
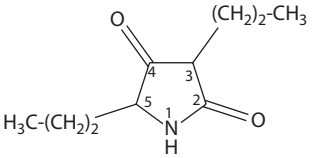
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
61.	3279-76-3	2-Pyridinol, 6-methyl- {2(1*H*)-pyridinone, 6-methyl-} 	568b, 1360, 1371, 1375a, 1586, 2761, 2762, 2765–2767, 2773, 2775, 3410, 3553, 4249, 5811b		1360, 1375a
62.	19006-81-6	2-Pyridinol, 4-phenyl- {2(1*H*)-pyridinone, 4-phenyl-}	642, 4249	642, 4249	
63.		2-Pyridinol-5-butanoic acid, γ-oxo- {2(1*H*)-pyridinone-5-butanoic acid, γ-oxo-} 		1101, 4249	
64.		2-Pyridinol-5-pentanoic acid, δ-oxo- {2(1*H*)-pyridinone-5-pentanoic acid, δ-oxo-}		1101, 4249	
65.	70969-38-9	2(1*H*)-Pyridinone, 5-(3,4-dihydro-2*H*-pyrrol-5-yl)- {2-pyridinol, 5-(3,4-dihydro-2*H*-pyrrol-5-yl)}		2226, 4249	
66.	39954-19-3	2(1*H*)-Pyridinone, 3,6-dihydroxy- {2,3,6-pyridinetriol} 		1101, 4249	
67.	5154-01-8	2(1*H*)-Pyridinone, 5-hydroxy- {2,5-pyridinediol} 		1101, 4249, 4918	
68.	626-06-2	2(1H)-Pyridinone, 6-hydroxy- {2,6-pyridinediol} 		1101, 4249, 4918	
69.	694-85-9	2(1*H*)-Pyridinone, 1-methyl- 	568b, 2767, 3553, 4249, 4570a, 5811b	404, 568b, 984, 2389, 2544, 4249	
70.	40316-88-9	2(1*H*)-Pyridinone, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {nicotone}	2224, 2228, 2724, 3308, 4249	2226, 4249, 4572	
71.	10516-09-3	2(1*H*)-Pyridinone, 5-(1-methyl-2-pyrrolidinyl)-,(S)-		554, 1101, 2226, 4249	
72.	1445-73-4	4(1*H*)-Pyridinone, 1-methyl-	568b, 4249		

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
73.		2-Pyridinol, 5-(2,3,4,5-tetrahydropyridinyl)-		1101, 4249	
					
74.	71-30-7	2(1*H*)-Pyrimidinone, 4-amino- {cytosine}	2539, 4249	120, 2270, 4249	
					
75.	34939-17-8	2(1*H*)-Pyrimidinone, 4,5-dimethyl-	3553, 4249		
76.	67383-34-0 3059-71-0	4(1*H*)-Pyrimidinone, 2,5-dimethyl-	3553, 4249, 5811, 5811a, 5811b		
77.	6622-92-0	4(1*H*)-Pyrimidinone, 2,6-dimethyl-	3553, 4249		
78.	34916-78-4	4(1*H*)-Pyrimidinone, 5,6-dimethyl-	3553, 4249		
79.	16858-16-5	4(1*H*)-Pyrimidinone, 6-methyl-2-propyl-	3559, 4249		
80.	121197-26-0	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-(2-methylpropyl)-	3429a, 4249	5811b	
81.	121197-16-8	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-propyl-	3429a, 4249	5811b	
82.	121197-27-1	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-bis(2-methylpropyl)-	3429a, 4249		
83.	121197-23-7	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dibutyl-	3429a, 4249	5811b	
84.	121197-14-6	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dipropyl-	3429a, 4249	5811b	
					
85.	121197-21-5	2*H*-Pyrrole-2,4(3*H*)-dione, 5-(2-methylpropyl)-3-propyl-	3429a, 4249	5811b	
86.	121197-24-8	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-(2-methylpropyl)-	3429a, 4249	5811b	
87.	121213-26-1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-propyl-	3429a, 4249	5811b	
88.	121197-25-9	2,4-Pyrrolidinedione, 3-butyl-5-propylidene-	3429a, 4249	5811b	
89.	121197-20-4	2,4-Pyrrolidinedione, 5-butyl-3-propylidene-	3429a, 4249	5811b	
90.	121197-28-2	2,4-Pyrrolidinedione, 3-butylidene-5-(2-methylpropyl)-	3429a, 4249	5811b	
91.	121197-18-0	2,4-Pyrrolidinedione, 3-butylidene-5-propyl-	3429a, 4249	5811b	
92.	121197-17-9	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-(2-methylpropylidene)-	3429a, 4249	5811b	
93.	121197-22-6	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-propylidene-	3429a, 4249	5811b	
94.	121197-19-1	2,4-Pyrrolidinedione, 3-(2-methylpropylidene)-5-propyl-	3429a, 4249	5811b	

(*continued*)

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

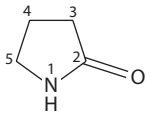
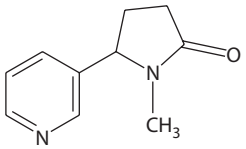
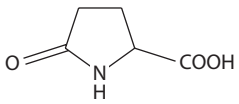
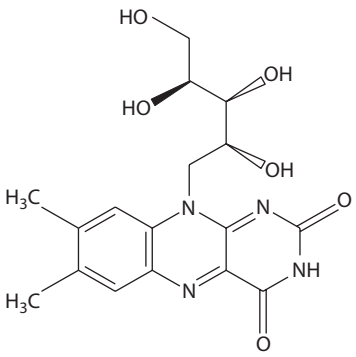
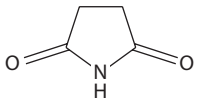
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
95.	121197-15-7	2,4-Pyrrolidinedione, 5-propyl-3-propylidene-	3429a, 4249	5811b	
96.	616-45-5	2-Pyrrolidinone {γ-butyrolactam} 	568b, 1350, 1354, 1371, 1375, 1375a, 1375b, 1586, 2545, 2570, 2761, 2765, 2766, 2773, 2775, 2857, 3255, 3386, 3398, 3410, 3553, 3557, 3559, 4249	568b, 2389, 2544, 3430, 3491, 3550, 3905, 3974a, 4249	1354, 1375a
97.	932-17-2	2-Pyrrolidinone, 1-acetyl-	568b, 4249		
98.		2-Pyrrolidinone, 1,?-dimethyl-	3553, 4249		
99.	5075-92-3	2-Pyrrolidinone, 1,5-dimethyl-	568b, 4249		
100.	88-12-0	2-Pyrrolidinone, 1-ethenyl-	568b, 4249		
101.	2687-91-4	2-Pyrrolidinone, 1-ethyl-	568b, 4249		
102.	872-50-4	2-Pyrrolidinone, 1-methyl-	568b, 2570, 2775, 3255, 3386, 3410, 3553, 3559, 4249, 5811b	404, 568b, 2339a, 2389, 2544, 3491, 3550, 3905, 4249, 5811b	
103.	2555-05-7	2-Pyrrolidinone, 3-methyl-	568b, 1360, 1375a, 1586, 2767, 3255, 4249		1360, 1375a
104.	2996-58-9	2-Pyrrolidinone, 4-methyl-	3559, 4249	2917a, 4249	
105.	108-27-0	2-Pyrrolidinone, 5-methyl-	568b, 2570, 2767, 3553, 4249, 5811b		
106.	75202-09-4	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-	3553, 4249	3797, 4249, 5811b	
107.	486-56-6	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, (S)- {cotinine} 	353, 437, 469a, 568b, 761, 830a, 1078, 1063–1066, 1068–1074, 1084, 1099, 1100, 1360, 1365, 1375a, 1567a, 1568, 1580, 1586, 1673, 1695, 1700, 1702, 1719, 1751, 2228, 2482, 2543, 2601a, 2724, 2761, 2762, 2765, 2767, 2773, 2775, 2799a, 2839, 2939, 3054, 3056, 3057, 3059, 3190, 3255, 3257, 3265, 3302, 3308, 3386, 3398, 3410, 3491, 3553, 3559, 3739–3742, 3972, 3992, 4249, 4407, 5035, 5508, 5565, 5811b	64, 120, 504, 553, 568b, 689, 830a, 984, 995, 998, 1012, 1226a, 1385, 1567a, 1568, 1702, 1712, 2338, 2359, 2724, 2917a, 2939, 2995, 3056, 3059, 3444, 3477, 3491, 3549, 3550, 3797, 3972–3974, 3974a, 4236, 4249, 4921, 5011, 5508, 5685, 5735, 5811b	1360, 1375a
108.	15569-85-4 36508-80-2	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, 1-oxide {cotinine 1-oxide}	2482, 4249		
109.	61892-90-8	2-Pyrrolidinone, 1-(2-oxopropyl)-	568b, 3553, 4249		
110.	5980-06-3	2-Pyrrolidinone, 5-(3-pyridinyl)-, (S)- {norcotinine}	568b, 2767, 3302, 3553, 3557, 3797, 4249, 5811b	568b, 3797, 4249, 4666, 5811b	
111.	98-79-3	5-Pyrrolidinone-2-carboxylic acid {5-oxoproline} 		2597a, 3052, 4249	
112.	54036-77-0	2*H*-Pyrrol-2-one	2387, 4249		2387
113.	61892-80-6	2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-3-ethyl-4-methyl-	568b, 3553, 4249		
114.		2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-4-ethyl-3-methyl-	568b, 4249		
115.	62003-47-8	2*H*-Pyrrol-2-one, 1,3-dihydro-5-(3-pyridinyl)-	568b, 2767, 4249		
116.	4031-15-6	2*H*-Pyrrol-2-one, 1,5-dihydro-	1360, 1375a, 4249		1360, 1375a

TABLE 17.13 (continued)
Lactams in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
117.	13950-21-5	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-		2917a, 4249	
118.	78210-72-7	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-5-(1-methylethylidene)-	568b, 1587, 4249, 5811b		
119.	4030-23-3	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4,5-trimethyl-	568b, 1365, 2767, 3553, 4249, 5811b		
120.	4030-22-2	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4-dimethyl-	568b, 1365, 2767, 2775, 3553, 4249, 5811b		
121.	51088-90-5	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-	568b, 3553, 4249, 5811b		
122.	4030-24-4	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-4-ethyl-	1063–1066, 1068–1074, 3553, 4249, 5811b		
123.		2*H*-Pyrrol-2-one, 1,5-dihydro-4,5-dimethyl-3-ethyl-	568b, 1063–1066, 1068–1074, 2775, 3553, 4249		
124.	27406-77-5	2*H*-Pyrrol-2-one, 1,5-dihydro-3-methyl-	568b, 2767, 2773, 2775, 3553, 3559, 4249, 5811b		
125.	766-36-9	2*H*-Pyrrol-2-one, 1,5-dihydro-3-ethyl-4-methyl-	568b, 1063–1066, 1068–1074, 3553, 3559, 4249, 5811b		
126.	78210-71-6	2*H*-Pyrrol-2-one, 1,5-dihydro-3-ethyl-5-methylene-	568b, 1586, 1587, 3559, 4249, 5811b		
127.	115600-67-4	2*H*-Pyrrol-2-one, 1,5-dihydro-4-ethyl-	3559, 4249		
128.	766-45-0	2*H*-Pyrrol-2-one, 1,5-dihydro-4-ethyl-3-methyl-	568b, 1063–1066, 1068–1074, 3553, 4249, 5811b		
129.	53598-99-5	2*H*-Pyrrol-2-one, 1,5-dihydro-4-methyl-	568b, 4249		
130.	19179-12-5	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-	568b, 3553, 4249, 5811b		
131.	19943-28-3 36357-32-1	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-methyl-, (3R-trans)-	568b, 3553, 4249, 5811b		
132.	5654-86-4	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	2601a		
133.	61949-29-9	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-propyl-	5811, 5811a, 5811b		
134.	26626-89-1	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-propyl-, (3S-trans)-	3553, 4249		
135.		Pyrrolo[1,2-*a*]pyrazine-1,4-dione, 3-(1-methylethyl)-	568b, 4249		
136.	61891-74-5	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, tetrahydro-	5811, 5811a, 5811b		
137.	83-88-5	Riboflavin 		120, 1941, 2270, 3973, 4249, 5079	
138.	146-17-8	Riboflavin 5′-(dihydrogen phosphate) 		4249, 4956	

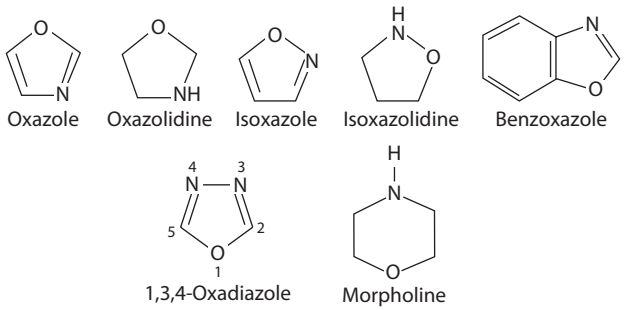


FIGURE 17.9 Parent structures of the oxazoles and oxazines identified in tobacco and tobacco smoke.

(3215) tabulated 5868 identified compounds in tobacco and tobacco smoke. By functional groups, 3044 compounds had been identified in tobacco, 3996 had been identified in smoke, and 1172 were identified in both tobacco and tobacco smoke. A large portion of the oxazole- and oxazine-related compounds in tobacco and tobacco smoke was originally identified by employees at the Research and Development Department of R.J. Reynolds Tobacco Company (RJRT) who were highly proficient in the isolation and identification of compounds in tobacco and tobacco smoke. From 1955 until 1988, they reported on 19 (of the 44) oxazole- and oxazine-related compounds in smoke and 6 (of the 14) oxazole- and oxazine-related compounds in burley, Maryland, flue-cured, Oriental, and Perique tobaccos (965, 1075, 1360, 1364, 1375a, 1586, 1587, 1590, 2270, 2337, 2339a 2761, 2762, 2765, 2766, 2767, 2769, 2775, 2777, 3547, 3549, 3550, 3553, 3557). Demole (4570a) at Firmenich [Geneva (Switzerland)], under contract to RJRT, identified 25 additional oxazoles in cigarette smoke condensate.

Oxazole- and oxazine-related compounds do not appear to be endogenous in green tobacco but are found in tobaccos that undergo heat treatments during curing and tobacco processing (965, 1590, 2337, 2339c, 2359). Additionally, it is known that in certain biomolecules, oxazoles can result from the cyclization and oxidation of serine or threonine nonribosomal peptides (17D02). Whether similar reactions occur in tobacco is not known. The Maillard or nonenzymatic browning reaction has generated much interest over the past 70 years [Nagodawithana (17D07)]. The Maillard reaction mainly involves the reaction of free amino groups of amino acids and reducing sugars (17D07). The principal chemistry of this reaction was reviewed by Hodge in 1953 (17D03). The aromas in most thermally processed foods, such as bread, cereal products, roasted peanuts, and roasted coffee, are generated during Maillard reactions [Maga (17D05, 17D06)]. Numerous heterocyclic compounds arising from the Maillard reaction have been identified in food and model systems. These heterocycles include furans, thiazoles, thiophenes, oxazoles, pyrroles, pyridines, and pyrazines (17D07). Several mechanisms have been proposed for the formation of oxazole- and oxazine-related compounds in food flavors, including the Strecker degradation (17D04). For example, hydroxy acid amides can react with acetone to produce oxazoles. Similar reaction products from the Maillard reaction and Strecker degradation are known in tobacco (965, 1590, 2337, 2339c, 2359).

Maga (17D06) has reviewed the occurrence of oxazoles and oxazolines in a variety of processed food systems. Most of them possess green, sweet, and nutty aroma qualities and have been identified in coffee, soy sauce, wheat, and cooked beef, and some of them have very low odor thresholds. In 1976, Leffingwell discussed how certain flavorants (reaction products) can be produced in tobacco and tobacco smoke (2337): "Because of the complexity of the chemical interactions and transformations involved, the types and ratios of active flavor products formed by nonenzymatic browning are dependent on the reaction conditions which may occur during aging or during the smoking process itself."

One of the flavorants discussed by Leffingwell (2337) that was identified in tobacco by Lloyd et al. (2389) was 3,4-dihydro-3-oxo-4-(phenylmethyl)-1*H*-pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde. This particular tobacco flavor has a hot peppery characteristic (2337). Leffingwell and Alford (2339a) and Li et al. (2359) have reported that 2,4,5-trimethyloxazole has a boiled beef, nutty, sweet, and green flavor in Perique and burley tobacco, respectively. The application of oxazole- and oxazine-related flavor compounds to tobacco is not normally undertaken because the flavor and aroma characteristics of these compounds are rather weak. No oxazole- or oxazine-related compound was included in either the Doull et al. list (1053) of individual flavor compounds used by one or more of the U.S. cigarette manufacturers or individual flavor compounds used outside the United States [see Tables 1 and 7A in (3266)].

Agrochemical residues containing an oxazole-related functionality that have been found on tobacco include Clomazone®, a broad spectrum herbicide; Phosalone, an organophosphate commonly used as an insecticide; and Vinclozolin®, a common fungicide. Dimethomorph® or Acrobat® is a common fungicide used on tobacco that contains morpholine functionality.

Analytical measurements for the determination and quantification of oxazole- and oxazine-related compounds in tobacco and tobacco smoke include gas chromatography (GC) with packed or capillary columns, high-performance liquid chromatography (HPLC) usually with reverse phase (RP) columns, and mass spectrometry (MS) methods (GC-MS and LC-MS).

Table 17.14 lists the distribution of oxazole- and oxazine-related compounds identified in tobacco and tobacco smoke. A total of 63 compounds have been identified: 9 are benzoxazole derivatives, 4 are isoxazole derivatives, 30 are oxazole derivatives, 4 are oxazolidine derivatives, and 9 are morpholine derivatives. Fifteen of the compounds are found in tobacco, 51 are found in tobacco smoke, and only 3 have been reported in both tobacco and tobacco smoke. Table 17.15 lists the 63 oxazole- and oxazine-related compounds identified in tobacco and/or tobacco smoke.

TABLE 17.14
Distribution of Oxazole- and Oxazine-Related Compounds Identified in Tobacco and Tobacco Smoke

Oxazole-Related Compounds	Total No. of Compounds	Smoke	Tobacco	Both	Agrochemical Product
Benzoxazole	9	8	1	0	1
Isoxazole	5	2	3	0	1
Oxazole	35	34	2	1	0
Oxazolidine	5	4	1	0	1
Morpholine	9	3	8	2	1
Total	63	51	15	3	4

17.5 AZA-ARENES

An aza-arene was defined as a fused-ring compound with two or more fused rings and consisting only of carbon, hydrogen, and nitrogen. Alkyl-substituted derivatives were also included in the aza-arene category. Overall, many of the aza-arenes are structurally comparable to the polycyclic aromatic hydrocarbons (PAHs) but include at least one nitrogen in the ring. In his early 1954 compilation of reported tobacco smoke components, Kosak (2170) listed no fused-ring polycyclic nitrogen compounds in tobacco smoke, the class of compounds subsequently termed the aza-arenes. Five years later, the only fused-ring *N*-heterocyclic compound listed by Johnstone and Plimmer (1971) as a tobacco smoke component was the bicyclic compound quinoline. Except for the replacement of a –CH═ linkage with a nitrogen (–N═) at the 1 position, quinoline is structurally similar to the PAH naphthalene (Figure 17.10). However, the reference cited by Johnstone and Plimmer was to the 1929 study by Gabelya and Kipriyanov (1263) who described the identification of quinoline in a "destructive distillate" of tobacco not in a sample of tobacco smoke prepared by a tobacco smoking procedure. A similar identification of benzo[*a*]pyrene (B[*a*]P) in the destructive distillate of tobacco by Roffo (3323, 3325) was criticized by Wynder and Hoffmann (4319, 4332) who asserted that a tobacco destructive distillate was not tobacco smoke.

In 1960, Van Duuren et al. (4027), in an extension of their studies on the tumorigenic PAHs in mainstream cigarette smoke condensate (CSC), described their findings on tumorigenic *N*-heterocyclic compounds in the CSC. They reported the identification of dibenz[*a,h*]acridine {I}, dibenz[*a,j*]acridine {II}, and 7*H*-dibenzo[*c,g*]carbazole {III} (Figure 17.11) in CSC at per cigarette levels of 0.1, 2.7, and 0.7 ng, respectively. These levels were substantially less than that of the reported per cigarette yield of B[*a*]P in the late 1950s or early 1960s. Similar to the situation noted earlier that quinoline is a nitrogen analog of naphthalene, dibenz[*a,h*]acridine {I} is a nitrogen analog of dibenz[*a,h*]anthracene (DB[*a,h*]A) {IV}. These two compounds are dimensionally similar. Over five decades ago, these three *N*-heterocyclics had been reported as tumorigenic to mouse skin [cf. summary by Hartwell (1544)]. Two of these compounds, dibenz[*a,h*]acridine and dibenz[*a,j*]acridine, were also reported by Van Duuren et al. to be present in the pyrolysates (750°C, nitrogen atmosphere) from both nicotine and pyridine.

Contradictory findings have been reported on the presence or absence of these three *N*-heterocyclic compounds; e.g., Wynder and Hoffmann (4319, 4332) reported that members of their research group—Candeli et al. (587)—were able to confirm the presence of dibenz[*a,j*]acridine but not dibenz[*a,h*]acridine in mainstream CSC. The per cigarette yield of dibenz[*a,j*]acridine reported by Candeli et al. was significantly greater than that reported by Van Duuren et al. (4027) [cf. 10.0 ng/cig *vs.* 2.7 ng/cig]. Other than brief mentions by Wynder and Hoffmann (4319, 4332) of the results obtained by Candeli et al. (587) on dibenz[*a,j*]acridine in CSC, the experimental procedures involved in its identification do not appear to have been published in the usual way in a peer-reviewed journal. At a mainstream smoke (MSS) yield for dibenz[*a,j*]acridine of 2.7 or 10.0 ng/cig as reported by Van Duuren et al. and Candeli et al., respectively, it is difficult to understand why no confirmation of the presence of this aza-arene has been reported by highly competent investigators from the early 1960s through the mid-1990s! Similarly, no confirmations of the presence of dibenz[*a,h*]acridine or 7*H*-dibenzo[*c,g*]carbazole have been presented to date. Studies on these and other aza-arenes in cigarette MSS or nicotine pyrolysates are described briefly in the following paragraphs. The question remains as follows: Was the preliminary isolation procedure (vacuum distillation of the smoke condensate at 100°C, 0.5 mm pressure) used by Van Duuren et al. (4027) responsible for the formation of the dibenzacridines and the dibenzocarbazole?

In 1970, Kaburaki et al. (2006) reported the results of their detailed study of the pyrolysis of nicotine at various temperatures in air and in an inert atmosphere (nitrogen). They did not report the identification of the two tumorigenic benzacridines reported previously by Van Duuren et al. (4027) as identified components in their nicotine pyrolysates.

TABLE 17.15
Oxazole- and Oxazine-Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

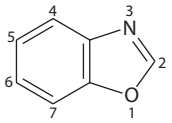
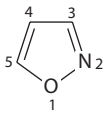
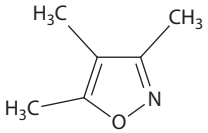
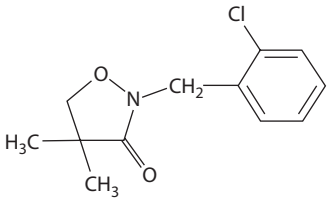
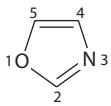
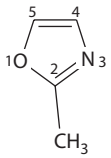
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Oxazole-related compounds					
1.	273-53-0	Benzoxazole {1-oxa-3-azaindene} 	568b, 1587, 4249, 5811b		
2.		Benzoxazole, C_2-alkyl-	568b, 1587, 4249		
3.	72692-90-1	Benzoxazole, 2,4-dimethyl-	568b, 1586, 1587, 2767, 3224, 3557, 4249		
4.	5676-58-4	Benzoxazole, 2,5-dimethyl-	568b, 2767, 2769, 3553, 3557, 3733–3735, 3750, 3752, 4249		
5.	72692-91-2	Benzoxazole, 4,6-dimethyl-	568b, 1587, 4249, 5811b		
6.	78210-58-9	Benzoxazole, 5,7-dimethyl-	568b, 1164, 1587, 4249, 5811b		
7.	78210-57-8	Benzoxazole, 7-ethyl-	568b, 1587, 4249, 5811b		
8.	95-21-6	Benzoxazole, 2-methyl-	568b, 1360, 1375a, 1586, 1884, 2761, 2762, 2765–2767, 2769, 2775, 3224, 3553, 3557, 3733–3735, 3750, 3752, 4249, 5811b		1360, 1375a
9.	288-14-2	Isoxazole 		2917a	
10.	300-87-8	Isoxazole, 3,5-dimethyl-		568b, 2917a, 4249	
11.	5765-44-6	Isoxazole, 5-methyl-	568b, 4249		
12.	10557-82-1	Isoxazole, trimethyl- = isoxazole, 3,4,5-trimethyl- 	568b, 1360, 1375a, 2761, 2762, 2765, 2766, 2769, 2777, 4249		1360, 1375a
13.	81777-89-1	3-Isoxazolidinone 2-[(2-chlorophenyl) methyl]-4,4-dimethyl- {Clomazone®} 		2913a, 3633	
14.	60918-97-0	1,3,4-Oxadiazol-2-amine, *N*-(4-bromophenyl)-5-(1-naphthalenylmethyl)-		4249	
15.	288-42-6	Oxazole 	568b, 4249		

TABLE 17.15 (continued)
Oxazole- and Oxazine-Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
16.		Oxazole, 2-butyl-4,5-dimethyl-	4570a		
17.		Oxazole, 5-butyl-2,4-dimethyl-	4570a		
18.		Oxazole, 2-butyl-4-methyl-	4570a		
19.		Oxazole, 4-butyl-2-methyl-	4570a		
20.	7208-05-1	Oxazole, 2,4-dimethyl-	568b, 4249, 4570a, 4800		
21.	33318-74-0	Oxazole, 2,4-dimethyl-5-ethyl-	568b, 4249, 4570a		
22.		Oxazole, 2,4-dimethyl-5-(2-methylpropyl)-	4570a		
23.		Oxazole, 2,4-dimethyl-5-propyl-	4570a		
24.	23012-11-5	Oxazole, 2,5-dimethyl-	568b, 1075, 1364, 1587, 4249, 5811b		
25.		Oxazole, 2,5-dimethyl-4-ethyl-	4570a		
26.		Oxazole, 2,5-dimethyl-4-(2-methylpropyl)-	4570a		
27.	20654-94-8 20662-83-3	Oxazole, 4,5-dimethyl-	568b, 1075, 1364, 1370, 1590, 4240, 4570a		
28.	53833-30-0	Oxazole, 4,5-dimethyl-2-ethyl-	4570a		
29.		Oxazole, 4,5-dimethyl-2-(1-methylpropyl)-	4570a		
30.		Oxazole, 4,5-dimethyl-2-(2-methylpropyl)-	4570a		
31.	24667-03-6	Oxazole, 2-ethyl-4-methyl-	568b, 4570a		
32.	42463-54-7	Oxazole, 2-ethyl-5-methyl-	568b, 4570a		
33.	53833-20-8	Oxazole, 4-ethyl-2-methyl-	568b, 4249		
34.	53833-28-6	Oxazole, 4-ethyl-5-methyl-	568b, 4249		
35.	53833-29-7	Oxazole, 5-ethyl-2-methyl-	568b, 4249		
36.	29584-92-7	Oxazole, 5-ethyl-4-methyl-	568b, 4249		
37.	23012-10-4	Oxazole, 2-methyl- 	1371, 1590, 4239, 4570a		
38.		Oxazole, 2-(2-methylpropyl)-	4570a		
39.		Oxazole, 2-(3-methylbutyl)-	4570a		
40.		Oxazole, 2-methyl-4-(2-methylpropyl)-	4570a		
41.		Oxazole, 4-(2-methylpropyl)-	4570a		
42.		Oxazole, 4-methyl-2-(2-methylpropyl)-	4570a		
43.		Oxazole, 4-methyl-5-(2-methylpropyl)-	4570a		
44.		Oxazole, 4-methyl-2-propyl-	4570a		
45.	27744-95-2	Oxazole, 4-methyl-5-propyl-	4570a		
46.	53833-31-1	Oxazole, 5-methyl-2-propyl-	568b, 4249		
47.		Oxazole, 4-pentyl-	4570a		
48.	20662-84-4	Oxazole, trimethyl- = 2,4,5-trimethyloxazole	568b, 4249, 4570a	568b, 2339a, 2359, 4249	
49.	2346-26-1	2,4-Oxazolidinedione	568b, 1884, 3224, 3553, 3557, 4249, 5811b		

(*continued*)

TABLE 17.15 (continued)
Oxazole- and Oxazine-Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

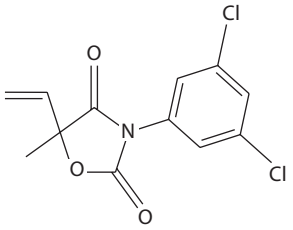
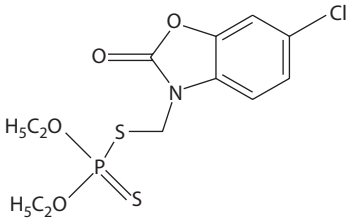
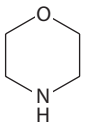
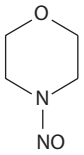
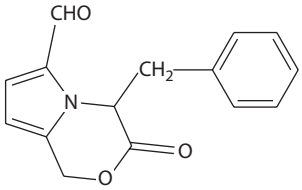
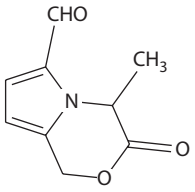
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
50.	50471-44-8	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- {Vinclozolin®} 		2650a	
51.		2,4-Oxazolidinedione, 5-ethyl-1-methyl-	3224, 3553, 3557, 4249		
52.	27770-23-6	2,4-Oxazolidinedione, 5-methyl-	568b, 1884, 3224, 3553, 3557, 4249, 5811b		
53.	58628-98-1	2-Oxazolidinone, 4.5-dimethyl-	568b, 4249		
54.	2310-17-0	Phosphorodithioic acid, *S*-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl)methyl] *O,O*-diethyl ester {Phosalone®} 		3381, 4271a	
		Oxazine-related compounds			
55.	110-91-8	Morpholine 		568b, 3973, 4249	
56.	110488-70-5	Morpholine, 3-(3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl)- (Dimethomorph®; Acrobat®)		2892a, 3633	
57.	147688-58-2	Morpholine, 2,2-dimethyl-		3951	
58.	59-89-2	Morpholine, 4-nitroso- {*N*-nitrosomorpholine (NMOR)} 	31, 126a, 203, 471, 478, 485, 510, 746c, 1058, 1059, 1727, 1842, 2442, 2443, 3255, 3257, 4010, 4011, 5811b	468, 478, 498, 510, 1217, 1727, 1740, 1741, 1773, 3256, 3265, 3300, 3973, 3974b, 4010, 4011, 4249, 5001, 5496, 5811b	
59.	70699-77-3	3-Morpholinepropanamide, 2-oxo-6-(1,2,3,4-tetrahydroxybutyl)-, [3S-[3α,6α(1R*,2S*,3S*)]]-		1863a	

TABLE 17.15 (continued)
Oxazole- and Oxazine-Related Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
60.	15769-88-7	2*H*-1,2-Oxazine, tetrahydro-2-methyl-6-(3-pyridinyl)-, (-)-{MPTO}	568b, 1587, 2270, 2761, 4249, 5811b	568b, 2270, 3547, 3549, 3550, 4249	
61.	71607-95-9	2*H*-1,2-Oxazine, tetrahydro-3-(1-methylethyl)-6-(3-pyridinyl)-	568b, 1587, 4249, 5811b		
62.	60026-28-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-3-oxo-4-(phenylmethyl)- 		965, 2337, 2389, 2544, 3491, 4249	
63.	35674-33-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde,3,4-dihydro-4-methyl-3-oxo- 		965, 2544, 3491, 4249, 5811b	

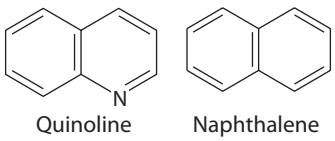


FIGURE 17.10 Quinoline and naphthalene.

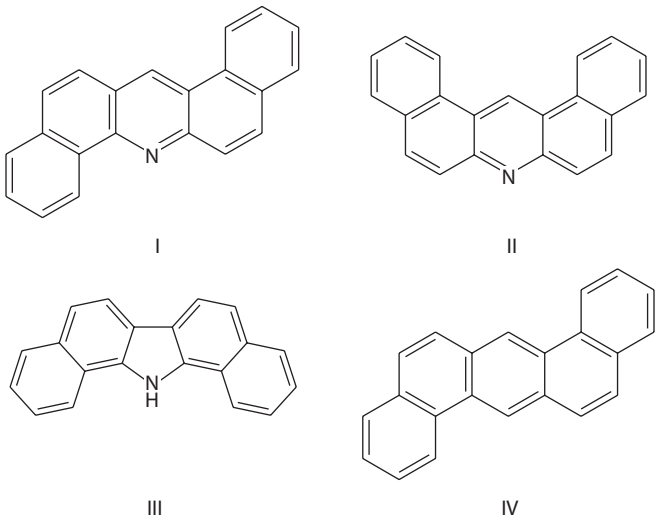


FIGURE 17.11 Some polycyclic components of tobacco smoke.

From their study of the pyrolysis of several nitrogenous components of tobacco, including nicotine, Schmeltz et al. (3499) reported:

> We could not detect benzo(a)pyrene in nicotine pyrolyzates, nor could we confirm the presence of the physiologically active dibenzacridines and dibenzcarbazole [sic] reported in tobacco smoke and in nicotine and pyridine pyrolyzates by Van Duuren [4027].

In their review of the pyrogenesis of tobacco smoke components, Chortyk and Schlotzhauer (722) emphasized these reported findings, i.e., the failures of several groups of investigators to confirm the presence of the two dibenzacridines and the 7*H*-dibenzo[*c*,*g*]carbazole in nicotine pyrolysates. They wrote:

> Since nicotine is the most abundant and best known tobacco alkaloid, its pyrolysis has been thoroughly studied [Woodward et al. (4275a), Jarboe and Rosene (1923a)]. More recent work [Kaburaki et al. (2006)] on the pyrolysis of nicotine and various alkyl-pyridines has resulted in a proposed mechanism for the thermal degradation of nicotine…Schmeltz [Schmeltz et al. (3499)] also studied nicotine and identified a number of previously unreported compounds in the nicotine pyrolysates… These included pyrrole, acenaphthene, indole, skatole, and anthracene and/or phenanthrene. However, the presence of dibenzacridines and dibenzcarbazole, previously reported in nicotine and pyridine pyrolysates, could not be confirmed [Van Duuren et al. (4027)].

Schmeltz and Hoffmann (3491) in their review of the *N*-containing components of tobacco and tobacco smoke discussed the generation of various pyridines from nicotine during both the actual smoking process and pyrolysis. Schmeltz and Hoffmann did report the identification by Van Duuren et al. (4027) of the two dibenzacridines in cigarette smoke and nicotine pyrolysate. They did not, however, comment on the reports issued between 1960 and 1977 of the inability of several other groups of investigators [Candeli et al. (587), Kaburaki et al. (2006), Schmeltz et al. (3499)] to confirm the 1960 findings of Van Duuren et al. (4027).

In 1979, Schmeltz et al. (3512) reported their results from an elaborate study on the fate of radiolabeled nicotine during pyrolysis and during the actual smoking of a radiolabeled nicotine-treated cigarette. Their major findings included the following: (1) Under combustion–tube pyrolysis conditions, nicotine in either silica gel matrix (pyrolysis temperatures at 600°C, 750°C, or 900°C) or tobacco matrix (pyrolysis temperature at 600°C) underwent extensive degradation to a mixture of pyridines, quinolines, arylnitriles, and aromatic hydrocarbons. (2) In a burning cigarette during actual smoking, a substantial portion of the nicotine (about 41%) remains intact, 12.5% is oxidized to carbon dioxide, as much as 11% is degraded to volatile alkylpyridines, and negligible amounts are converted to neutral or acidic components of the particulate phase. (3) Dibenz[*a,h*]acridine and dibenz[*a,j*]acridine reported nearly two decades earlier by Van Duuren et al. (4027) were not identified in this study by Schmeltz et al. (3512). They noted:

> In ongoing studies* we are now identifying those compounds that are formed from nicotine only as minor compounds (<0.1%) which nevertheless can contribute to the toxicity of the smoke. To this group of minor smoke constituents having nicotine as a precursor belong the dibenzacridines [Van Duuren et al. (4027)]…

(4) From the experimental results, the authors reached the following conclusion: "Pyrolysis experiments may be of limited value for establishing the fate of nicotine and possibly other tobacco components in a burning cigarette." (5) The pyrolysis system used in this study [cf. Higman et al. (1648)] was designed, according to Higman et al., to be the optimum simulation of the smoking process. Obviously, nicotine did not behave in this pyrolysis system as it did in the burning cigarette during actual smoking.

Critical examination of the text and the conclusions expressed in the 1979 Schmeltz et al. publication on the fate of nicotine during pyrolysis and during actual smoking reveals that at least two of the authors (Hoffmann, Schmeltz) have definitely changed their opinion with regard to their long-held view on the supposed equivalence of compound behavior during pyrolysis and actual smoking; e.g., Wynder and Hoffmann (4332) earlier wrote in support of this equivalence:

> Most pyrolysis studies with tobacco, tobacco extracts, extract fractions, individual components, and tobacco additives are performed in a nitrogen atmosphere. This procedure has often been criticized on the grounds that many of the toxic constituents formed during smoking of tobacco products occur as a result of combustion in air rather than in a nitrogen atmosphere. This criticism, however, cannot be maintained in view of studies by Newsome and Keith [2780] which demonstrated that a reducing rather than an oxidizing atmosphere exists at the cone region of a burning cigarette.

With regard to the dibenzacridines and the dibenzocarbazole from nicotine during pyrolysis and the smoking process, Table 17.16 summarizes the current state of knowledge.

For example, authors of numerous articles in the 1980s [Hoffmann and Wynder (1808)], in the 1990s [Hoffmann and Hecht (1727), Hoffmann et al. (1773), Occupational Safety and Health Administration (OSHA) (2825), Hoffmann and Hoffmann (1740, 1741)], and in the 2000s [Hoffmann and Hoffmann (1743), Hoffmann et al. (1744), and Fowles and Bates (1217)] on the toxicants in tobacco and tobacco smoke repeatedly listed dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole as tumorigenic or adversely biologically active MSS components despite the following: (1) The presence of these three aza-arenes in MSS had not been confirmed in several investigations conducted between 1963 and 1990 (3260). (2) Between 1990 and 2000, additional studies failed to confirm their presence in MSS (2021, 3414). (3) Several summaries of the attempts to confirm the findings of Van Duuren et al. have been published (172, 3260, 3265). In 2002, Rustemeier et al. (3370) did report the presence of dibenz[*a,j*]acridine in the MSSs from several ingredient-treated cigarettes. All yields were reported as less than 2.72 ng/cig. It might have been appropriate in view of the Rustemeier et al. to have provided more meaningful information on its presence.

Other tumorigens in cigarette MSS, including several the presence of which was and is suspect, have been listed since the early 1960s.

In 1960, Mold et al. (2592) reported the isolation and identification of the tricyclic *N*-heterocyclic 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) {V} (Figure 17.12) from CSC and demonstrated its relationship to its precursor in tobacco, the amino acid proline. Obviously, pyrocoll is not an aza-arene but an amide. Rodgman and Cook (3279) reported the identification of indole, carbazole, and several alkylated indoles and carbazoles in CSC and confirmed the presence of 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) {V} described previously by Mold et al. (2592). Rodgman and Cook also assessed previously reported biological studies on indole, 3-methylindole (skatole), and carbazole: none was reported to be tumorigenic in laboratory animals [Hartwell (1544), Shubik and Hartwell (3664)].

Poindexter and Carpenter (2972) identified 9*H*-pyrido [3,4-*b*]indole (norharman) {VI} and 1-methyl-9*H*-pyrido [3,4-*b*] indole (harman) {VII} (Figure 17.12) isolated from CSC.

* No report of the confirmation of the presence of the dibenzacridines (or the dibenzocarbazole) as a result of these ongoing studies has been found to date.

TABLE 17.16
Dibenz[*a,h*]acridine {I}, Dibenz[*a,j*]acridine {II}, and 7*H*-Dibenzo[*c,g*]carbazole {III} in Nicotine Pyrolysates (Pyr) and Mainstream CSC

	Dibenz[*a,h*]acridine		Dibenz[*a,j*]acridine		7*H*-Dibenzo[*c,g*]carbazole	
Investigators	**Pyr**	**CSC**	**Pyr**	**CSC**	**Pyr**	**CSC**
Van Duuren et al. (4027)	Yes	Yes	Yes	Yes	No	Yes
Candeli et al. (587); Wynder and Hoffmann (4319, 4332)	NE	No	NE	Yes	NE	NE
Kaburaki et al. (2006)	No	NE	No	NE	NE	NE
Schmeltz et al. (3499)	No	NE	No	NE	No	NE
Schmeltz et al. (3512)	No	No	No	No	No	No
Snook (3733)	NE	No	NE	No	NE	No
Snook et al. (3750)	NE	No	NE	No	NE	No
Grimmer et al. (1409)	NE	No	NE	No	NE	No
Kamata et al. (2021)	NE	No	NE	No	NE	NE
Sasaki and Moldoveanu (3414)	NE	No	NE	No	NE	NE
Rustemeier et al. (3370)	NE	No	NE	Yes	NE	NE

Yes, compound identified; No, compound not found or identified; NE, substrate not examined for compound in question.

Examination of these results indicates that Van Duuren et al. (4027) reported the identification of the three *N*-heterocyclic compounds {I, II, and III} in MS CSC and two of them {I and II} in a nicotine pyrolysate, whereas Candeli et al. (587) failed to identify {I} but did identify {II} in MS CSC. The 1963 Candeli et al. findings on {II} in MS CSC were not confirmed in 1979 by investigators (3512) from the same laboratory: Hoffmann participated in both the 1963 and 1979 studies. Two studies (3499, 3512) confirmed the 1960 report by Van Duuren et al. that 7*H*-dibenzo[*c,g*]carbazole {III} was not present in a nicotine pyrolysate.

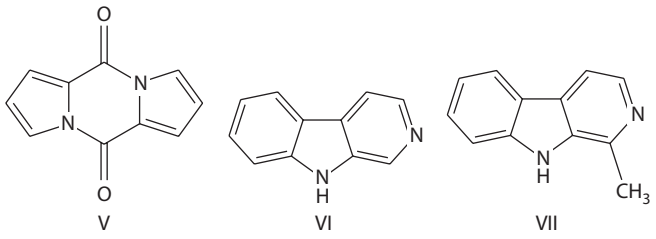


FIGURE 17.12 Some amino-acid-derived *N*-heterocyclics identified in tobacco smoke.

They reported the yield of the total harmans in burley and flue-cured smokes to be between 15 and 20 µg/g of tobacco smoked, values 40–50 times that of the total harmans in the unsmoked tobaccos. Since the weight of tobacco in cigarettes sold at that time approximated 1 g, the delivery of these two compounds was about 15–20 µg/cig. They concluded from experiments with radiolabeled tryptophan that the harmans (found to be radiolabeled in the smoke) were generated pyrogenetically from a reaction between aldehydes (formaldehyde for norharman, acetaldehyde for harman) and the tryptophan in tobacco. Schmeltz et al. (3505) reported 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) {V}, 9*H*-pyrido[3,4-*b*]indole (norharman) {VI}, and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) {VII} in tobacco smoke. Testa and Testa (3886, 3887) also confirmed the presence of 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) in CSC.

In 1964, the Advisory Committee to the U.S. Surgeon General (3999) briefly discussed only four fused-ring *N*-heterocyclic compounds in tobacco smoke: quinoline plus the two dibenzacridines (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine) and the dibenzocarbazole (7*H*-dibenzo[*c,g*]carbazole) reported by Van Duuren et al. (4027).

In his 1968 review of tobacco and tobacco smoke composition, Stedman (3797) discussed the identification of tumorigenic *N*-heterocyclic compounds [dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]carbazole] reported by Van Duuren et al. (4027) as well as the identification of the following *N*-heterocyclic compounds: 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), 9*H*-pyrido[3,4-*b*]indole (norharman), 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), and 9*H*-pyrido[2,3-*b*]indole.

In his early 1970s outline of recent research on tobacco and tobacco smoke composition, Wakeham (4103) noted the reported presence of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) in cigarette smoke and discussed their possible formation by reaction of tryptophan and an aldehyde. As noted by Rodgman (3253a), the structure of the aldehyde reacting with tryptophan ultimately dictates the structure of alkylated norharmans found in CSC (see Table 17.17).

In addition to 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), Izard et al. (1899) reported the identification of its homolog methyl-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (methylpyrocoll) in CSC.

During a presentation at the 1975 TCRC and in a 1977 publication on their study of the water-soluble portion of CSC, Schumacher et al. (3553) reported the identifications of 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (octahydropyrocoll), and 2-ethyl-9*H*-pyrido[2,3-*b*]indole.

TABLE 17.17
Chronology of Selected Aza-Arenes: Dibenz[*a,h*]acridine, Dibenz[*a,j*]acridine, 7*H*-Dibenzo[*c,g*]carbazole, Quinoline

Year	Event
1929	Gabelya and Kipriyanov (1263) reported the identification of quinoline in a destructive distillate from tobacco. Destructive distillation of tobacco is not considered to be equivalent to the tobacco smoking process [see comments by Wynder and Hoffmann (4319, 4332)]
1935	Barry et al. (194) (members of the Kennaway group in the United Kingdom) compared the tumorigenicity of dibenz[*a,h*]anthracene (DB[*a,h*]A) with that of heterocyclic compounds in which one or both of the *meso*-carbons were replaced by nitrogen. The aza-arene dibenz[*a,h*]acridine was found to be less tumorigenic (mouse skin) than its PAH counterpart DB[*a,h*]A. They also reported that the tumorigenicity of dibenz[*a,j*]acridine was less than that of dibenz[*c,h*]acridine
1937	In the first reported investigation of the tumorigenicity of 7*H*-dibenzo[*c,g*]carbazole, Boyland and Brues (421a) reported that mice skin painted with it developed carcinomas at the painting site
1937	Bachmann et al. (137a) reported that dibenz[*a,j*]acridine injected subcutaneously induced sarcomas in mice; i.e., dibenz[*a,j*]acridine was sarcogenic. Its sarcogenicity was relatively weak compared to that noted for similarly injected PAHs
1940	Badger et al. (140) reported that oral administration to 10 mice of 5 mg/week/mouse of dibenz[a,h]acridine resulted in one mouse with an epithelioma and papilloma of the forestomach; another mouse showed stomach papillomas. Duration of the experiment was 627 days Similar administration of dibenz[a,j]acridine (10 mice, 5 mg/week/mouse) gave no tumors in 572 days. In their introduction, the authors stated: "There is now little doubt that cigarette smoking is the major factor concerned with the ever-increasing incidence of bronchogenic carcinoma in men. Both cigarette-tobacco tars and particulates from air pollution contain various carcinogenic polynuclear compounds"
1940	In their study of the response of the lungs of strain A[a] mice to various compounds, Andervont and Shimkin (79) demonstrated that 20 of 20 strain A mice given a single injection of 0.5 mg of dibenz[*a,h*]acridine in 0.1 mL of tricaprylin developed multiple adenomas in 14 weeks but no sarcomas at the injection site. All 14 mice administered a single injection of 1 mg of dibenz[*a,h*]acridine in 0.3 mL of sesame oil developed multiple adenomas in 40 weeks but no sarcomas at injection site. Andervont and Shimkin also compared the response of the lungs of strain A mice to a single intravenous injection of 0.25 mg of each of nine compounds dispersed in 0.25 mL of water. Among the nine compounds were DB[*a,h*]A, B[*a*]P, benz[*a*]anthracene (B[*a*]A), dibenz[*a,h*]acridine, and 7*H*-dibenzo[*c,g*]carbazole. A calculated "carcinogenic index" [% tumor-bearing animals *x* mean number of adenomas in animals showing a positive response for each of these compounds at 8, 14, and 20 weeks] gave the following sequence: DB[*a,h*]A > 7*H*-dibenzo[*c,g*]carbazole > B[*a*]P > dibenz[*a,h*]acridine > B[*a*]A
1946	Dubinin and Chelintsev (1075a) reported quinoline, isoquinoline, and several substituted pyridines in a pyrolysate of anabasine, a tobacco alkaloid structurally related to nicotine
1951	Hartwell (1544) listed several studies in which dibenz[*a,j*]acridine and 7*H*-dibenzo[*c,g*]carbazole were reported to be tumorigenic in skin-painting (epitheliomas) and subcutaneous-injection (sarcomas) experiments
1954	At the International Cancer Congress, São Paolo, a new short-term test was reported by Smith (3722a). By this test, the "tumorigenicity" of a test compound could be estimated in less than a week *vs*. the 18–20 months required in skin-painting studies. The extent and rapidity of the disappearance of the sebaceous glands after 4 daily applications of the test compound (PAHs, aza-arenes, etc.) were considered to be related to the tumorigenicity of the test compound. Because of the absence of the ultimate end point—a tumor—this test did not receive the endorsement originally anticipated
1954	Kosak (2170) did not list quinoline as a tobacco smoke component, perhaps because it was reported as a component of a destructive distillate of tobacco rather than a component of tobacco smoke. However, he did list B[*a*]P as a questionable tobacco smoke component even though it too was identified in a destructive distillate of tobacco by Roffo (3323, 3325)
1956	Lacassagne et al. (2247a) reported the tumorigenicity of dibenz[*a,h*]acridine and dibenz[*a,j*]acridine to the skin and subcutaneous tissue of mice. The tumorigenicity of 76 other unsubstituted and substituted benzacridines was also cataloged. The authors noted: "All [angular benzacridines] have a characteristic odor which is reminiscent of cigar smoke" Since 1967, two unsubstituted angular benzacridines (benz[*a*]acridine, benz[*c*]acridine) and over a dozen of their alkyl-substituted derivatives have been identified in tobacco smoke (1409, 2021, 2120, 2132, 2596a, 3300, 3337, 3339, 3499, 3750, 3752)
1957	In the first supplement to Hartwell's 1951 compilation of compounds tested for tumorigenicity, Shubik and Hartwell (3664) summarized the results of additional published studies on the tumorigenicity of 7*H*-dibenzo[*c,g*]carbazole in mice and rats
1959	Johnstone and Plimmer (1971) listed quinoline as a tobacco smoke component, but the reference cited was the report of Gabelya and Kipriyanov (1263) who identified quinoline in a destructive distillate of tobacco
1960	Van Duuren et al. (4027) vacuum distilled a solution of the basic portion of 250 g of cigarette "tar" at 100°C/0.5 mm pressure. The residue (10 g) was successively chromatographed on alumina and several Whatman papers. Bands corresponding to the aza-arenes dibenz[*a,h*]acridine and dibenz[*a,j*]acridine were rechromatographed until their ultraviolet absorption and fluorescence spectra were identical with those of authentic samples. Chromatography of the neutral fraction of the CSC gave an isolate whose properties were identical with an authentic sample of 7*H*-dibenzo[*c,g*]carbazole. No 7*H*-dibenzo[*a,g*]carbazole was detected. The estimated amounts of dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole isolated from the "tar" were 0. 1, 2.7, and 0.7 ng/cig, respectively. They estimated the levels of B[*a*]P and DB[*a,h*]A in the same CSC to be 5.0 and 0.5 ng/cig[b], respectively. Van Duuren et al. noted: "It is clear that the heterocyclics here described make a significant contribution to the reported carcinogenicity of tobacco tars"

TABLE 17.17 (continued)
Chronology of Selected Aza-Arenes: Dibenz[*a,h*]acridine, Dibenz[*a,j*]acridine, 7*H*-Dibenzo[*c,g*]carbazole, Quinoline

Year	Event
1960	Van Duuren et al. (4027) also investigated the possibility that pyridine and nicotine were precursors of these nitrogen heterocyclics. Pyrolysis of pyridine or nicotine (750°C, nitrogen atmosphere) yielded pyrolysates in which dibenz[*a,h*]acridine and dibenz[*a,j*]acridine were identified by the same procedures used with CSC. As in the CSC case, dibenz[*a,j*]acridine was more plentiful than dibenz[*a,h*]acridine in the pyridine and nicotine pyrolysates. No 7*H*-dibenzo[*c,g*]carbazole was found in either pyrolysate
1960	Van Duuren et al., citing unpublished data by Nelson et al. (2689d) on mouse-skin painting with the basic fraction of CSC, noted that the skin-painting experiments gave negative results and attributed this finding to the fact that: "The basic fraction used in those experiments would not have been sufficient to yield skin tumors even if the benzacridines had been as potent for the skin as benzo[a]pyrene, which is not the case. They also noted that Wynder and Wright (4354) reported weak tumorigenicity with more concentrated fractions from the basic fraction"
1961/1962	Balasubrahmanyam and Quin (175) identified quinoline, isoquinoline, and various substituted pyridines in the pyrolysates from the tobacco alkaloids nornicotine and myosmine
1962	Van Duuren (4022a) described methods for the separation and identification of 7*H*-dibenzo[*c,g*]carbazole in cigarette MSS
1962	Rodgman and Cook (3279) reported the isolation in crystalline form and the identification of a series of homologous indoles (indole, skatole, etc.) as well as several carbazoles from cigarette MSS
1963	Candeli et al. (587) investigated the aza-arenes in CSC with the method described by Van Duuren et al. in 1960. It was noted: "With some modifications, this method …by Candeli et al…enabled us to isolate from 100 cigarettes 1.0 µg. [dibenz[a,j]acridine]. The presence of [dibenz[a,h]acridine] could not be confirmed"
1963	Wynder and Hoffmann (4317) described the results of mouse-skin-painting tests with dibenz[*a,j*]acridine applied in 0.5% and 0.1% acetone solutions three times weekly to the backs of 20 Swiss female mice. After 12–14 months, tumors were induced in 16 (80%) and 15 (75%) mice, respectively, with 60% of the animals in each test developing carcinomas. Wynder and Hoffmann (4332) offered the following explanation for the difference between these extremely high results and the much lower one reported by Lacassagne et al. (2247a): "This relatively high tumor response in mouse skin (compared to the findings of Lacassagne et al.) might be partially explained by the high purity of the compounds, due mainly to the absence of the 'Morgan's base' [a dihydro-dibenz[*a,j*]acridine]. Only by repeated column chromatography on alumina can a [dibenz[*a,j*]acridine] be isolated that is free of the dihydro product (absence of N-H band in infrared absorption spectrum)" In another study reported by Wynder and Hoffmann (4317), mouse skin was initiated with a single application of 300 µg of 7,12-dimethylbenz[a]anthracene and then painted with a 0.5% solution of dibenz[a,j]acridine, three times weekly. The same tumor response was observed as with dibenz[a,j]acridine alone except that the tumors appeared 2–3 months earlier. The investigators interpreted this finding as indicating: "There is no significant tumor-promoting activity of [dibenz[a,j]acridine], despite its strong hyperplastic effect"
1964	The report of the 1964 Advisory Committee to the U.S. Surgeon General (3999) identified dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole as carcinogenic polycyclic compounds isolated from cigarette smoke, classified them as weakly carcinogenic, and listed their amounts in cigarette MSS as 0.1, 2.7, and 0.7 ng/cig. The report also listed quinoline as a tobacco smoke component
1964	In addition to discussing the dibenzacridines and dibenzocarbazole in tobacco smoke and the two dibenzacridines in a nicotine pyrolysate reported by Van Duuren et al. (4027), Wynder and Hoffmann (4319) discussed the identification by Jarboe and Rosene (1923a) of quinoline in a nicotine pyrolysate produced at 600°C–900°C in an inert atmosphere
1964	Kuhn (2228) reviewed the pyrogenesis of aza-arenes from tobacco and nicotine. The dibenzacridines were tabulated with reference to the 1960 paper of Van Duuren et al. (4027). He listed quinoline as a pyrolysis product of nicotine and nornicotine but not as a tobacco smoke component
1964	Testa and Testa (3886) report quinoline as a tobacco smoke component. Its presence was subsequently confirmed by Grob and Völlmin (1427) and Kaburaki et al. (1992a)
1965	Sawicki et al. (3419a) identified dibenz[*a,h*]acridine and dibenz[*a,j*]acridine in polluted air in the amounts of 80 and 40 ng/1000 m^3 of air, respectively
1968	Stedman (3767) wrote: "The presence of the dibenzacridines and 7*H*-dibenzo[*c,g*]carbazole in cigarette smoke…is of special interest since these compounds are carcinogenic and may contribute to the weak tumorigenic activity of the basic fraction in laboratory animals [Wynder and Wright (4354); Wynder and Hoffmann (4319)]" *Note*: Stedman apparently missed the point that 7H-dibenzo[c,g]carbazole, because of its structure, was not present in the basic fraction but was found in the neutral fraction of CSC [see Van Duuren et al. (4027)]
1969	Rothwell and Whitehead (3339) improved the method of isolation of 7*H*-dibenzo[*c,g*]-carbazole from complex mixtures such as CSC by formation of complexes of the aza-arenes and PAHs with purines
1970	In a study of the composition of nicotine pyrolysates (400°C, 500°C, 550°C, 600°C, 650°C, 700°C, 800°C; nitrogen and air atmospheres), Kaburaki et al. (2006) were unable to confirm the presence of the aza-arenes (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine) reported by Van Duuren et al. in 1960 for nicotine pyrolysis (750°C, nitrogen atmosphere). Because there is sufficient overlap between the pyrolysis conditions used by Kaburaki et al. and by Van Duuren et al., the profound difference in composition results (presence vs. absence of the aza-arenes in question) cannot be explained by minor differences in pyrolysis conditions

(*continued*)

TABLE 17.17 (continued)
Chronology of Selected Aza-Arenes: Dibenz[*a,h*]acridine, Dibenz[*a,j*]acridine, 7*H*-Dibenzo[*c,g*]carbazole, Quinoline

Year	Event
	In addition, the tumorigenicity of 7*H*-dibenzo[c,g]carbazole was compared with that of B[α]P: "Weekly administration of 3 mg of 7*H*-dibenzo[c,g]carbazole for 15 weeks resulted in 13% more animals dying with respiratory tract cancer than died with same dose level of B[α]P. With lower total dose levels (15 mg) of B[α]P only, 30% of the animals developed respiratory tract tumors vs. 89% of the animals treated with the same dose of 7*H*-dibenzo[c,g]carbazole. The tumors in the 7*H*-dibenzo[c,g]carbazole group appeared earlier than those in the B[α]P-treated group"
1972	Schmeltz et al. (3499) studied the pyrolysis (800°C–860°C, nitrogen atmosphere) of nitrogen-containing materials (tobacco, tobacco pigment, nicotine) and reported: "We could not detect benzo(a)pyrene in nicotine pyrolyzates, nor could we confirm the presence of the physiologically active dibenzacridines and dibenzcarbazole reported in tobacco smoke and in nicotine and pyridine pyrolyzates by Van Duuren…"
	Here again, the slight difference in the temperature (750°C *vs*. 800°C–860°C) of the inert atmosphere (nitrogen) pyrolysis cannot explain the profound difference in the compositional findings (presence *vs*. absence of the aza-arenes in question)
1973	The IARC working group reported that skin painting with dibenz[*a,h*]acridine induced skin tumors in mice (1864a). Subcutaneous injection into mice produced sarcoma at the injection site plus an increased incidence of pulmonary adenomas. In 1973, dibenz[*a,h*]acridine had not been tested by other administration routes or in other species. The IARC noted that no human data were available, but it did note: "Coal tar and other materials which are known to be carcinogenic to man may contain [dibenz[*a,h*]acridine]"
	The IARC concluded that dibenz[*a,j*]acridine induced skin tumors in mice following topical application. At the highest dose tested by subcutaneous injection, it induced sarcomas at the injection site and an increased incidence of pulmonary adenomas. Negative results were obtained by the oral route in the mouse, but the test was considered inadequate because of the small number of animals tested. Dibenz[*a,j*] acridine had not been tested in other species at that time. No human data were available, but the IARC considered that some materials known to be carcinogenic to man may contain dibenz[*a,j*]acridine
1973	The IARC working group considered 7*H*-dibenzo[*c,g*]carbazole to be: "Carcinogenic in the mouse, rat, hamster, and possibly in the dog. It has both a local and a systemic carcinogenic effect. Following oral administration in the mouse, forestomach tumors and hepatomas occurred; intratracheal administration to hamsters produced tumors of the respiratory tract. In comparison with benzo[*a*]pyrene, [7*H*-dibenzo[*c,g*] carbazole] appears to be a stronger respiratory tract carcinogen for the hamster"
	Though 7*H*-dibenzo[c,g]carbazole had been reported as a component of CSC, no case reports or epidemiological data concerning human exposure were available
1976	In his review on polycyclic tumorigens, Dipple (983) labeled dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole as "carcinogenic heterocyclic compounds" with "slight" activity. However, in a later review in 1984, Dipple et al. (984) revised the assessment of 7*H*-dibenzo[*c,g*]carbazole, listing it as a highly potent tumorigen
1976	Wynder and Hoffmann (4347) listed dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole as: "Tumorigenic agents identified in the particulate phase of tobacco smoke, each possessing low biological activity and only traces detected in the smoke of 100 cigarettes. Dibenz[*a,j*]acridine was detected in amounts of 1.0 µg/100 cigarettes [10 ng/cig]"
	They categorized dibenz[*a,j*]acridine and dibenz[*a,h*]acridine as "known animal carcinogens" but noted that these aza-heterocyclic compounds are "minor carcinogens" in tobacco smoke
1976	Hoffmann et al. (1780) reported that the basic fraction of CSC which contains dibenz[*a,h*]acridine and dibenz[*a,j*]acridine was not tumorigenic to mouse skin [cf. Wynder and Wright (1957) Wynder and Hoffmann (4319, 4332)]
1977	Schmeltz and Hoffmann (3491), in their review of *N*-containing compounds in tobacco and tobacco smoke discussed the benzacridines: "Nicotine has…been shown to produce on pyrolysis the animal carcinogens, dibenz[*a,h*]acridine…and dibenz[*a,j*]-acridine…both of which are present in tobacco smoke…Acridans have been reported in smoke… Subsequent dehydrogenation of the acridans could lead to acridines. The only examples of the latter reported in smoke are two benzacridines [dibenz[*a,h*]acridine, dibenz[*a,j*]acridine]; these have been shown to form during pyrolysis from nicotine… A dibenzocarbazole [7*H*-dibenzo[*c,g*]carbazole]…has also been reported in tobacco smoke… The last three fused ring compounds cited are tumorigenic in the experimental animal"
	Schmeltz and Hoffmann listed quinoline as both a tobacco and a tobacco smoke component as well as an "animal carcinogen (rat liver)"
1979	In a brief section of the chapter on cigarette smoke composition, the aza-arenes (including dibenz[a,h]acridine, dibenz[a,j]acridine, and 7*H*-dibenzo[c,g]carbazole), their tumorigenicity, and their mutagenicity were discussed in the 1979 Surgeon General's report (4005). The report noted: "Mutagens thus far identified in cigarette smoke are: Quinoline (MS 1.7 µg/cigarette; SS 18 µg/cigarette), all seven isomeric methylquinolines (MS 0.7 µg/cigarette; SS 8 µg/cigarette)… Quinoline induces hepatomas when fed in high doses to rats…"
1979	Rinkus and Legator (3157) reported dibenz[*a,h*]acridine and dibenz[*a,j*]acridine to be mutagenic substances in the Ames *S. typhimurium* test
1979	Schmeltz et al. (3512) studied the fate of radiolabeled nicotine during pyrolysis and during actual smoking in a burning cigarette spiked with radiolabeled nicotine. The radiolabeled nicotine was pyrolyzed (nitrogen atmosphere) from a silica gel matrix at several temperatures (600°C, 750°C, and 900°C) and from a tobacco matrix at 600°C. None of the three aza-arenes—dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*] carbazole—identified by Van Duuren et al. (4027) in CSC were found in the smoke study by Schmeltz et al. Neither of the two dibenzacridines reported by Van Duuren et al. in a nicotine pyrolysate was found in the several nicotine pyrolysates generated by Schmeltz et al. (3512)
	The differences concerning the presence or absence of these aza-arenes in several such studies involving CSCs and/or nicotine pyrolysates were summarized by Rodgman (3255, 3257)

TABLE 17.17 (continued)
Chronology of Selected Aza-Arenes: Dibenz[*a,h*]acridine, Dibenz[*a,j*]acridine, 7*H*-Dibenzo[*c,g*]carbazole, Quinoline

Year	Event
1982	In the 1982 Surgeon General's report (4010), the aza-arenes dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole were described as "tumor-initiating agents in the particulate phase of tobacco smoke" and their MSS levels as 0.1, 3–10, and 0.7 ng/cig respectively. It was noted, from data provided by Hoffmann et al. (1781, 1782), that dibenz[*a,j*]acridine possessed much higher tumorigenic activity than dibenz[*a,h*]acridine and 7*H*-dibenzo[*c,g*]carbazole [cf. Dipple et al. (983)]
1982	Adams et al. (35) reported the identification and quantitation of quinoline (0.2–1.3 µg/cig), isoquinoline (0.1–0.9 µg/cig), and the seven isomeric methylquinolines (0.5–2.5 µg/cig) in the MSS of several commercial cigarettes. They noted: "Quinoline is the most abundant aza-arene in [mainstream] cigarette smoke"
1984	In their review of polycyclic aromatic tumorigens, Dipple et al. (983) classified dibenz-[*a,h*]acridine and dibenz[*a,j*]acridine as possessing only *slight* tumorigenicity. They classified 7*H*-dibenzo[*c,g*]carbazole as possessing *high* tumorigenicity (same category as 1,2-dihydro-benz[*j*]aceanthrylene (cholanthrene), 3-methyl-1,2-dihydro-benz[*j*]aceanthrylene (3-methylcholanthrene), 7,12-dimethylbenz[*a*]anthracene, and B[*a*]P)
1984	In their review of tumorigenic aromatic amines in which fused-ring polycyclic amines are discussed, Garner et al. (1275a) neither mention nor list quinoline as a tumorigenic compound
1985/86	The IARC (1870) in its 1986 report on its 1985 deliberations found sufficient evidence to classify dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole as carcinogenic in laboratory animals. The IARC noted that "nicotine is a specific precursor for the two acridines," totaling ignoring contradictory evidence from several groups of investigators who were unable to confirm the presence of these dibenzacridines in nicotine pyrolysates. The IARC listed quinoline as a smoke component but did not include it in its tabulation of compounds *vs*. "the degree of evidence [for carcinogenicity] in animals (and humans)"
1986	Hoffmann and Wynder (1808) published a list of components classified as toxicants and/or tumorigens in tobacco and smoke. Much of the information in their report on quinoline, dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole had been provided to the IARC for inclusion in its 1986 article (1870)
1990	Hoffmann and Hecht (1727), in their compilation of 43 "tumorigenic components of tobacco and tobacco smoke," listed dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]-carbazole, and quinoline as tumorigenic aza-arenes in CSC. This list was subsequently used by the EPA (1990) in its attempt to have environmental tobacco smoke classified as a Group A (human) carcinogen. Hoffmann and Hecht paid little attention to the discrepancies between the 1960 report of Van Duuren et al. on the presence of these aza-arenes in CSC and nicotine pyrolysates and later reports from other investigators who failed to confirm the Van Duuren findings on these compounds either in CSC or nicotine pyrolysates [see Table 17.16]
	In their tabulation, Hoffmann and Hecht listed quinoline with no comment as to its carcinogenicity as reported in the "IARC evaluation of evidence of carcinogenicity in laboratory animals [and] in humans." In their text, they noted: "Quinoline, a liver carcinogen in rats…and in newborn mice…, is present in cigarette smoke at a concentration of 1-2 µg/cigarette [Dong et al. (1042)]"
1991	In a memorandum to the EPA, Rodgman (3255) summarized the inconsistencies between the 1960 findings reported by Van Duuren et al. on dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole in nicotine pyrolysates and/or mainstream CSC *vs*. the findings in the comparable 1963 study of Candeli et al. [reported by Wynder and Hoffmann (4319, 4332)], the 1970 study of Kaburaki et al. (2006), the 1972 and 1979 studies of Schmeltz et al. (3499, 3512), and the 1986 and 1987 reports by Grimmer et al. (1409). The expanded summary is shown in Table 17.16. Summaries of the studies of benzacridines in cigarette smoke by Kamata et al. (2021) and Sasaki and Moldoveanu (3414) were added
	A possible explanation of the differences in the results concerning the presence or absence of these three aza-arenes in mainstream CSC may be the differences between cigarettes fabricated in 1960 and those fabricated more recently after the 1970s. The pre-1960 cigarettes were substantially higher in nicotine. However, there does not appear to be a logical explanation for the difference in the results (presence *vs*. absence) of these three compounds in nicotine pyrolysates prepared in 1960, 1963, 1970, 1972, and 1979. Post-1960 advances in analytical technology should have improved the ability to isolate/identify low levels of these three aza-arenes
1994	OSHA (2825), in its goals for clean air legislation, presented its own list of 43 tobacco smoke components tumorigenic in animals or man. Its list differed slightly from that of Hoffmann and Hecht (1727). OSHA included the three aza-arenes reported by Van Duuren et al. (4027) but omitted quinoline
1994	In a response to the OSHA (2825) publication, Rodgman (3257) presented the information in Table 17.16 as reasons why the benzacridines and the benzocarbazole should be removed from the list. Valid scientific reasons for deleting other listed components were also presented
1997	Hoffmann and Hoffmann (1740) revised the 1990 Hoffmann–Hecht list of "43 tumorigenic components" of tobacco smoke (1727), expanding the list to 60 components by deleting chrysene and crotonaldehyde in agreement with the OSHA (2825) list and by adding 19 other components, including the 8 *N*-heterocyclic amines known as the "cooked food" mutagens. Still retained in the Hoffmann–Hoffmann 1997 list were the aza-arenes quinoline, dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole
1998	In a letter to the editors of Beiträge Tabakforschung zur International, Hoffmann and Hoffmann (1741) submitted a list of biologically active components of cigarette MSS, including the four aza-arenes quinoline, dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole

(*continued*)

TABLE 17.17 (continued)
Chronology of Selected Aza-Arenes: Dibenz[*a,h*]acridine, Dibenz[*a,j*]acridine, 7*H*-Dibenzo[*c,g*]carbazole, Quinoline

Year	Event
2000	Fowles and Bates (1217) included dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole in their list of tobacco and tobacco smoke toxicants
2001	Hoffmann and Hoffmann (1743) in their list of tobacco and tobacco smoke toxicants again included dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole despite the numerous reports of research that failed to confirm the 1960 Van Duuren et al. reported finding.
	Hoffmann et al. (1744) again included dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole in their list of tobacco and tobacco smoke toxicants
2003	Rodgman (3265) assessed the various published reports in which numerous tobacco and tobacco smoke components were classified as toxicants (1217, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 2825). The numerous deficiencies and errors in the reports were cataloged

[a] The strain A mouse was developed for lung tumor research in laboratory animals. Without treatment of any kind, 70%–90% of strain A mice develop adenomas, a type of lung tumor, between 12 and 18 months of age [Shimkin (3652)].

[b] It is interesting to note the deliveries recorded by Van Duuren et al. for B[*a*]P (5 ng/cig) and DB[*a,h*]A (0.5 ng/cig) and compare them to values subsequently listed by Hoffmann and Hecht (1727) and Hoffmann and Hoffmann (1740) who listed a range for B[*a*]P of 20–40 ng/cig and a single value for DB[*a,h*]A of 4 ng/cig! Why did these authors not acknowledge the values reported by Van Duuren et al?

The results of research in Japan in the late 1970s brought attention not to any aza-arenes themselves but to a group of their amine derivatives, many of which showed inordinately high mutagenicity in the Ames test with several strains of *Salmonella typhimurium*. The originally studied source was cooked foodstuffs and pyrolysis products from several amino acids which resulted in their being described as "cooked food" mutagens. Later, they became known as the *N*-heterocyclic amines. When the *N*-heterocyclic amines were shown to be tumorigenic in addition to being highly mutagenic and subsequently identified in tobacco smoke, they were included by Hoffmann and his colleagues in their numerous lists of tobacco smoke tumorigens published in 1997 and later (1740, 1741, 1743, 1744). The *N*-heterocyclic amines had not been included in their numerous lists published between 1986 and 1997 (1727, 1773, 1806) nor in similar lists by IARC (1870) and OSHA (2825). Even though their number in tobacco smoke is low, we decided to discuss them in a separate chapter that follows this one on aza-arenes.

In the 1979 Surgeon General's report (4005), the aza-arenes dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]carbazole, quinoline, and alkylated quinolines in CSC were discussed but not the presence or biological properties of any of the "cooked food" mutagens identified in tobacco smoke. In the 1982 report of the Surgeon General [see Table 10, p. 214 in (4010)], 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) were classified as "toxic and tumorigenic agents of cigarette smoke" in amounts of 3.2–8.1 and 1.1–3.1 µg/cig, respectively, in mainstream CSC. None of the other highly mutagenic *N*-heterocyclic amine mutagens present in tobacco smoke were discussed.

Table 17.17 lists, with appropriate citations, the chronology of the studies pertinent to the aza-arenes and other polycyclic nitrogen compounds in tobacco smoke. A similar chronology of studies pertinent to the *N*-heterocyclic amines, the "cooked food" mutagens, is presented in a subsequent chapter.

17.5.1 Alternate Exposures to Aza-Arenes

In the several lists of tumorigenic components in tobacco and/or tobacco smoke, three *N*-heterocyclic compounds (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole) appear on the list of 43 by Hoffmann and Hecht (1727) and OSHA (2825) and the list of 60 by Hoffmann and Hoffmann (1740). Quinoline was on several lists but was omitted from the OSHA list (Table 17.18).

In Table 17.19 are listed the many tobacco smoke components similar in structure to those listed in Table 17.18.

Even though, as indicated in Table 17.16 and the text accompanying it, the presence of the three pentacyclic *N*-heterocyclic compounds in tobacco smoke is equivocal, the alternate exposure to them and similar components is discussed in the following.

In their 1956 review of angular benzacridines and dibenzacridines and their tumorigenicity, Lacassagne et al. (2247a) made the following interesting observation, pertinent to the alleged "carcinogenicity" of benzene, frequently used as a solvent in tumorigenicity studies in the 1930s, 1940s, and 1950s:

> These molecules [the angular benzacridines] are very soluble in benzene and acetone (two solvents currently used for the investigations of carcinogenic activity)…

In addition to the exposure to acridines and benzacridines in tobacco smoke, other exposures to various acridines and benzacridines have been cataloged in the scientific literature. Many of the sources (Table 17.20) comprise environmental pollutants.

Unlike the PAHs and the *N*-nitrosamines, nontobacco smoke exposure to the acridines/benzacridines does not include foods. However, exposures other than tobacco smoke to polycyclic nitrogen compounds include exposures to the

TABLE 17.18
Summary of Lists of Tumorigenic Aza-Arenes in Tobacco Smoke

Component	Ho & He[b]	OSHA[c]	Ho & Ho[d]	MS Level wt/cig[d]	IARC Evaluation[a] of Evidence of Tumorigenicity in	
					Laboratory Animals	Humans
Quinoline	x	…	x	1–2 µg	…	…
Dibenz[*a,h*]acridine	x	x	x	0.1 ng	Sufficient	…
Dibenz[*a,j*]acridine	x	x	x	3–10 ng	Sufficient	…
7*H*-Dibenzo[*c,g*]carbazole	x	x	x	0.7 ng	Sufficient	…

[a] See IARC (1870).
[b] Ho & He, Hoffmann and Hecht (1727).
[c] OSHA, OSHA (2825).
[d] Ho & Ho, Hoffmann and Hoffmann (1740).

TABLE 17.19
Tobacco Smoke Components Related to Aza-Arenes in Tumorigen Lists[a]

Quinolines [35][b]	Acridines [28][b]	Carbazoles [20][b]
Quinoline	Acridine	9*H*-Carbazole
Quinoline, 5-amino-	Acridine, 9,10-dihydro-	9*H*-Carbazole, 2-amino-
Quinoline, butyl-	Acridine, 9,10-dihydro- (four homologs)	9*H*-Carbazole, dimethyl- (four isomers)
Quinoline, dihydro-	Acridine, ethyl-	9*H*-Carbazole, 9-ethyl-
Quinoline, dihydroethyl- (three isomers)	Acridine, methyl-	9*H*-Carbazole, methyl- (five isomers)
Quinoline, dihydromethyl- (three isomers)	Acridine, propyl-	9*H*-Carbazole, tetramethyl-
Quinoline, dimethyl- (five isomers)		9*H*-Carbazole, trimethyl-
Quinoline, ethyl- (two isomers)	Benz[*a*]acridine	
Quinoline, methyl- (six isomers)	Benz[*a*]acridine, dimethyl-	11*H*-Benzo[*a*]carbazole
Quinoline, (1-methylethyl)-		
Quinoline, methyltetrahydro- (two isomers)	Benz[*c*]acridine	5*H*-Benzo[*b*]carbazole
Quinoline, propyl-	Benz[*c*]acridine, dimethyl- (five isomers)	
Quinoline, tetrahydro- (two isomers)	Benz[*c*]acridine, methyl- (five isomers)	7*H*-Benzo[*c*]carbazole
Quinoline, tetramethyl-	Benz[*c*]acridine, trimethyl- (two isomers)	
Quinoline, trimethyl-		1*H*-Dibenzo[*a,c*]carbazole
	Dibenz[*a,h*]acridine	
Quinolinecarbonitrile (two isomers)		13*H*-Dibenzo[*a,i*]carbazole
	Dibenz[*a,i*]acridine	
8-Quinolinol		7*H*-Dibenzo[*c,g*]carbazole
8-Quinolinol, 7-methyl-	Dibenz[*a,j*]acridine	
	Dibenz[*c,h*]acridine	

[a] Omitted from the list are the *N*-heterocyclic amines discussed in a subsequent chapter.
[b] Number in square bracket = number of reported components.

N-heterocyclic amines, the so-called cooked food mutagens, in a variety of foods.

In Table 17.21 are listed, with appropriate citations, the 343 aza-arenes and other polycyclic nitrogen compounds reported in tobacco and tobacco smoke.

Table 17.22 summarizes the variation in the structures of the aza-arene compounds identified in tobacco and/or tobacco smoke. Of particular interest with regard to the 343 aza-arenes cataloged in Table 17.21 is that only 25 of the 343 have been identified as tobacco components. Of 25, just 18 have been identified in both tobacco and smoke. The number of aza-arenes identified in smoke is 336. Those isolated from and/or identified in tobacco in greater than trace amounts include 1*H*-indole, 2,3-dihydro-1*H*-indole, 9*H*-pyrido[3,4-*b*] indole (norharman), 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), 1*H*-purine, and quinoline.

Because of their classification as significant tumorigens in tobacco smoke (1740, 1741, 1743, 1744) and their inordinately high mutagenicity in the Ames test with *S. typhimurium* (2327c, 3828c), the amino derivatives of several aza-arenes

TABLE 17.20
Aza-Arene Sources Other than Tobacco Smoke

Acridine/Benzacridine Source	Reference
Automobile exhaust	3419b, 4247a
Coal-fired residential furnace emission	1407b
Coal distillate	1334c, 2210a
Coal tar	2261a, 2534a
Crude oil	1407a, 3519c
High boiling petroleum distillate	2519a
Industrial stack effluent	3419a
Urban suspended particulate matter	35, 636a, 1040a, 3419c
CSC	1884, 3491

are discussed in detail in a subsequent chapter (Section 17.6) devoted to the *N*-heterocylic amines identified in tobacco smoke. However, in addition to the *N*-heterocylic amines, several aza-arene-related fused *N*-containing-ring compounds with two or more ring nitrogens plus various functional groups have been identified in tobacco and/or tobacco smoke. Classic examples of such compounds in tobacco include adenosine, 5′-adenylic acid, and many purines. Table 17.23 lists many such components identified in tobacco and/or tobacco smoke. Examination of the structures of the various derivatives indicates the inclusion of a variety of functional groups, e.g., amino, carboxylic acid, carboxamide, hydroxyl, and various carbohydrates. It should be noted that Table 17.23 does not include the nine *N*-heterocylic amines because they are described and discussed in detail in Section 17.6. In contrast to the aza-arenes which occur predominately in tobacco smoke, 65 of the 88 components with functional groups listed in Table 17.23 were identified in tobacco, and only 29 have been identified to date in tobacco smoke.

17.6 *N*-HETEROCYCLIC AMINES

Although not originally classified at the time as "cooked food" mutagens, several amino-acid-derived *N*-heterocylic compounds were identified in cigarette smoke condensate (CSC) in the early 1960s: 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) {I} by Mold et al. (2592) and 9*H*-pyrido[3,4-*b*]indole (norharman) {II} and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) {III} by Poindexter and Carpenter (2972) (Figure 17.13).

Proline is the precursor in tobacco of 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) {I} in tobacco smoke. Tryptophan is the major precursor in tobacco of 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) {II} and 9*H*-pyrido[3,4-*b*]indole (norharman) {III}, as well as indole and its alkylated homologs, in tobacco smoke.

In the late 1970s, Japanese investigators—in their detailed studies of components of various "cooked foods"—isolated and identified the first of a series of *N*-heterocylic amines as pyrolysis products of several amino acids. Sugimura et al. (3829) reported the isolation and identification of 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (designated as Trp-P-1) {IV} and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) {V} (Figure 17.14) from tryptophan pyrolysates.

Yamamoto et al. (4365a) reported the isolation and identification of the mutagenic *N*-heterocylic amines 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) {VI} and 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2) {VII} from glutamic acid pyrolysates. Yoshida and Matsumoto (4388) and Matsumoto et al. (2492) reported the identification of 2-amino-9*H*-pyrido[2,3-*b*]indole (AαC) {VIII} and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC) {XIII–IX} in CSC (Figure 17.14).

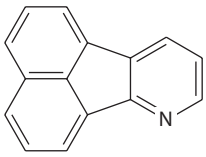
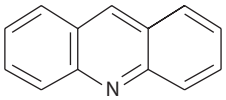
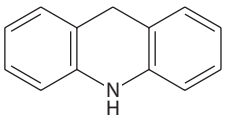
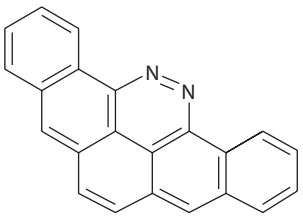
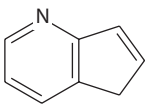
A unique feature of several of compounds {IV–VII} was their inordinately high mutagenicity in the Ames system (*Salmonella typhimurium*). Mutagenic activities on a revertant/μg basis as determined in the Ames test with *S. typhimurium* strains TA 98 and TA 100 for several of these compounds are shown in Table 17.24 [Sugimura (3828c), Lee et al. (2327c)]. To put in perspective the extremely high values for the mutagenic activities listed in Table 17.24, it should be noted that the mutagenic activity of benzo[*a*]pyrene (B[*a*]P) (strain TA 98) when tested under the same conditions is about 200 revertant/μg of B[*a*]P. In separate studies, Levitt et al. (2355a) and Nagao et al. (2667b) demonstrated the mutagenicity of the previously identified tobacco smoke components 9*H*-pyrido[3,4-*b*]indole (norharman) {II} and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) {III}.

Heckman and Best (1587) reported the identification of nearly 270 previously unidentified and confirmation of over 150 previously identified *N*-containing components in CSC. These included several components structurally similar to some of the *N*-heterocylic amines 9*H*-pyrido[2,3-*b*]indole, 2-methyl-9*H*-pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-9*H*-pyrido[2,3-*b*]indole, 2-pentyl-9*H*-pyrido[2,3-*b*]indole, 1-butyl-9*H*-pyrido[3,4-*b*]indole, 1-propenyl-9*H*-pyrido[3,4-*b*]indole, and a partially characterized norharman.

In addition to their mutagenicity in the Ames test (*S. typhimurium*), several of the mutagenic *N*-heterocylic amines were subsequently reported to be tumorigenic to laboratory animals. They were reported to be tumorigenic, particularly in feeding experiments, to several laboratory animal species. The tumorigenicity in mice of 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) was reported by Matsukura et al. (2491a) and in rats by Hosaka et al. (1835a). Takayama et al. (3862d) demonstrated the tumorigenicity in rats of 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2).

Ohgaki et al. (2849b) described the tumorigenicity in mice, and Takayama et al. (3862b) described the tumorigenicity in rats of 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) and 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2). 2-Amino-3-methylimidazo[4,5-*f*]quinoline (IQ) {X} was reported to be tumorigenic in rats by Takayama et al. (3862c) and Tanaka et al. (3865c) and in mice by Ohgaki et al. (2849, 2849a). Ohgaki et al. (2849, 2849a) also reported the tumorigenicity in mice of 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ)

TABLE 17.21
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	206-49-5	Acenaphtho[1,2-b]pyridine {7-azafluoranthene} 	3750, 4249		
2.	260-94-6	Acridine {benzo[*b*]quinoline} 	515, 568b, 1041, 1042, 1334f 1409, 2114, 2120, 2142, 3255, 3337–3339, 3505, 3733–3735, 3750, 3752, 4249, 5811b		
3.	92-81-9	Acridine, 9,10-dihydro- {acridan} 	568b, 2120, 4249, 5811b		
4.	6267-02-3	Acridine, 9,10-dihydro-9,9-dimethyl- {9,9-dimethylacridan}	658, 1767, 2550, 2552, 2553, 2724, 3308, 3491, 3797, 4342, 5811b		
5.	26914-16-9	Acridine, 9,10-dihydro-9,9-dimethyl-(1-methylethyl)-	2552		
6.	63451-42-3	Acridine, 9,10-dihydro-9,9-dimethyl-2-(1-methylethyl)-	2550, 2552, 2724, 3491, 4249, 5811b		
7.	64828-44-0	Acridine, ethyl-	2141, 4249, 5811b		
8.	54116-90-4	Acridine, methyl-	2132, 4249, 5811b		
9.	64828-45-1	Acridine, propyl-	2141, 4249, 5811b		
10.	55751-83-2	Acridine, 2-ethyl-	568b, 4249		
11.	65789-44-8	Acridine, 4-ethyl-	568b, 4249		
12.	4740-12-9	Acridine, 3-methyl-	568b, 4249		
13.	189-58-2	Anthra[9,1,2-*cde*]benzo[*h*]cinnoline 	3339, 4249		
14.	89126-45-4	Azafluoranthene	5811		
15.	8047-67-4	Azaindene 	1884, 2141		
16.	89126-46-5	Azapyrene	5811		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

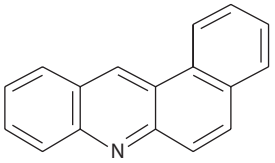
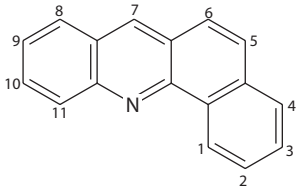
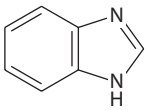
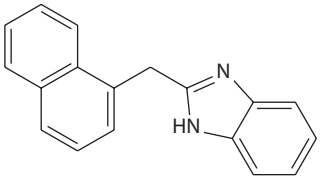
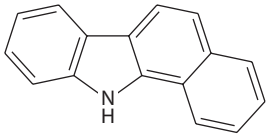
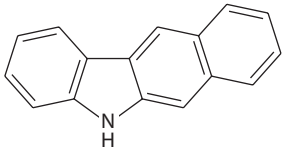
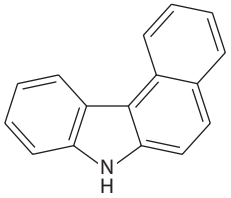
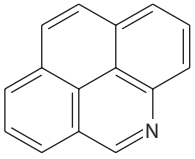
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
17.	225-11-6	Benz[*a*]acridine 	1409, 2120, 2596a, 3300, 3337–3339, 3499, 4249, 5811b		
18.	53-69-0	Benz[*a*]acridine, 8,10-dimethyl-	1409, 4249		
19.	17401-48-8	Benz[*a*]acridine, 9,12-dimethyl-	5811, 5811a, 5811b		
20.	225-51-4	Benz[*c*]acridine 	1409, 2021, 2120, 596a, 3300, 3337–3339, 3499, 3733–3735, 3750, 3752, 4249, 5811b		
21.	10567-95-0	Benz[*c*]acridine, 5,7-dimethyl-	4249		
22.	71265-19-5	Benz[*c*]acridine, 6,9-dimethyl-	2120, 2132, 4249, 5811b		
23.	963-89-3	Benz[*c*]acridine, 7,9-dimethyl-	3300, 4249		
24.	2381-40-0	Benz[*c*]acridine, 7,10-dimethyl-	2021, 3300, 4249		
25.	32740-01-5	Benz[*c*]acridine, 7,11-dimethyl-	2021, 4249		
26.	3340-94-1	Benz[*c*]acridine, 7-methyl-	1409, 2021, 3300, 4249		
27.	14319-90-5	Benz[*c*]acridine, 8-methyl-	2021, 4249		
28.	33942-93-7	Benz[*c*]acridine, 9-methyl-	2021, 4249		
29.	7230-71-9	Benz[*c*]acridine, 10-methyl-	2021, 4249		
30.	67028-20-0	Benz[*c*]acridine, 11-methyl-	2021, 4249		
31.	58430-01-6	Benz[*c*]acridine, 7,9,10-trimethyl-	2021, 4249		
32.	51787-42-9	Benz[*c*]acridine, 7,9,11-trimethyl-	2021, 4249		
33.	51-17-2	1*H*-Benzimidazole 	568b, 1587, 2543, 2773, 2775, 3255, 3398, 3491, 3797, 3888, 4249, 5811b		
34.		1*H*-Benzimidazole, C_2-alkyl-	568b, 2777, 3553, 3559, 4249		
35.	5851-44-5	1*H*-Benzimidazole, 2-butyl-	568b, 1587, 4249, 5811b		
36.	72692-74-1	1*H*-Benzimidazole, dimethyl-	4249		
37.	2876-08-6	1*H*-Benzimidazole, 1,2-dimethyl-	568b, 1587, 4249, 5811b		
38.	582-60-5	1*H*-Benzimidazole, 5,6-dimethyl-	568b, 4249		
39.	72692-75-2	1*H*-Benzimidazole, ethyl-	2570, 4249		
40.	7035-68-9	1*H*-Benzimidazole, 1-ethyl-	568b, 4249		
41.	1848-84-6	1*H*-Benzimidazole, 2-ethyl-	568b, 4249		
42.		1*H*-Benzimidazole, 2-(2-ethylphenylmethyl)-	568b, 4249		
43.	30304-58-6	1*H*-Benzimidazole, methyl-	3553, 4249		
44.	1632-83-3	1*H*-Benzimidazole, 1-methyl-	3255, 3398, 4249, 5811b		
45.	615-15-6	1*H*-Benzimidazole, 2-methyl-	568b, 2767, 3553, 4249, 5811b		
46.	946-18-9	1*H*-Benzimidazole, 2-(3-methylbutyl)-	568b, 1587, 4249, 5811b		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
47.	42268-60-0	1*H*-Benzimidazole, 2-(1-naphthalenylmethyl)-	5811, 5811a, 5811b		
					
48.	82326-40-7	1*H*-Benzimidazole, 2-(2-naphthalenylmethyl)-	568b, 1587, 4249		
49.	5851-46-7	1*H*-Benzimidazole, 2-pentyl-	568b, 4249		
50.	3363-56-2	1*H*-Benzimidazole, 2,5,6-trimethyl-		568b, 2917a, 4249	
51.	67526-84-5	Benzocarbazole	1884, 3735		
52.	64859-55-8	Benzocarbazole, dimethyl-	3733–3735, 3750, 3752, 5811b		
53.	64859-54-7	Benzocarbazole, methyl-	3733–3735, 3750, 3752, 5811b		
54.	239-01-0	11*H*-Benzo[*a*]carbazole	3499, 3733–3735, 3750, 3752, 4249		
					
55.	243-28-7	5*H*-Benzo[*b*]carbazole	3337–3339, 3499, 3733–3735, 3750, 3752, 4249, 5811b		
					
56.	205-25-4	7*H*-Benzo[*c*]carbazole	3499, 3733–3735, 3750, 3752, 4249		
					
57.		Benzoisoquinoline	3733, 3750, 3752		
58.		Benzoisoquinoline, dimethyl-	3733–3735, 3750, 3752, 4249		
59.		Benzoisoquinoline, methyl-	3733–3735, 3750, 3752, 4249		
60.		Benzoisoquinoline, tetramethyl-	3733, 3750, 3752		
61.		Benzoisoquinoline, trimethyl-	3733–3735, 3750, 3752, 4249		
62.	194-03-6	Benzo[*lmn*]phenanthridine {thebenidine}	2132		
					

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

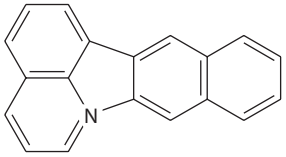
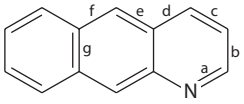
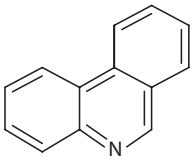
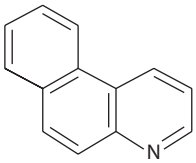
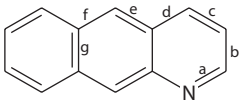
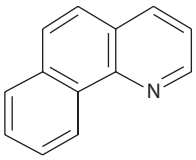
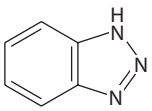
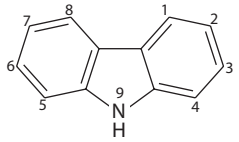
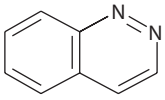
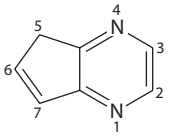
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
63.	30907-88-1	6*H*-Benzo[*c*]pyrido[3,2,1-*jk*]carbazole 	3339, 4249		
64.	39327-16-7	Benzoquinoline {benzo[*g*]quinoline} 	1649, 3733, 3750, 3752, 4249		
65.		Benzoquinoline, dimethyl-	3733, 3750, 3752		
66.	88813-63-2	Benzoquinoline, methyl-	1649, 3733, 3750, 3752, 4249		
67.		Benzoquinoline, tetramethyl-	3733, 3750, 3752		
68.		Benzoquinoline, trimethyl-	3733, 3750, 3752		
69.	229-87-8	Benzo[*c*]quinoline {phenanthridine; 9-azaphenanthrene} 	172, 568b, 1409, 1544, 1645, 3733–3735, 3741, 3750, 3752, 4249	172, 568b, 4249	
70.	85-02-9	Benzo[*f*]quinoline {1-azaphenanthrene} 	568b, 1409, 3733, 3750, 3752, 4249, 5811b		
71.	260-36-6	Benzo[*g*]quinoline 	1649, 3733, 3750, 3752, 4249, 5811a		
72.	230-27-3	Benzo[*h*]quinoline {4-azaphenanthrene} 	172, 568b, 1041, 1042, 1409, 1899, 2142, 2908, 3255, 3491, 3733, 3750, 3752, 4249, 5811b	172, 568b, 4249	
73.	63042-66-0	Benzo[h]quinoline, 2,3,4-trimethyl-	5811		
74.	95-14-7	1*H*-Benzotriazole {1,2,3-triaza-1*H*-indene} 	568b, 1667, 4249		
75.		Carbazole	1649, 2060, 2724, 3096, 3491, 3505, 4249, 5869a		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
76.	86-74-8	9*H*-Carbazole {dibenzo[*b*,*d*]pyrrole} 	127, 239, 515, 568b, 1172, 1373, 1426, 1427, 1765, 1767, 2596a, 2552, 2724, 2767, 2799a, 2939, 3191, 3251, 3279, 3300, 3302, 3308, 3485, 3491, 3493, 3505, 3506, 3557, 3741, 3797, 3886, 3887, 4248, 4249, 4342, 4407, 5811b		
77.		9*H*-Carbazole, alkyl-	1899, 3279, 3485, 3491, 3506, 4249		
78.		9*H*-Carbazole, 9-alkyl-	1560, 1899, 3491, 3493, 4249		
79.	30642-38-7	9*H*-Carbazole, dimethyl-	1650, 1652, 1762, 1765, 2724, 3279, 3308, 3485, 3491, 3506, 3732, 3757a, 4249, 5811b		
80.	14171-85-8	9*H*-Carbazole, 1,9-dimethyl-	1373, 1762, 1781, 2510, 3491, 4249, 5811b		
81.	24075-47-6	9*H*-Carbazole, 2,9-dimethyl-	1373, 1762, 1781, 2510, 3491, 4249, 5811b		
82.	24075-48-7	9*H*-Carbazole, 3,9-dimethyl-	1373, 1762, 1781, 2510, 3491, 4249, 5811b		
83.	24075-49-8	9*H*-Carbazole, 4,9-dimethyl-	1373, 1762, 1781, 2510, 3491, 4249, 5811b		
84.	71277-85-5	9*H*-Carbazole, ethyl-	1730, 1765, 4249		
85.	86-28-2	9*H*-Carbazole, 9-ethyl-	1373, 1781, 2510, 3479, 4249, 5811b		
86.	27323-29-1	9*H*-Carbazole, methyl-	127, 1765, 2141, 2570, 2939, 3251, 3279, 3308, 3485, 3491, 3506, 3797, 4249, 4332, 5811b		
87.	6510-65-2	9*H*-Carbazole, 1-methyl-	568b, 1765, 2724, 3491, 4249, 5811b		
88.	3652-91-3	9*H*-Carbazole, 2-methyl-	568b, 1765, 2724, 3491, 4249, 5811b		
89.	4630-20-0	9*H*-Carbazole, 3-methyl-	568b, 1765, 2724, 3491, 4249, 5811b		
90.	3770-48-7	9*H*-Carbazole, 4-methyl-	568b, 1765, 2724, 3491, 4249, 5811b		
91.	1484-12-4	9*H*-Carbazole, 9-methyl-	1762, 1781, 2510, 2724, 3300, 3491, 4005–4007, 4009–4011, 4249, 5811b		
92.	64844-53-7	9*H*-Carbazole, tetramethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
93.	64844-51-5	9*H*-Carbazole, trimethyl-	1650, 1652, 3732, 3757, 4249, 5811b		
94.	253-66-7	Cinnoline {1,2-diazanaphthalene} 	568b, 2132, 4249		
95.	63863-33-2	Cinnoline, dihydro-	2141, 4249		
96.	14722-38-4	Cinnoline, 4-methyl-	568b, 1587, 4249, 5811b		
97.	25042-83-5	5*H*-Cyclopentapyrazine 	1587, 4249		
98.	23747-47-9	5*H*-Cyclopentapyrazine, 6,7-dihydro-	568b, 4249		
99.	38917-63-4	5*H*-Cyclopentapyrazine, 6,7-dihydro-2,3-dimethyl-	1587, 1587a, 4249, 5811b		
100.		5*H*-Cyclopentapyrazine, 6,7-dihydro-5,7-dimethyl-	4570a		
101.	38917-60-1	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-ethyl-	1587, 1587a, 1590, 4249, 5811b		
102.	52517-53-0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-ethyl-	568b, 4249		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

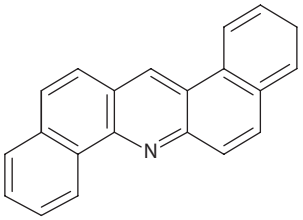
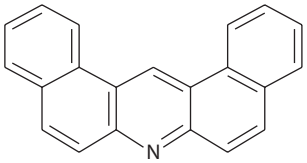
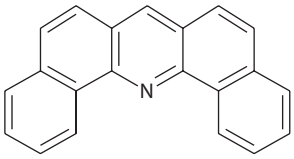
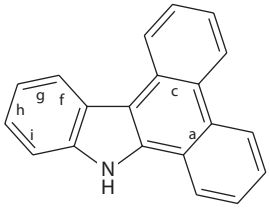
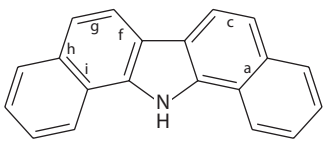
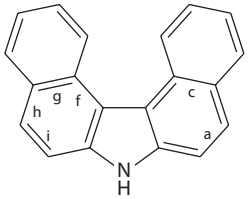
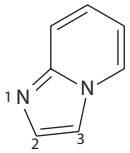
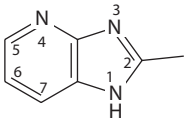
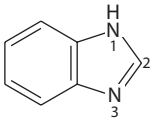
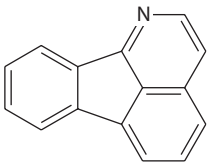
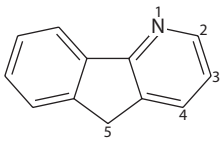
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
103.	23747-46-8	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-methyl-	1587, 1587a, 4249, 4570a, 5811b	1590	
104.	23747-48-0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-methyl-	1587, 1587a, 1590, 4249, 4570a, 5811b	174b, 3266	
105.	61891-57-4	5*H*-Cyclopentapyrazine, dimethyl-	2570, 3553, 4249, 5811b		
106.	61929-05-3	5*H*-Cyclopentapyrazine, 2,3-dimethyl-	568b, 4249		
107.	65129-00-2	5*H*-Cyclopentapyrazine, 2-ethyl-	568b, 4249		
108.	226-36-8	Dibenz[*a,h*]acridine 	126a, 139, 172, 239, 587, 1148, 1217, 1373, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1802, 1808, 1842, 1870, 1871, 2228, 2724, 2825, 2939, 3059, 3255, 3257, 3260, 3265, 3279, 3300, 3302, 3308, 3414, 3491, 3512, 3714, 3733–3735, 3741, 3750, 3752, 3797, 3999, 4005, 4009–4011, 4027, 4249, 4319, 4327, 4332, 5512, 5811b, 5869a		
109.	226-92-6	Dibenz[*a,i*]acridine	3337–3339, 4249		
110.	224-42-0	Dibenz[*a,j*]acridine 	126a, 172, 239, 587, 603, 1148, 1217, 1373, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1802, 1808, 1842, 1870, 1871, 2229, 2724, 2825, 2939, 3059, 3255, 3257, 3260, 3265, 3279, 3300, 3302, 3308, 3370, 3414, 3491, 3512, 3714, 3733–3735, 3750, 3752, 3797, 3999, 4005–4007, 4009–4011, 4027, 4249, 4317, 4319, 4327, 4332, 5512, 5811b, 5869a		
111.	224-53-3	Dibenz[*c,h*]acridine 	3337–3339, 4249		
112.	34442-52-9	1*H*-Dibenzo[*a,c*]carbazole 	3337–3339, 4249		
113.	207-84-1	7*H*-Dibenzo[*a,g*]carbazole	4249		
114.	239-63-4	5*H*-Dibenzo[*a,i*]carbazole	5811b		
115.	239-64-5	13*H*-Dibenzo[*a,i*]carbazole 	2120, 4249, 5811, 5811a		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
116.	194-59-2	7*H*-Dibenzo[*c,g*]carbazole 	126a, 172, 239, 587, 1148, 1217, 1373, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1802, 808, 1842, 1870, 1871, 2724, 2825, 2939, 3255, 3257, 3059, 3255, 3257, 3260, 3265, 3279, 3300, 3302, 3414, 3491, 3512, 3714, 3733–3735, 3750, 3752, 3797, 3999, 4005, 4009–4011, 4027, 4249, 4319, 4327, 4332, 5512, 5811b, 5869a		
117.	28641-62-5	5*H*-Dibenzo[*c,g*]carbazole	4249		
118.		1*H*-Imidazo[2.1-*a*]isoquinoline	568b, 4249		
119.	274-76-0	Imidazo[1,2-*a*]pyridine 	568b, 879, 3559, 4249		
120.		Imidazo[1,2-*a*]pyridine, C_2-alkyl-	3559		
121.	875-80-9	Imidazo[1,2-*a*]pyridine, 2,3-dimethyl-	568b, 3553, 3559, 4249, 5811b		
122.		1*H*-Imidazo[4,5-*b*]pyridine, methyl-	3559		
123.	68175-07-5	1*H*-Imidazo[4,5-*b*]pyridine, 2-methyl- 	568b, 1587, 3559, 4249, 5811b		
124.	27582-20-3	1*H*-Imidazo[4,5-*b*]pyridine, 7-methyl-	568b, 1587, 3559, 4249, 5811b		
125.	271-44-3	1*H*-Indazole 	568b, 4249		
126.	34879-87-3	1*H*-Indazole, 1,6-dimethyl-		2917a	
127.	206-56-4	Indeno[1,2,3-*ij*] isoquinoline{1-azafluoranthene} 	1041, 3733–3735, 3750, 3752, 4249		
128.		Indeno[1,2,3-*ij*]isoquinoline, dimethyl-	3733, 3750, 3752, 4249		
129.		Indeno[1,2,3-*ij*]isoquinoline, methyl-	3733, 3750, 3752, 4249		
130.	244-99-5	5*H*-Indeno[1,2-*b*]pyridine {4-azafluorene} 	1409, 1587, 1899, 3491, 3733–3735, 3750, 3752, 4249		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

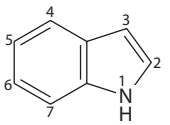
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
131.		5*H*-Indeno[1,2-*b*]pyridine, dimethyl-	3733, 3750, 3752, 4249		
132.		5*H*-Indeno[1,2-*b*]pyridine, methyl-	3733, 3750, 3752, 4249		
133.	120-72-9	1*H*-Indole {2,3-benzopyrrole} 	127, 172, 239, 568b, 722, 884, 918a, 1063–1066, 1068–1074, 1099, 1329, 1330, 1332, 1333, 1360, 1361, 1364, 1365, 1371, 1375, 1375a, 1375b, 1388–1390, 1423, 1426, 1427, 1437, 1580, 1586, 1649, 1744, 1765, 1767, 1778, 1842, 1881, 1898, 2005, 2060, 2387, 2493, 2506–2508, 2510, 2524a, 2537, 2543, 2545, 2552, 2553, 2570, 2601a, 2630, 2683, 2724–2727, 2731, 2735, 2596a, 2761, 2762, 2765–2767, 2773, 2775, 2799a, 2857, 2939, 3081, 3082, 3251, 3255–3257, 3265, 3279, 3286, 3300, 3302, 3308, 3386, 3397, 3410, 3491, 3493, 3504, 3506, 3555, 3557, 3559, 3729, 3733, 3741, 3750, 3752, 3797, 3886, 3887, 3890, 4249, 5034, 5512, 5811b	172, 404, 543a, 568b, 937, 984, 1063–1066, 1068–1074, 1256, 1590a, 2093, 2282, 2339a, 2386, 2389, 2544, 2611, 2917a, 3198, 3219, 3430, 3491, 3547, 3549, 3550, 3555, 3973, 4249, 5811b	1330, 1332, 1360, 1375a, 2387, 2506 (0), 2507 (0)
134.		1*H*-Indole, alkyl-	568b, 3251, 3279, 3286, 3504, 3506, 3559, 4249		
135.	55191-12-3	1*H*-Indole, 1,3-dibutyl-	2601a		
136.	496-15-1	1*H*-Indole, 2,3-dihydro- {indoline}	5034	984, 2339a, 4249	
137.	6872-06-6	1*H*-Indole, 2,3-dihydro-2-methyl-		2917a	
138.		1*H*-Indole, 2,3-dihydro-3-(3-pyridinyl)-	1587, 4249		
139.	78210-52-3	1*H*-Indole, 2,3-dihydro-3-(3-pyridinylmethyl)-	568b, 1587, 4249, 5811b		
140.	29930-57-2	1*H*-Indole, dimethyl-	127, 1365, 1373, 1778, 1898, 2543, 2545, 2570, 2727, 2731, 2735, 2773, 2939, 3251, 3255, 3279, 3286, 3308, 3410, 3491, 3504, 3506, 4249, 4332, 5811b		
141.	875-79-6	1*H*-Indole, 1,2-dimethyl-	568b, 1063–1066, 1068–1074, 1365, 1427, 1757, 2724, 3491, 3741, 4249, 5811b		
142.	875-30-9	1*H*-Indole, 1,3-dimethyl-	568b, 1063–1066, 1068–1074, 1580, 1757, 2510, 2570, 2767, 3081, 3082, 2767, 3491, 3741, 4249, 5811b		
143.	27816-52-0	1*H*-Indole, 1,4-dimethyl-	568b, 1748, 1757, 2510, 3491, 3741, 4249, 5811b		
144.	27816-53-1	1*H*-Indole, 1,5-dimethyl-	1063–1066, 1068–1074, 1748, 1757, 2510, 3491, 3741, 4249, 5811b		
145.	5621-15-8	1*H*-Indole, 1,6-dimethyl-	568b, 1748, 1757, 2510, 3491, 3741, 4249, 5811b		
146.	5621-16-9	1*H*-Indole, 1,7-dimethyl-	1748, 1757, 2510, 3491, 3741, 4249, 5811b		
147.	91-55-4	1*H*-Indole, 2,3-dimethyl-	568b, 933, 1375, 1375b, 1586, 2724, 2767, 3557, 4407, 4249, 5811b		
148.	1196-79-8	1*H*-Indole, 2,5-dimethyl-	568b, 4249, 4669, 5811b		
149.		1*H*-Indole, 2,6-dimethyl-	568b, 4249		
150.	3189-12-6	1*H*-Indole, 3,5-dimethyl-	568b, 4249, 5811b		
151.	5621-14-7	1*H*-Indole, 3,7-dimethyl-	568b, 1586, 2767, 2769, 3557, 3733–3735, 3750, 3752, 4249		
152.	54020-53-0	1*H*-Indole, 5,7-dimethyl-	568b, 4249		
153.	64844-47-9	1*H*-Indole, dimethylethyl-	1765, 1778, 2724, 3733, 3735, 3750, 3752, 4249, 5811b		
154.	64844-49-1	1*H*-Indole, dimethylpropyl-	1650, 1652, 3732, 3757, 4249, 5811b		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
155.	97542-81-9	1*H*-Indole, ethyl-	430, 1650, 1652, 2387, 2543, 2545, 2570, 2767, 3732, 3757, 4249, 5811b, 1D01		2387
156.	10604-59-8	1*H*-Indole, 1-ethyl-	568b, 1747, 1757, 2510, 3491, 3741, 4249, 5811b		
157.	3484-18-2	1*H*-Indole, 2-ethyl-	1364, 1371, 1765, 1777, 2724, 2775, 3410, 3650, 4249, 4332		
158.	1484-19-1	1*H*-Indole, 3-ethyl-	568b, 1360, 1364, 1373, 1375, 1375a, 1375b, 1426, 1417, 1586, 1757, 1765, 1778, 2543, 2545, 2724, 2761, 2762, 2765–2767, 2773, 2777, 3410, 3491, 3557, 3650, 3797, 4249, 5811b		1360, 1375a
159.	68742-28-9	1*H*-Indole, 5-ethyl-	3734, 4249		
160.	64844-45-7	1*H*-Indole, ethylmethyl-	3735, 4249, 5811b		
161.	64844-50-4	1*H*-Indole, ethylpropyl-	3733–3735, 3750, 3752, 4249, 5811b		
162.	27323-28-0	1*H*-Indole, methyl-	127, 430, 1371, 1426, 1898, 2387, 2506, 2507, 2543, 2545, 2570, 2727, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 3251, 3279, 3286, 3308, 3410, 3491, 3504, 3506, 4249, 5811b	3430, 5811b	2387, 2506 (0), 2507 (0)
163.	603-76-9	1*H*-Indole, 1-methyl-	568b, 1427, 1580, 1587, 1757, 1781, 2510, 3081, 3082, 3300, 3491, 3493, 3559, 3741, 4009–4011, 4249, 4570a, 5811b		
164.	95-20-5	1*H*-Indole, 2-methyl-	568b, 884, 1063–1066, 1068–1074, 1364, 1426, 1427, 2387, 2601a, 3255, 3308, 3491, 4249, 5811b	404, 568b, 4249	2387
165.	83-34-1	1*H*-Indole, 3-methyl- {skatole}	293, 568b, 722, 918a, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1360, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1388–1390, 1426, 1427, 1580, 1586, 1744, 1765, 1778, 1842, 1880, 1898, 2387, 2510, 2537, 2545, 2683, 2724–2727, 2732, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2939, 3081, 3082, 3251, 3255, 3266, 3279, 3286, 3302, 3308, 3386, 3397, 3410, 3491, 3504, 3506, 3553, 3557, 3559, 3650, 3797, 3886, 3887, 4249, 4407, 5512, 5811b	568b, 1053, 3266, 4249	1330, 1332, 1360, 1375a, 2387
166.	16096-32-5	1*H*-Indole, 4-methyl-	568b, 3255, 4249, 4579		
167.	614-96-0	1*H*-Indole, 5-methyl-	568b, 1063–1066, 1068–1074, 1364, 1426, 1427, 3255, 3491, 4249, 5811b		
168.	3420-02-8	1*H*-Indole, 6-methyl-	568b, 4249, 4570		
169.	933-67-5	1*H*-Indole, 7-methyl-	568b, 1063–1066, 1068–1074, 1364, 1426, 1427, 3491, 4249, 5811b		
170.		1*H*-Indole, (1-methylethyl)-	1778		
171.	64844-52-6	1*H*-Indole, methylphenyl-	2724, 5811, 5811a, 5811b		
172.	64844-46-8	1*H*-Indole, methylpropyl-	3504, 3733–3735, 3750, 3752, 4249, 5811b		
173.		1*H*-Indole, 1-phenyl-	568b, 4249		
174.	948-65-2	1*H*-Indole, 2-phenyl-	568b, 942, 1765, 2724, 4249	568b, 1854, 4249	
175.	1504-16-1	1*H*-Indole, 3-phenyl-	568b, 942, 1765, 2724, 3491, 4249, 4332, 5811b		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

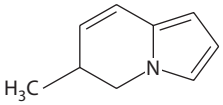
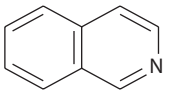
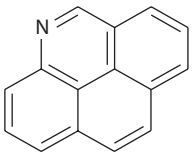
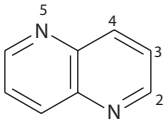
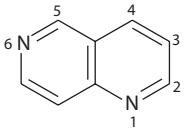
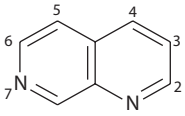
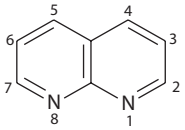
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
176.	64844-44-6	1*H*-Indole, propyl-	3504, 3506, 3733–3735, 3750, 3752, 4249, 5811b		
177.	1859-92-3	1*H*-Indole, 3-propyl-	1364, 1765, 1778, 2724, 3491, 4249, 5811b		
178.	64844-48-0	1*H*-Indole, tetramethyl-	3504, 3733–3735, 3750, 3752, 4249, 5811b		
179.	30642-36-5	1*H*-Indole, trimethyl-	127, 1364, 1373, 1778, 2543, 2724, 2731, 2733, 2735, 2767, 2939, 3251, 3279, 3286, 3308, 3491, 3504, 3506, 3557, 3888, 4249, 4332		
180.	1971-46-6	1*H*-Indole, 1,2,3-trimethyl-	568b, 1063–1066, 1068–1074, 2724, 2727, 2731, 2735, 2767, 3491, 3557, 4249, 5811b		
181.	10299-63-5	1*H*-Indole, 2,3,4-trimethyl-	5811, 5811a, 5811b		
182.	21296-92-4	1*H*-Indole, 2,3,5-trimethyl-	933, 3734, 3741, 4249, 5811b		
183.	22072-35-1	1*H*-indole, 2,3,6-trimethyl-	5811, 5811a, 5811b		
184.	27505-78-8	1*H*-Indole, 2,3,7-trimethyl-	5811, 5811a, 5811b		
185.		1*H*-Indole, 4.5.6-trimethyl-	568b, 4249		
186.	54340-99-7	1*H*-Indole, 5,6,7-trimethyl-	2570, 4249		
187.	1761-10-0	Indolizine, 3-methyl-		984, 4249	
188.	1761-11-1	Indolizine, 6-methyl- 	568b, 1587, 4249, 5811b		
189.	119-65-3	Isoquinoline 	27, 35, 167, 172, 568b, 722, 1099, 1360, 1371, 1375a, 1586, 1649, 1880, 2008, 2228, 2327c, 2543, 2724–2727, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3308, 3386, 3397, 3398, 3463, 3491, 3499, 3729, 3733–3735, 3750, 3752, 3797, 4249, 5034, 5811b	172, 568b, 4249, 5811b	1360, 1375a
190.	64828-50-8	Isoquinoline, butyl-	2141, 4249, 5811b		
191.	7661-38-3	Isoquinoline, 1-butyl-	568b, 1587, 4249		
192.	64973-79-1	Isoquinoline, dihydro-	2132, 4249, 5811b		
193.	65312-77-8	Isoquinoline, dihydroethyl-	2141, 4249, 5811b		
194.	65312-79-0	Isoquinoline, dihydromethyl-	2141, 4249, 5811b		
195.		Isoquinoline, dimethyl-	3733, 3750, 3752		
196.	64828-51-9	Isoquinoline, ethyl-	1042, 4249, 5811b		
197.	58853-80-8	Isoquinoline, methyl- {several methylquinolines detected in MSS}	568b, 1587, 3733, 3750, 3752, 4249, 5811b		
198.	1721-93-3	Isoquinoline, 1-methyl-	568b, 1587, 3386, 4249, 5811b		
199.	4965-09-7	Isoquinoline, 1-methyl-1,2,3,4-tetrahydro-	568b, 4249		
200.	1125-80-0	Isoquinoline, 3-methyl-	568b, 1587, 4249, 5811b		
201.	64828-49-5	Isoquinoline, (1-methylethyl)-	2141, 4249, 5811b		
202.	65312-75-6	Isoquinoline, methyltetrahydro-	2141, 2765, 2766, 4249, 5811, 5811a, 5811b		
203.	64849-98-5	Isoquinoline, propyl-	2141, 4249, 5811b		
204.	29832-78-8	Isoquinoline, tetrahydro-	1360, 1369, 1375a, 2141, 2761, 2762, 4249, 5811b		1360, 1375a
205.	91-21-4	Isoquinoline, 1,2,3,4-tetrahydro-	568b, 4249		
206.	36556-06-6	Isoquinoline, 5,6,7,8-tetrahydro-	568b, 4249		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
207.	313-80-4	Naphtho[2,1,8-*def*]quinoline {1-azapyrene} 	2120, 3733–3735, 3741, 3750, 3752, 4249, 5811b		
208.		Naphtho[2,1,8-*def*]quinoline, dimethyl-	3733, 3750, 3752		
209.		Naphtho[2,1,8-*def*]quinoline, methyl-	3733, 3750, 3752		
210.		Naphtho[2,1,8-*def*]quinoline, trimethyl-	3733, 3750, 3752		
211.		Naphthyridine	2141		
212.		Naphthyridine, C_2-alkyl-	4248		
213.		Naphthyridine, 3-butyryl-	1587		
214.		Naphthyridine, 3-methyl-	1587		
215.	254-79-5	1,5-Naphthyridine {1,5-diazanaphthalene; pyrido[3,2-*b*]pyridine} 	568b, 1587, 2132, 2141, 4249		
216.	18937-71-8	1,5-Naphthyridine, 3-methyl-	568b, 1587, 4249, 5811b		
217.	253-72-5	1,6-Naphthyridine {1,6-diazanaphthalene; pyrido[4,3-*b*]pyridine} 	1587, 2132, 4249		
218.	14757-43-8	1,6-Naphthyridine, 3-methyl-	568b, 1587, 4249, 5811b		
219.	253-69-0	1,7-Naphthyridine {1,7-diazanaphthalene; pyrido[3,4-*b*]pyridine} 	2141, 4249, 5811b		
220.		1,8-Naphthyridine, 3-butanoyl-	568b, 4249		
221.	254-60-4	1,8-Naphthyridine {1,8-diazanaphthalene; pyrido[2,3-*b*]pyridine} 	2141, 3255, 4249		
222.	14757-45-0	1,8-Naphthyridine, 2,6-dimethyl-	4249		
223.	14759-22-9	1,8-Naphthyridine, 3-methyl-	568b, 1587, 2327c, 4249		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

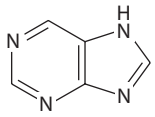
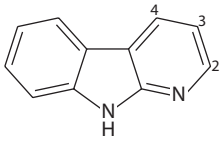
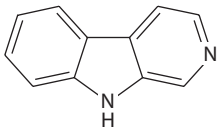
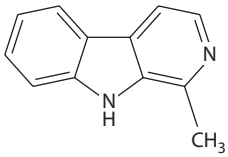
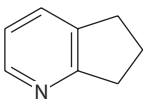
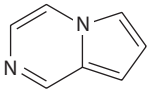
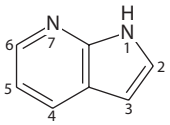
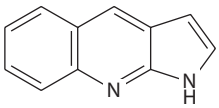
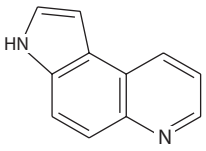
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
224.	120-73-0	1*H*-Purine 		2939, 3215, 3973, 4249, 5079, 5413	
225.	51953-03-8	9*H*-Purine-		568b, 4249	
226.		Pyridoindole	1587		
227.		Pyridoindole, butyl-	1587		
228.		Pyridoindole, C_3-alkyl-	1587		
229.	80700-46-5	Pyridoindole, *N*-methyl-	3733, 3750, 3752, 5811a		
230.	244-76-8	1*H*-Pyrido[2,3-b]indole 	1587, 2724, 3302, 3491, 3797, 3888, 4249		
231.	72693-00-6	1*H*-Pyrido[2,3-*b*]indole, 1-butyl-	568b, 1587, 4249		
232.	61893-11-6	1*H*-Pyrido[2,3-*b*]indole, 2-ethyl-	568b, 3553, 4249		
233.	17276-85-8	1*H*-Pyrido[2,3-*b*]indole, 2-methyl-	568b, 1587, 4249, 5811b		
234.	76162-60-2	1*H*-Pyrido[2,3-*b*]indole, 3-methyl-	1587, 4249		
235.	78210-53-4	1*H*-Pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-	568b, 1587, 4249		
236.	78210-54-5	1*H*-Pyrido[2,3-*b*]indole, 2-pentyl-	568b, 1587, 4249		
237.	245-08-9	5*H*-Pyrido[3,2-*b*]indole	5811a		
238.	244-69-9	5*H*-Pyrido[4,3-*b*]indole	568b, 4249		
239.	244-63-3 8001-81-8	9*H*-Pyrido[3,4-*b*]indole, ?-methyl- = {?-methylnorharman} β-carboline = 2-azacarbazole} 	179a, 179b, 568b, 635, 1375, 1375b, 1587, 1702, 1898, 1899, 2142, 2354a, 2450, 2484a, 2601a, 2678, 2724, 2939, 2972, 3059, 3255, 3279, 3302, 3308, 3491, 3505, 3733–3735, 3739–3742, 3750, 3752, 3797, 3952, 4103, 4249, 4389, 4390, 4407, 4763, 5811b	568b, 1702, 2972, 3491, 3797, 3973, 3974a, 4249, 4763	
240.	10371-85-4	9*H*-Pyrido[3,4-*b*]indole, 1-butyl-	1587, 4249, 5811b		
241.	20127-61-1	9*H*-Pyrido[3,4-*b*]indole, 1-ethyl-	568b, 3553, 4249		
242.	5667-11-8	9*H*-Pyrido[3,4-*b*]indole, methyl- = {methylnorharman} {?-methylnorharman}	3739–3741		
243.	486-84-0	9*H*-Pyrido[3,4-*b*]indole, 1-methyl- = {harman} {1-methylnorharman} 	126b, 172, 179a, 179b, 237, 568b, 635, 1375, 1375b, 1445, 1587, 1674, 1702, 1898, 2133, 2142, 2354a, 2450, 2484a, 2601a, 2678, 2724, 2939, 2972, 3059, 3255, 3279, 3302, 3308, 3491, 3505, 3553, 3733–3735, 3739–3741, 3742, 3750, 3752, 3797, 3952, 4103, 4249, 4332, 4389, 4390, 5811b	172, 568b, 1702, 2972, 3491, 3797, 3973, 3974a, 4249	
244.	78210-55-6	9*H*-Pyrido[3,4-*b*]indole, 1-(1-propenyl)-	568b, 1587, 4249, 5811b		
245.	533-37-9	5*H*-1-Pyrindine, 6,7-dihydro- 	568b, 1371, 1587, 4249, 5811b		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
246.	274-45-3	Pyrrolo[1,2-*a*]pyrazine 	568b, 1351, 1587, 1587a, 3410, 3553, 4249, 5811b		
247.		Pyrrolo[1.2-*a*]pyrazine, 3,6-dimethyl-	568b, 4249		
248.	274-40-8	Pyrrolo[1,2-*a*]pyridine	4249		
249.	271-63-6	1*H*-Pyrrolo[2,3-*b*]pyridine {7-azaindole} 	568b, 879, 2724, 3386, 3491, 3733, 3750, 3752, 3797, 3888, 4249, 5811b		
250.		1*H*-Pyrrolo[2,3-*b*]pyridine, C_3-alkyl-	1587, 4249		
251.		1*H*-Pyrrolo[2,3-g]pyridine, diethyl-	3733, 3750, 3752, 4249		
252.	78249-85-1	1*H*-Pyrrolo[2,3-b]pyridine, ethyl-	568b, 1587, 3733, 3750, 3752, 4249, 5811b		
253.	72692-80-9	1*H*-Pyrrolo[2,3-*b*]pyridine, methyl- {at least 4-methyl isomers other than the 1- and 2-methyl- compounds}	568b, 1371, 1587, 2543, 2552, 2773, 2775, 3255, 3410, 3559, 3733, 3750, 3752, 4249, 5811b		
254.	27257-15-4	1*H*-Pyrrolo[2,3-*b*]pyridine, 1-methyl-	568b, 1370, 1587, 3255, 3559, 5811b		
255.	23612-48-8	1*H*-Pyrrolo[2,3-*b*]pyridine, 2-methyl-	568b, 1587, 3559, 4249		
256.		1*H*-Pyrrolo[2,3-*g*]pyridine, diethyl-	3733–3735, 3750, 3752, 4249		
257.		1*H*-Pyrrolo[2,3-*g*]pyridine, dimethyl-	3733–3735, 3750, 3752, 4249		
258.		1*H*-Pyrrolo[2,3-*g*]pyridine, ethylmethyl-	3733–3735, 3750, 3752, 4249		
259.		1*H*-Pyrrolo[2,3-*g*]pyridine, (1-methylethyl)-	3733–3735, 3750, 3752, 4249		
260.		1*H*-Pyrrolo[2,3-*g*]pyridine, methyl-(1-methylethyl)-	3733–3735, 3750, 3752, 4249		
261.		1*H*-Pyrrolo[2,3-*g*]pyridine, pentamethyl-	3733–3735, 3750, 3752, 4249		
262.		1*H*-Pyrrolo[2,3-*g*]pyridine, trimethyl-	3733–3735, 3750, 3752, 4249		
263.		Pyrroloquinoline	3733–3735, 3750, 3752, 4249		
264.		Pyrroloquinoline, dimethyl-	3733, 3750, 3752, 4249		
265.		Pyrroloquinoline, methyl-	3733, 3750, 3752, 4249		
266.		Pyrroloquinoline, trimethyl-	3733, 3750, 3752, 4249		
267.	268-91-7	1*H*-Pyrrolo[2,3-*b*]quinoline 	3733–3735, 3750, 3752, 4249		
268.	233-36-3	1*H*-Pyrrolo[2,3-*f*]quinoline 	3733–3735, 3750, 3752, 4249		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

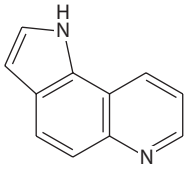
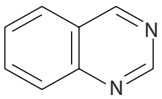
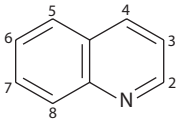
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
269.	232-85-9	3*H*-Pyrrolo[3,2-*f*]quinoline 	3733–3735, 3750, 3752, 4249		
270.	253-82-7	Quinazoline {1,3-benzodiazine} 	568b, 1587, 4249, 5811b		
271.	64811-59-2	Quinazoline, dihydro-	4249, 5811b		
272.	64828-47-3	Quinazoline, ethyl-	2141, 4249, 5811b		
273.	64828-48-4	Quinazoline, methyl-	2141, 4249, 5811b		
274.	700-79-8	Quinazoline, 2-methyl-	568b, 4249		
275.	700-46-9	Quinazoline, 4-methyl-	1587, 4249, 5811b		
276.	91-22-5	Quinoline {1-azanaphthalene} 	27, 35, 126a, 126b, 167, 172, 174b, 174c, 237, 402, 568b, 688, 722, 1077a, 1099, 1148, 1217, 1263, 1360, 1371, 1375, 1375a, 1375b, 1386, 1426, 1427, 1437, 1445, 1586, 1647, 1649, 1656, 1674, 1727, 1740, 1741, 1743, 1744, 1773, 1839, 1842, 1853b, 1880, 1881, 2006, 2132, 2133, 2134a, 2142, 2228, 2270, 2543, 2545, 2724–2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2939, 3007, 3140, 3190, 3255, 3257, 3265, 3300, 3302, 3308, 3386, 3397, 3398, 3410, 3463, 3491, 3499, 3557, 3559, 3729, 3733–3735, 3750, 3752, 3992, 4010, 4011, 4249, 4319, 4407, 4570a, 4830, 4921, 5034, 5079, 5512, 5811b, 5836, 25A84	172, 568b, 937, 2339a, 2359, 2389, 2544, 2917a, 3491, 3547, 3973, 3974a, 3974b, 4249, 5811b	1360, 1375a
277.		Quinoline, C_3-alkyl-	568b, 1587, 2570, 4249		
278.		Quinoline, alkyl-2-methyl-	3386		
279.		Quinoline, alkyl-3-methyl-	4249		
280.		Quinoline, alkyl-4-methyl-	4249	937, 3491	
281.	53452-65-6	Quinoline, butyl-	2132, 4249, 5811b		
282.	7634-74-4	Quinoline, 6-butyl-	568b, 4249		
283.		Quinoline, 7-butyl-	568b, 4249		
284.	2051-28-7	Quinoline, decahydro-	5811		
285.	29968-14-7	Quinoline, dihydro-	4249		
286.	65312-76-7	Quinoline, dihydroethyl-	2141, 4249, 5811b		
287.	65312-78-9	Quinoline, dihydromethyl-	2141, 4249, 5811b		
288.	28351-04-4	Quinoline, dimethyl-	568b, 1587, 2132, 2543, 2570, 2724–2727, 2731, 2732, 2735, 2767, 2773, 2775, 3491, 3733, 3750, 3752, 4249, 4570a, 5811, 5811a, 5811b		
289.	1198-37-4	Quinoline, 2,4-dimethyl-	568b, 4249		
290.	26190-82-9	Quinoline, 2,5-dimethyl-	440, 441, 4249		
291.	877-43-0	Quinoline, 2,6-dimethyl-	440, 441, 568b, 3491, 4249, 5811b	5811b	
292.	1463-17-8	Quinoline, 2,8-dimethyl-	568b, 1587, 4249, 5811b		

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
293.		Quinoline, 3.6-dimethyl-	1041, 1042, 2142, 3255, 4249		
294.	2623-50-9	Quinoline, 5,8-dimethyl-	568b, 1587, 4249, 5811b		
295.	53123-73-2	Quinoline, ethyl-	1041, 1042, 1644, 1645, 2132, 2141, 2142, 3255, 4249, 4570a, 5811b		
296.	1613-34-9	Quinoline, 2-ethyl-	568b, 1587, 4249, 5811b		
297.	56717-33-0	Quinoline, 2-ethyl-5,6,7,8-tetrahydro-	568b, 1587, 4249, 5811b		
298.	1873-54-7	Quinoline, 3-ethyl-	568b, 4249		
299.	19020-26-9	Quinoline, 4-ethyl-	568b, 1587, 2141, 4249, 5811b		
300.	65745-66-6	Quinoline, 5-ethyl-	568b, 4249		
301.	7661-47-4	Quinoline, 7-ethyl-	568b, 4249		
302.	78249-84-0	Quinoline, 7-ethyl-5,6,7,8-tetrahydro-	568b, 1587, 4249, 5811b		
303.	19655-56-2	Quinoline, 8-ethyl-	568b, 4249		
304.	27601-00-9	Quinoline, methyl-	27, 35, 167, 1041, 1042, 1360, 1375a, 1426, 1427, 1644, 1645, 1649, 2132, 2142, 2543, 2570, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765, 2766, 2773, 2777, 3255, 3491, 3559, 4249, 4570a, 5811b		1360, 1375a
305.	65312-74-5	Quinoline, methyltetrahydro-	2765, 2766, 4249, 5811b		
306.	78249-82-8	Quinoline, methyl-1,2,3,4-tetrahydro- {several isomers present in MSS}	568b, 1587, 4249, 5811b		
307.	91-63-4	Quinoline, 2-methyl-	27, 35, 568b, 1041, 1042, 2142, 2545, 3386, 3733, 3750, 3752, 4249		
308.	2617-98-3	Quinoline, 2-methyl-5,6,7,8-tetrahydro-	568b, 1587, 4249, 5811b		
309.	612-58-8	Quinoline, 3-methyl-	27, 35, 568b, 1041, 1042, 2327c, 3733, 3750, 3752, 4249		
310.	28712-62-1	Quinoline, 3-methyl-5,6,7,8-tetrahydro-	5811		
311.	491-35-0	Quinoline, 4-methyl-	27, 35, 568b, 1041, 1042, 2142, 2327c, 2570, 2769, 2773, 3255, 3386, 3733, 3750, 3752, 4249, 5811b	937	
312.	7661-55-4	Quinoline, 5-methyl-	27, 35, 1041, 1042, 2142, 3255, 3733, 3750, 3752, 4249		
313.	91-62-3	Quinoline, 6-methyl-	27, 35, 568b, 1041, 1042, 3733, 3750, 3752, 4249, 5811b		
314.	612-60-2	Quinoline, 7-methyl-	27, 35, 1041, 1042, 2142, 3255, 3386, 3733, 3750, 3752, 4249, 5811b		
315.	78249-83-9	Quinoline, 7-methyl-5,6,7,8-tetrahydro-	568b, 1587, 4249, 4570a, 5811b		
316.	611-32-5	Quinoline, 8-methyl-	27, 35, 1041, 1042, 1587, 2142, 2570, 2769, 3255, 3733–3735, 3750, 3752, 4249		
317.	1333-53-5	Quinoline, (1-methylethyl)-	2132, 2141, 4249, 5811b		
318.	17507-24-3	Quinoline, 2-(1-methylethyl)-	568b, 4249		
319.	17507-25-4	Quinoline, 4-(1-methylethyl)-	568b, 4249		
320.	64828-52-0	Quinoline, propyl-	1041, 1042, 2132, 2141, 2142, 3255, 4249, 5811b		
321.	7661-53-2	Quinoline, 8-propyl-	568b, 4249		
322.	6294-65-1	Quinoline, 2-(3-pyridyl)-	568b, 4249		
323.		Quinoline, tetrahydro-	1360, 1375a, 2761, 2762		1360, 1375a
324.	635-46-1	Quinoline, 1,2,3,4-tetrahydro-	568b, 1587, 4249		
325.	10500-57-9	Quinoline, 5,6,7,8-tetrahydro-	568b, 1587, 4249, 4570a, 5811b		

(*continued*)

TABLE 17.21 (continued)
Aza-Arenes and Other Polycyclic Nitrogen Compounds in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

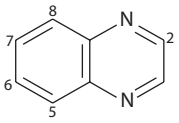
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
326.	76602-27-2	Quinoline, tetramethyl-	2132, 3733–3735, 3750, 3752, 4249		
327.	51366-52-0	Quinoline, trimethyl-	2132, 3733–3735, 3750, 3752, 4249		
328.	4945-28-2	Quinoline, 2,3,8-trimethyl-	568b, 1587, 4249, 5811b		
329.	91-19-0	Quinoxaline {1,4-benzodiazine} 	568b, 1587, 1587a, 1590, 2724, 3491, 3797, 3888, 4249, 4570a, 5811b		
330.	64811-58-1	Quinoxaline, dihydro-	568b, 3559, 4249, 5811b		
331.	72692-77-4	Quinoxaline, dimethyl-	568b, 1587, 3559, 4249		
332.	2379-55-7	Quinoxaline, 2,3-dimethyl-	568b, 4249		
333.	64828-46-2	Quinoxaline, ethyl-	2141, 4249, 5811b		
334.		Quinoxaline, 2-ethyl-	568b, 4249		
335.	37920-99-3	Quinoxaline, 2-ethyl-3-methyl-	568b, 4249		
336.	7251-61-8	Quinoxaline, 2-methyl-	568b, 1587, 3266, 4249, 5811b		
337.	38917-65-6	Quinoxaline, 2-methyl-5,6,7,8-tetrahydro-	568b, 1587, 1590, 2761, 2762, 2765, 2766, 2769, 2773, 2775, 2777, 4249, 5811b		
338.	13708-12-8	Quinoxaline, 5-methyl-		172a, 174b, 1053, 3266	
339.	64828-56-4	Quinoxaline, 7-methyl-	568b, 1075, 1587, 4249, 5811b		
340.	34413-35-9	Quinoxaline, 5,6,7,8-tetrahydro-	4570a	172a, 174b, 1053, 3266	
341.	72692-78-5	Quinoxaline, trimethyl-	568b, 1587, 4249, 5811b		
342.	195-84-6	Tricycloquinazoline	3337, 3339, 4249		
343.	28522-57-8	Tricycloquinazoline, 3-methyl-	3338, 3339, 4249		

TABLE 17.22
Structures of Aza-Arenes in Tobacco and Tobacco Smoke

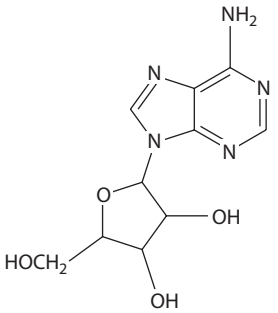
	Identified in Smoke				Present in Tobacco			
	No. of Nitrogens				No. of Nitrogens			
Ring Type	1	2	3	Total	1	2	4	Total
Bicyclic	130	66	4	200	15	4	2	21
Tricyclic	62	29	0	91	2	2	0	4
Tetracyclic	33	0	0	33	0	0	0	0
Pentacyclic	11	0	0	11	0	0	0	0
Hexacyclic	0	1	0	1	0	0	0	0
Total	236	96	4	336	17	6	2	25

and 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ), both compounds being components in broiled fish, fried beef, and beef extract. As indicated in Table 17.24, both 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ) (4367, 4368) and 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ) (2039) have been reported in tobacco smoke.

Rodgman (3253a) discussed the theoretical relationships (Figures 17.15 and 17.16) among glutamic acid {XII}, its possible degradation products, 4-aminobutanoic {XIII} and 2-aminobutanoic acid {XIV}, 2-amino-3-methylpyridine {XV} and 2-amino-6-methylpyridine {XVI}, 2-aminopyridine {XVII}, and the possible reactions between these substituted aminopyridines to form 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) {VI}, 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2) {VII}, and two similar products, 2-amino-9-methyldipyrido[1,2-*a*: 3′,2′-*d*]imidazole {XVII} and 2-amino-3,6-dimethyldipyrido[1,2-*a*:3′,2′-*d*]imidazole {XIX}, not yet identified in tobacco smoke or cooked foods. The aminobutanoic acids {XIII and XIV} and the aminopyridines {XV–XVII} noted in Figures 17.15 and 17.16 have been reported as tobacco smoke components.

Rodgman also discussed the already identified and other possible theoretical relationships (Figure 17.17) between tryptophan {XX} and 9*H*-pyrido[3,4-*b*]indole (norharman) {II}; its methyl homolog 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) {III} and other substituted norharmans {VI, R = C_2H_5, $CH_3CH{=}CH$, and *n*-C_4H_9}; the tryptophan pyrolysis products 3-amino-1,4-dimethyl-5*H*-pyrido-[4,3-*b*]indole

TABLE 17.23
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	58-61-7	Adenosine 		429b, 4249, 4828, 5540	
2.	60-92-4	Adenosine, cyclic 3′,5′-(hydrogen phosphate)		429b, 4249	
3.	139636-55-8	Adenosine, 2′-deoxyadenylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxyadenylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxycytidylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxy-		4249	
4.	146689-29-4	Adenosine,2′-deoxycytidylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxyguanylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxyguanylyl-(5′→3′)-2′-deoxy-		4249	
5.	28542-78-1	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-		2371a, 4249, 4523	
6.	6025-53-2	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*E*)-		683a, 2371a, 4066a, 4249	
7.	15896-46-5	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*Z*)-		2371a, 4249, 4582	
8.	26190-61-4	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-		2371a, 4249	
9.	53274-45-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*E*)-		2371a, 4249, 4778	
10.	52049-48-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*Z*)-		2371a, 4249, 4778	
11.	22663-55-4	Adenosine, *N*-(4-hydroxy-3-methylbutyl)-		960a, 2371a, 4249	
12.	7724-76-7	Adenosine, *N*-(3-methyl-2-butenyl)-		2371a, 4249, 4522	
13.	75081-82-2	Adenosine, *N*-[3-methyl-4-[(*O*-phosphono-β-*D*-glucopyranosyl)oxy]-2-butenyl]-, (*E*)-		429b, 4249, 4813	
14.	4294-16-0	Adenosine, *N*-(phenylmethyl)-		2371a	
15.	4294-16-0	Adenosine, *N*-(phenylmethyl)-		2371a	
16.	56-65-5	Adenosine 5′-(tetrahydrogen triphosphate)		429b	
17.	40922-97-2	Adenosine 5′-(tetrahydrogen triphosphate), *N*-(phenylmethyl)-		2371a	
18.	53-57-6	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4708	—

(*continued*)

TABLE 17.23 (continued)
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

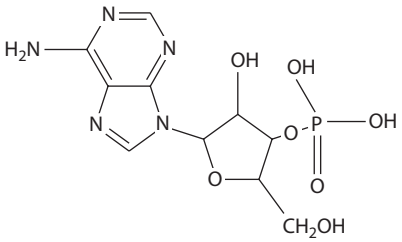
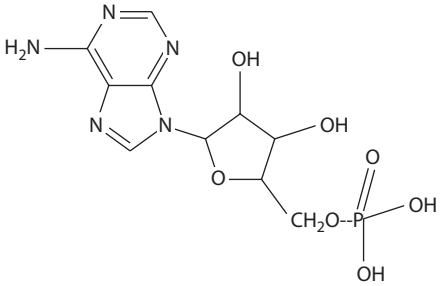
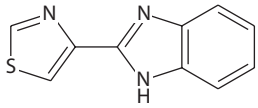
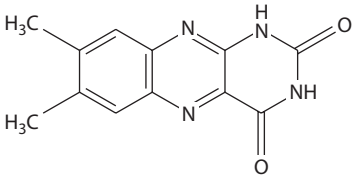
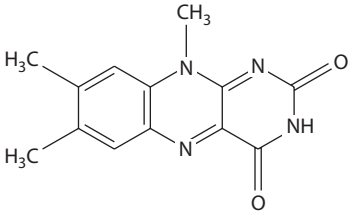
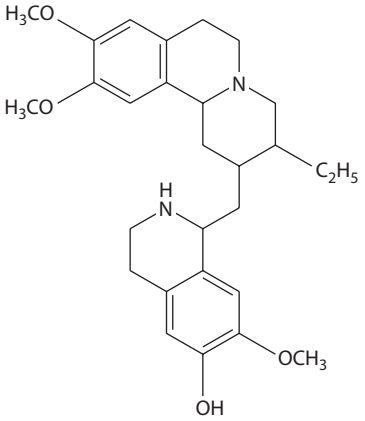
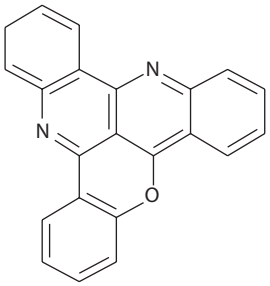
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
19.	53-59-8	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249	
20.	7298-93-3	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
21.	55030-93-8	Adenosine 5′-(trihydrogen diphosphate), *N*-(3-methyl-2-butenyl)-		429b	
22.	22732-83-8	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester		4249, 4617	
23.	40811-89-0	Adenosine 5′-(trihydrogen diphosphate), *N*-(phenylmethyl)-		2371a, 4249	
24.	58-68-4	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		429b, 4249, 4510	
25.	53-84-9	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		429b, 4249, 4670	
26.	84-21-9	3′-Adenylic acid 		429b, 4249, 4758	
27.	61-19-8	5′-Adenylic acid 		429b, 4249	
28.	20268-93-3	5′-Adenylic acid, *N*-(3-methyl-2-butenyl)-		4249, 4536	
29.	13484-66-7	5′-Adenylic acid, *N*-(phenylmethyl)-		4249	
30.	148-79-8	1*H*-Benzimidazole, 2-(4-thiazolyl)- 	568b, 2207, 4249	568b, 2207, 3633, 4249	
31.	4250-90-2	Benzo[*g*]pteridine-10(2*H*)-acetaldehyde, 3,4-dihydro-7,8-dimethyl-2,4-dioxo-		4249	

TABLE 17.23 (continued)
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
32.	1086-80-2	Benzo[*g*]pteridine-2,4(1*H*,3*H*)-dione, 7,8-dimethyl-		4249	
					
33.	1088-56-8	Benzo[*g*]pteridine-2,4(3*H*,10*H*)-dione, 7,8,10-trimethyl-		4249	
					
34.	483-17-0	Cephalin		5079, 5375	
					
35.	4607-33-4	Dibenzo[*b,h*][1]benzopyrano[2,3,4-*de*][1,6]naphthyridine	3339, 4249		
					

(*continued*)

TABLE 17.23 (continued)
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

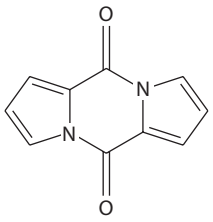
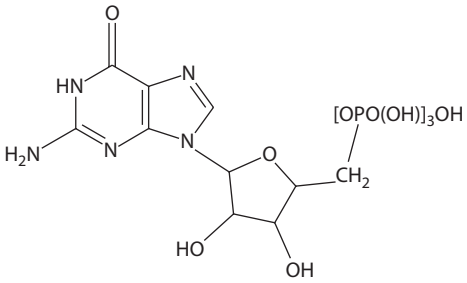
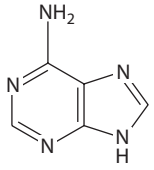
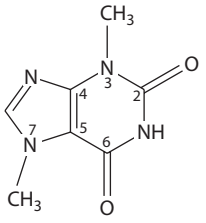
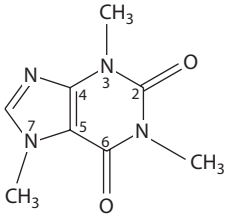
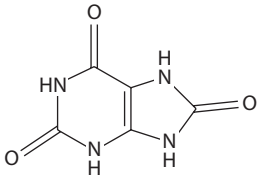
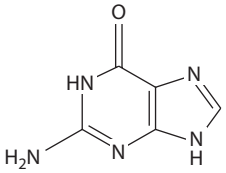
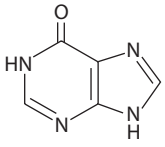
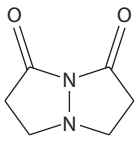
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
36.	484-73-1	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione {pyrocoll} 	127, 568b, 1364, 1371, 1586, 2387, 2543, 2545, 2592, 2724, 2767, 2773, 2775, 2939, 3059, 3251, 3255, 3279, 3308, 3410, 3491, 3505, 3553, 3886, 3887, 4249	5747	2387
37.	59017-02-6	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, 1,2,3,5a,8,10a-hexahydro-, (5aS-*cis*)-	3553, 4249		
38.		5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, 1,2,3,5a,8,10a-hexahydro-3-methyl-	3553, 4249		
39.	71277-95-7	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, methyl-	1899, 3491, 4249		
40.	6708-06-1	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, octahydro-	568b, 3553, 4249, 5811b		
41.	75039-16-6	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl, mono(dihydrogen phosphate) (ester), (*E*)-		4249, 4813	
42.	62512-96-3	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino) butyl		4249	
43.	86-01-1	Guanosine 5′-(tetrahydrogen triphosphate) 		4249	
44.	120293-52-9	1*H*-Imidazo[4,5-*c*]pyridine-4-propanoic acid, 4,6-dicarboxy-4,5,6,7-tetrahydro-, (4R-*cis*)-		4249	
45.	40000-89-3	1,8-Naphthyridin-2(1*H*)-one, 3-methyl-	3553, 4249		
46.	73-24-5	1*H*-Purin-6-amine {adenine} 		120, 568b, 2270, 2539, 2939, 3491, 3797, 3973, 3974a, 4249, 5079, 5189, 5311, 5435, 5436, 5478	
47.	525-79-1	1*H*-Purin-6-amine, *N*-(2-furanylmethyl)-		3973, 4249, 4509	
48.	2365-40-4	1*H*-Purin-6-amine, *N*-(3-methyl-2-butenyl)-		4249, 4590	
49.	1214-39-7	1*H*-Purin-6-amine, *N*-(phenylmethyl)-		3973, 4249, 4557	
50.	56159-42-3	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-		4249, 4603	
51.	38477-23-5	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-		4249, 4603	
52.	54538-20-4	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-		4249, 4620	
53.	69-89-6		5811b	429b, 2539, 2939, 4249, 5727	

TABLE 17.23 (continued)
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
54.	58-55-9	1*H*-Purine-2,6-dione, 3,7-dihydro-1,7-dimethyl-		568b, 4249	
55.	83-67-0	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- {theobromine} 	568b, 1375, 1375b, 2601a, 3255, 3257, 3265, 3553, 4249, 5811b	568b, 1204, 2313a, 4249	
56.	33073-01-7	1*H*-Purine-2,6-dione, 3,9-dihydro-1,9-dimethyl-	1587, 4249, 5811b		
57.	58-08-2	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine} 	568b, 1365, 1842, 3255, 3257, 3265, 3266, 3553, 4249, 5811b	568b, 1053, 3266, 4249, 4880	
58.		6*H*-Purine-2,6-dione, 1,7-dihydro-, C_3-alkyl-	1587, 4249		
59.	69-93-2	1*H*-Purine-2,6,8-trione, 7,9-dihydro- {uric acid} 	2170, 5079, 5456		
60.	73-40-5	6*H*-Purin-6-one, 2-amino-1,7-dihydro- {guanine} 	3797	120, 2270, 2539, 2939, 3491, 3797, 3973, 3974a, 4249, 5079, 5189, 5311, 5435	
61.	68-94-0	6*H*-Purin-6-one, 1,7-dihydro- {hypoxanthine} 		2539, 2939	
62.	61892-79-3	1*H*,7*H*-Pyrazolo[1,2-*a*]pyrazole-1,7-dione, tetrahydro- 	3553, 4249		

(*continued*)

TABLE 17.23 (continued)
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

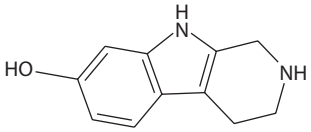
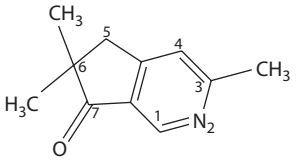
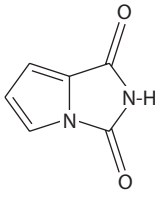
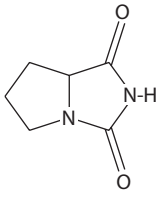
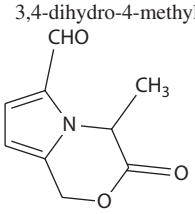
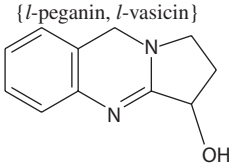
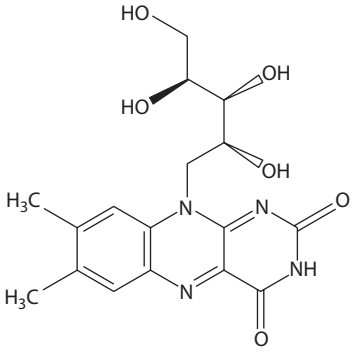
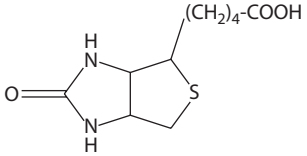
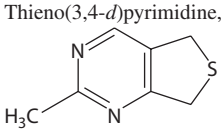
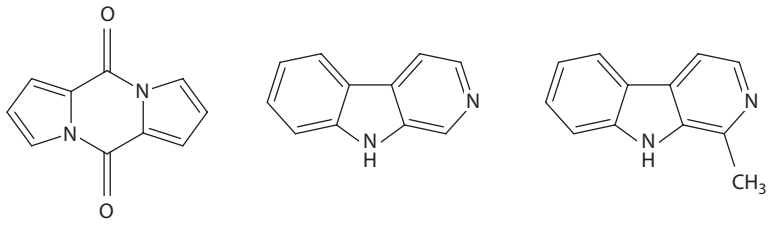
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
63.	33986-27-5	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methyl-2-butenyl)-		4249, 4665	
64.	33698-49-6	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methylbutyl)-		4249, 4665	
65.	34232-31-0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methyl-2-butenyl)-		4249, 4665	
66.	33986-28-6	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methylbutyl)-		4249, 4665	
67.	42438-90-4	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-, (S)-	2447a		
68.	40678-46-4	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-1-methyl-, (1S-*cis*)-	2447a		
69.	83177-17-7	3*H*-Pyrido[3,4-*b*]indol-7-ol; 1,2-dihydro-{1,2-dihydro-1-demethylharmalol}		2917a	
					
70.	78538-74-6	9*H*-Pyrido[3,4-*b*]indole-3-carboxamide, *N*-methyl-	2447a		
71.	50609-61-5	4*H*-Pyrido[1,2-*a*]pyrimidine-3-acetic acid, 9-hydroxy-4-oxo-, ethyl ester	2601a		
72.	3303-26-2	Pyrido[3,2-*d*]pyrimidin-4-ol, 2-methyl-		2917a	
73.	55713-43-4	7*H*-2-Pyrindin-7-one, 5,6-dihydro-3,6,6-trimethyl-		69, 939, 943, 3491, 4249	
					
74.	13939-91-8	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione	3553, 4249		
					
75.	5768-79-6	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione, tetrahydro-	568b, 3553, 4249, 5811b		
					

TABLE 17.23 (continued)
Derivatives of Fused *N*-Containing Ring Compounds with Two or More Nitrogens in the Rings

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
76.	35674-33-0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-4-methyl-3-oxo- 		965, 2544, 3491, 4249, 5811b	
77.	19179-12-5	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-	568b, 3553, 4249, 5811b		
78.	19943-28-3 36357-32-1	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-methyl-, (3R-*trans*)-	568b, 3553, 4249, 5811b		
79.	5654-86-4	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	2601a		
80.	61949-29-9	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-propyl-	5811, 5811a, 5811b		
81.	26626-89-1	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-propyl-, (3S-*trans*)-	3553, 4249		
82.		Pyrrolo[1,2-*a*]pyrazine-1,4-dione, 3-(1-methylethyl)-	568b, 4249		
83.	61891-74-5	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, tetrahydro-	5811, 5811a, 5811b		
84.	6159-55-3	Pyrrolo[2,1-*b*]quinazolin-3-ol, 1,2,3,9-tetrahydro- {*l*-peganin, *l*-vasicin} 		3763, 5079	
85.	83-88-5	Riboflavin 		120, 1941, 2270, 3973, 4249, 5079	
86.	146-17-8	Riboflavin 5′-(dihydrogen phosphate)		4249, 4956	
87.	58-85-5	1*H*-Thieno[3,4-*d*]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3aS-(3aα,4β,6aα)]- 		2408a, 4249, 4789	
88.	36267-71-7	Thieno(3,4-*d*)pyrimidine, 5,7-dihydro-2-methyl- 		1053, 3266, 17B22	

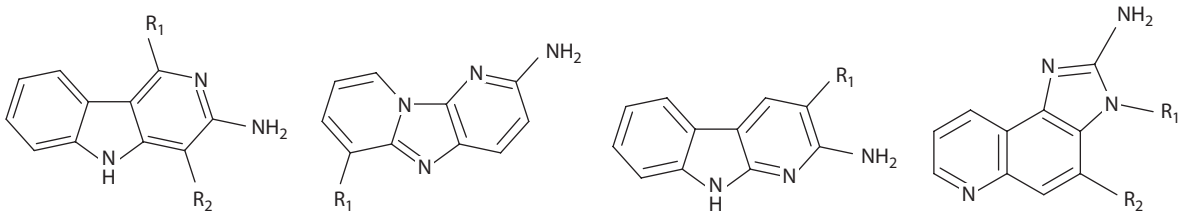


I 5*H*,10*H*-Dipyrrolo[1,2-*a*:1',2'-*d*]pyrazine-5,10-dione (pyrocoll)

II 9*H*-Pyrido[3,4-*b*] indole (norharman)

III 1-Methyl-9*H*-pyrido[3,4-*b*]indole (harman)

FIGURE 17.13 Pyrocoll, norharman, and harman.



IV $R_1 = R_2 = CH_3$
V $R_1 = CH_3$ $R_2 = H$

VI $R_1 = CH_3$
VII $R_1 = H$

VIII $R_1 = H$
IX $R_1 = CH_3$

X $R_1 = CH_3$ $R_2 = H$
XI $R_1 = R_2 = CH_3$

FIGURE 17.14 *N*-Heterocyclic amines, the "cooked food" mutagens.

TABLE 17.24
Mutagenic Activities of *N*-Heterocyclic Amines toward *S. typhimurium*[a]

Compound	Abbreviation	Identified in Tobacco Smoke	Mutagenic Activity, revertant/μg			
			TA98[b]	TA100[b]	TA98[c]	TA100[c]
Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-6-methyl-	Glu-P-1	Yes	49,000	3,200	73,000	4,000
Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-	Glu-P-2	Yes	1,900	1,200	600	400
5*H*-Pyrido[4,3-*b*]indole, 3-amino-1,4-dimethyl-	Trp-P-1	Yes	39,000	1,700	20,000	500
5*H*-Pyrido[4,3-*b*]indole, 3-amino-1-methyl-	Trp-P-2	Yes	104,200	1,800	103,000	2,000
9*H*-Pyrido[2,3-*b*]indole, 2-amino-	AαC	Yes	300	20	—	—
9*H*-Pyrido[2,3-*b*]indole, 2-amino-3-methyl-	MeAαC	Yes	200	120	—	—
Imidazo[4,5-*f*]quinoline, 2-amino-3-methyl-	IQ	Yes	433,000	7,000	222,000	11,000
Imidazo[4,5-*f*]quinoline, 2-amino-3,4-dimethyl-	MeIQ	Yes	661,000	30,000	1,327,000	70,000
9*H*-*P*yrido[3,4-*b*]indole	Nor-harman	Yes	—	—	—	—
9*H*-Pyrido[3,4-*b*]indole, 1-methyl-	Harman	Yes	—	—	—	—
Cigarette smoke condensate	CSC	—	—	—	2	1
Benzo[*a*]pyrene	B[*a*]P	Yes	—	—	200	—

[a] Tests with *S. typhimurium* involved use of S-9 mix.
[b] Ames test data with *S. typhimurium* reported by Sugimura (3828c).
[c] Ames test data with *S. typhimurium* reported by Lee et al. (2327c).

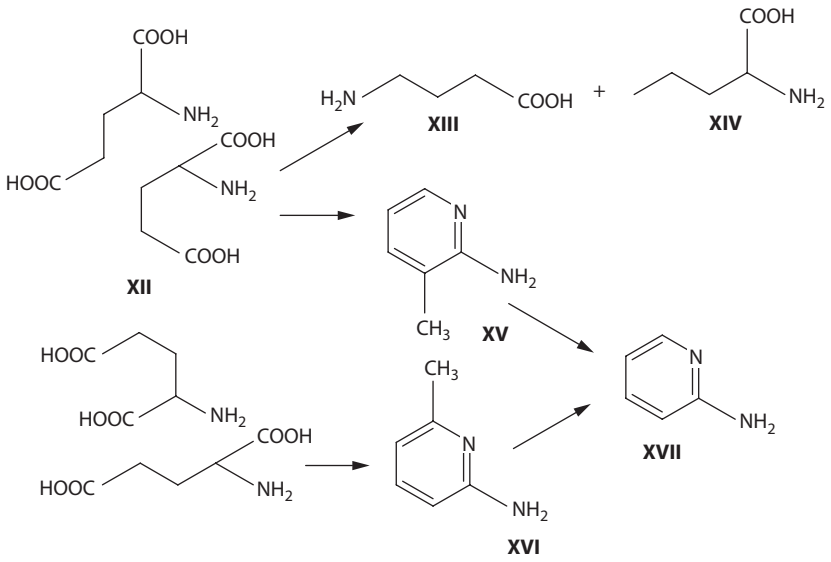


FIGURE 17.15 Theoretical conversion of glutamic acid {XVI} to aminobutanoic acids {XVII, XVIII} and aminopyridines {XIX–XXI}.

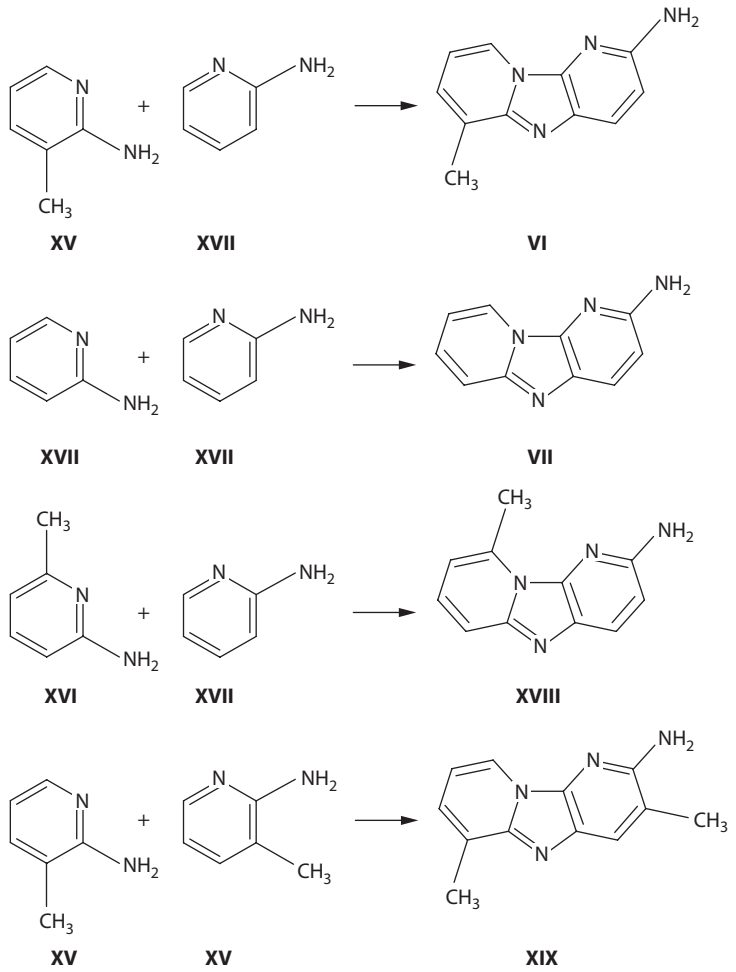


FIGURE 17.16 Theoretical routes for conversion of glutamic-acid-derived aminopyridines to possible tobacco smoke components.

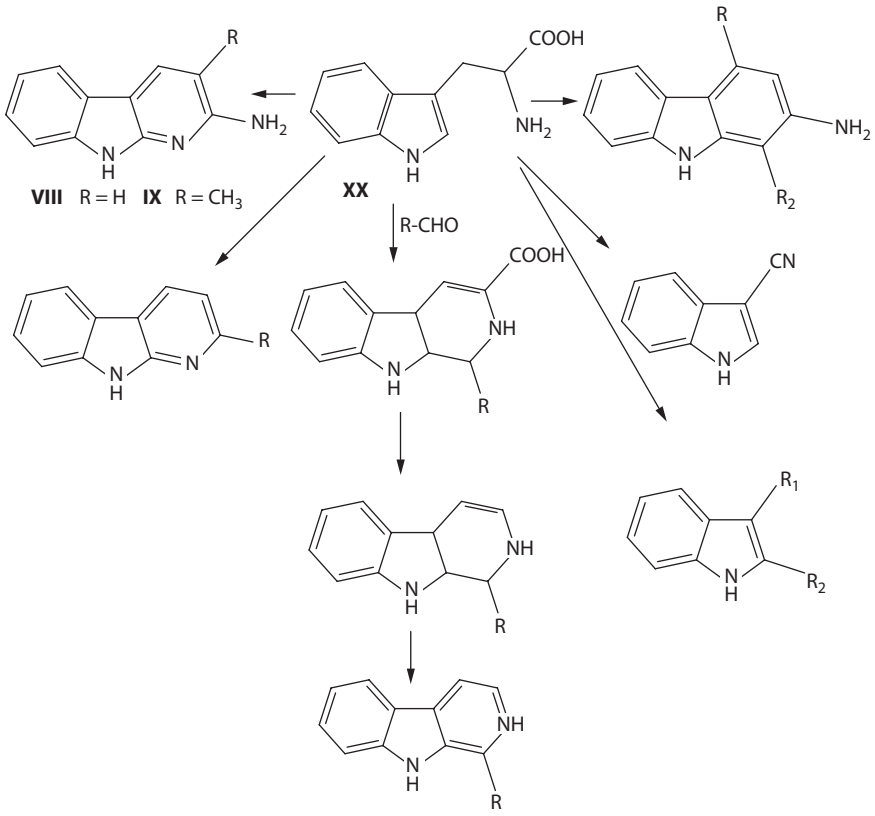


FIGURE 17.17 Possible tryptophan-derived compounds in tobacco smoke.

(Trp-P-1) {IV} and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*] indole (Trp-P-2) {V}; the alkyl- and dialkylindoles; indole-3-acetonitrile; the 2-amino-9*H*-pyrido[2,3-*b*]indoles [AαC {VIII} and MeAαC {IX}] plus other pyrido[2,3-*a*]indoles {R = H, CH_3, C_2H_5, $(CH_3)_2CHCH_2$, or n-C_5H_{11}} (see Table 17.29). All of the compounds noted in (Figure 17.16) have been reported as tobacco smoke components.

In the 1979 report of the U.S. Surgeon General (4005), the azaarenes dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*] carbazole, quinoline, and alkylated quinolines in CSC were discussed but not the presence or biological properties of the *N*-heterocyclic amines identified in tobacco smoke. However, in the 1982 report of the Surgeon General (4010), 9*H*-pyrido[3,4-*b*] indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) were classified as "toxic and tumorigenic agents of cigarette smoke" in amounts of 3.2–8.1 and 1.1–3.1 µg/cig, respectively, in mainstream CSC. None of the *N*-heterocyclic amines present in tobacco smoke were discussed.

Snook and Chortyk (3739, 3740) reported the cigarette mainstream smoke (MSS) yield of 9*H*-pyrido[3,4-*b*]indole (norharman) to be 1.2–13.4 µg/cig and that for 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) to be 0.3–3.8 µg/cig. They found a linear relationship between the yield of MSS "tar" and the yields of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman). In contrast to the 1962 findings of Poindexter and Carpenter (2972), Snook and Chortyk reported yields of these two compounds were not influenced by the tobacco type.

In his review of the studies of the mutagenicity of CSC, Demarini (933) discussed the significance of the findings of Yoshida and Matsumoto (4388) and Matsumoto et al. (2492) on the mutagenicity of 2-amino-9*H*-pyrido[2,3-*b*]indole (AαC) (80 ng/cig) and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*] indole (MeAαC) (7 ng/cig).

None of the authors contributing to the American Chemical Society's 1984 monograph [Searle (3568)] on chemical carcinogens mentioned the *N*-heterocyclic amines as mutagens and/or tumorigens.

Yamashita et al. (4367, 4368) identified and quantitated the following *N*-heterocyclic amines in mainstream CSC: 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ) (0.3 ng/cig), 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) (0.3 ng/cig), 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) (0.2 ng/cig), 2-amino-9*H*-pyrido[2,3-*b*]indole (AαC) (16.9 ng/cig), and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC) (1.6 ng/cig).

In his 1986 review of the isolation and identification of the *N*-heterocyclic amines, the high mutagenicity in the Ames test (*S. typhimurium*) of several of them, their tumorigenicity in laboratory animals, and their various sources, including

CSC, Sugimura (3828c) wrote the following about their importance as human carcinogens:

> Taking various factors into consideration, it is probably impractical and not realistic to make risk estimations from the carcinogenicity data on rodents given a single carcinogen. However, for a simple extrapolation of animal data for risk estimation, TD_{50} values, which are the doses needed to develop cancers in 50% of animals fed on carcinogens [IQ, Trp-P-1, Trp-P-2, Glu-P-1, Glu-P-2, AαC, and MeAαC] for their life time, have been calculated based on mouse experiments… If we assume the average TD_{50} value of heterocyclic amines should be about 8mg/kg/day, we can roughly estimate the risk of these carcinogenic heterocyclic amines for human beings. The intake of heterocyclic amines was calculated from available data on their quantities in foods. Apparently the human intake is about 0.0002% times the TD_{50} obtained from animal data. This means that heterocyclic amines may not be so serious for human cancer development.

Sugimura added:

> On the other hand, it is also true that human beings are being exposed to many heterocyclic amines and many other carcinogens with tumor promoters and/or suppressing factors for carcinogenesis. At this moment, it is honest to state that no solid information on the estimation of risk of heterocyclic amines has been obtained in any direction, either positive or negative.

As in the case of the carcinogens whose activity can be substantially reduced by anticarcinogens [see review by Rodgman (3255)], Lee et al. (2327c) reported that mainstream CSC significantly inhibited the mutagenicity of several of these *N*-heterocyclic amines when tested in the Ames assay with *S. typhimurium*, strain TA 98 in the presence of the S-9 mix. The *N*-heterocyclic amines tested included 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ), 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ), 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1), 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2), 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1), and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2). The mutagenic activities of these mutagens were suppressed as much as 80% by addition of 50–100 µg of CSC per plate. Enzymatic studies indicate that CSC is a potent inhibitor of cytochrome-P-450-dependent monooxygenase. Therefore, it appears that CSC exerts its antimutagenicity by inhibiting the P-450 system. Lee et al. (2327c) also reported that fractionation of CSC yields fractions that show low mutagenicity themselves but are significantly antimutagenic.

Although many of the *N*-heterocyclic amines are indeed present in cigarette MSS, it should be remembered that the major part of the research on this class of compounds was initiated and extended because of their presence in a great number of cooked foodstuffs consumed by a great number of people. When the *N*-heterocyclic amines were shown to be tumorigenic in addition to being highly mutagenic and subsequently identified in tobacco smoke, they were included by Hoffmann and his colleagues in their numerous lists of tobacco smoke tumorigens published in 1997 and later (1740, 1741, 1743, 1744). The *N*-heterocyclic amines had not been included in their numerous lists published between 1986 and 1997 (1727, 1773, 1806) nor in similar lists published by IARC (1870) and OSHA (2825). Table 17.25 summarizes some details of these *N*-heterocyclic amines in tobacco smoke.

Because of their concerns about the mutagenicity of numerous commonly consumed heated foods, many of the studies of the isolation, identification, and estimation of *N*-heterocyclic amines in heated foodstuffs or heated food components, particularly amine-containing components such as amino acids, proteins, and peptides, were conducted by Japanese investigators. This becomes obvious from examination of the authors and coauthors of the references listed in Table 17.26.

With the reporting of the Ames mutagenicity test with *S. typhimurium* in the mid-1970s and the demonstration of its utility, the number of studies on potential mutagenic systems and the mutagenicity–tumorigenicity relationship virtually exploded. By highly competent application of up-to-date isolation and characterization techniques plus utilization of the Ames test, Sugimura and his staff at the Japanese National Cancer Research Institute contributed significantly to our knowledge of the structures, properties, and precursors in foods of the *N*-heterocyclic amines. While the methodologies differed, the 1977 isolation/identification of the *N*-heterocyclic amines (Trp-P-1, Trp-P-2) from a tryptophan pyrolysate paralleled the historic 1932 isolation and identification of polycyclic aromatic hydrocarbons (PAHs) [B[*a*]P, benzo[e]pyrene (B[*e*]P), benz[*a*]anthracene (B[*a*]A), perylene] from coal tar. In the 1930s, the Kennaway group in the United Kingdom used ultraviolet spectrophotometry [Hieger (1631)] to monitor coal tar PAHs during their concentration and purification by repeated precipitations and recrystallizations of PAH–picric acid complexes [Cook et al. (796a, 797)]. In the mid-1970s, Sugimura et al. (3829a) in Japan used the Ames test (*S. typhimurium*, TA98 strain/S-9) to monitor tryptophan pyrolysate mutagens (Trp-P-1, Trp-P-2) during their concentration and purification by sequential chromatography on silicic acid, alumina, and CM-Sephadex® columns.

References to several early studies on the identification of biologically active compounds in heated foodstuffs are included in Table 17.26, e.g., the 1956 study by Kuratsune (2237) of PAHs such as B[*a*]P in roasted coffee and the similar mid-1960s studies of PAHs in broiled meat [Lijinsky and Shubik (2364a, 2364b)]. PAHs such as B[*a*]P were identified in both studies. The major concern of the early investigators was the possible presence of tumorigenic PAHs, particularly B[*a*]P, in the heated foodstuff. Of course, it

TABLE 17.25
Summary of Lists of Tumorigenic *N*-Heterocyclic Amines in Tobacco Smoke

	MSS Yield (ng/cig) Reported by					
Component	1986–1994 IARC (1870), Hoffmann and Wynder (1806), Hoffmann and Hecht (1727), Hoffmann et al. (1773), OSHA (2825)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)[a]	2001 Hoffmann and Hoffmann (1743), Hoffmann et al. (1744)	2001 Fowles and Bates (1217)	1997–2001 Smith et al. (3711–3713)
AαC[a]	NL	25–260	25–260	25–260	NL	ND–258
MeAαC	NL	2–37	2–37	NL	NL	1.6–37
Glu-P-1	NL	0.37–0.89	0.37–0.89	0.37–0.89	NL	ND–0.89
Glu-P-2	NL	0.25–0.88	0.25–0.88	0.25–0.88	NL	0.25–0.88
PhIP	NL	11–23	11–23	11–23	NL	ND–22.9
IQ	NL	0.26	0.3	0.3	NL	0.26–0.49
MeIQ	NL	NL	NL	NL	NL	0.28–0.75
Trp-P-1	NL	0.29–0.48	0.3–0.5	0.3–0.5	NL	0.19–0.3
Trp-P-2	NL	0.82–1.1	0.8–1.1	0.8–1.1	NL	ND–0.2

NL, not listed; ND, not detected.

[a] AαC, 2-amino-9*H*-pyrido[2,3-*b*]indole; MeAαC, 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole; Glu-P-1, 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole; Glu-P-2, 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole; PhIP, 2-amino-1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridine; IQ, 2-amino-3-methyl-3*H*-imidazo[4,5-*f*]quinoline; MeIQ, 2-amino-3,4-dimethyl-3*H*-imidazo[4,5-*f*]quinoline; Trp-P-1, 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole; Trp-P-2, 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole.

was subsequently demonstrated that B[*a*]P, in addition to its tumorigenicity to mouse skin, is also mutagenic in the Ames test. However, its specific mutagenicity is insignificant compared to that of several of the *N*-heterocyclic amines (see Table 17.24). The presence of PAHs in numerous foods was discussed previously.

From their studies of heated foods or food pyrolysates (30 different foods, including rice, flour, soy beans, fish, meat, eggs), Sugimura (3828b) reported the following:

- Mutagenicity was proportional to the protein content.
- Mutagenicity was proportional to the levels of specific amino acids (tryptophan, glutamic acid, etc.) in the constituent protein.
- Mutagenicity was dependent on water content and heating temperature, e.g., for foods with low water content, the mutagens appear at 300°C; for those with high water content, the mutagens appear at 400°C.

Estimates of daily exposures to PAHs and *N*-nitrosamines in foods, beverages, and other factors have been made by numerous investigators. Estimates of exposures to *N*-heterocyclic amines are limited. Part of the reason is the difference in time span since the particular class of compounds was found to be tumorigenic and/or mutagenic: Exposures to PAHs tumorigenic in laboratory animal bioassays have been studied for more than seven decades (since the early 1930s and the identification of B[*a*]P in coal tar by Cook et al. (796a, 797)) and exposures to *N*-nitrosamines tumorigenic in laboratory animal bioassays have been studied [Magee and Barnes (2441a)] since the mid-1950s. In contrast, exposures to *N*-heterocyclic amines tumorigenic in laboratory animal bioassays have only been studied for about 30 years (since the mid-1970s and the availability of the Ames test).

Sugimura (3828b) reported comparisons of the mutagenicities (Ames test) of various beverages (coffee, brandy, tea) and CSC. The data are summarized in Table 17.27.

As noted previously, Sugimura (3828c) reported in his 1986 review his estimate of the exposure of humans to *N*-heterocyclic amines with the limited data at his disposal. From his estimate, Sugimura concluded that at that time, *N*-heterocyclic amines might not be serious in human cancer development and no solid information on the estimation of risk of *N*-heterocyclic amines had been obtained in any direction, either positive or negative.

In another comparison of mutagenicities toward *S. typhimurium* TA98, Nagao et al. (2667c) calculated the B[*a*]P equivalency of extracts of charred fish and meat. Their data, with additions (charred food weight in ounces, cigarette equivalents based on B[*a*]P), are shown in Table 17.28.

Table 17.29 lists identified tobacco smoke components actually or possibly derived from the amino acids glutamic acid, tryptophan, or proline. In the mid-1980s, Rodgman (3253a) discussed both the known relationships as well as several theoretically possible relationships between the

TABLE 17.26
N-Heterocyclic Amines: Mutagenicity of Beverages, Heated Foods, and Heated Food Components

Food or Food Component	References
Foods, heated (grilled, broiled, etc.)	Felton and Knize (1177d), Matsumoto et al. (2492), Nagao et al. (2667a), Sugimura (3828c, 3828e, 3828f), Sugimura et al. (3829), Sugimura and Nagao (3929b), Tanaka et al. (3865b)
Beef, extract	Commoner et al. (790a), Hargraves and Pariza (1501a), Hayatsu et al. (1555b), Ohgaki et al. (2849a), Takayama et al. (3862c), Turesky et al. (3988b)
Beef, broiled, fried, and/or charred	Commoner et al. (790a), Felton et al. (1177d), Hayatsu et al. (1555a, 1555b), Jägerstad et al. (1916b), Kasai et al. (2037d), Lijinsky and Shubik (2364a, 2364b)[a], Nagao et al. (2667c), Ohgaki et al. (2849a), Takayama et al. (3862c), Yasuda et al. (4382a)
Cuttlefish, broiled	Ohgaki et al. (2849a), Yamaguchi et al. (4361a)
Eggs, fish, meat Flour, rice Soy beans	Sugimura and Nagao (3828b)
Fish, broiled, charred	Kasai et al. (2037c, 2037d), Nagao et al. (2667c), Yamaizumi et al. (4361b), Yasuda et al. (4382a)
Herring, broiled Mackerel, broiled Pike, broiled Sardine, broiled	Nagao et al. (2667f)
Sardine, broiled	Ohgaki et al. (2849a), Takayama et al. (3862c)
Protein pyrolysates	Matsumoto (2491c), Nagao et al. (2667f), Nebert et al. (2688a), Yoshida and Matsumoto (4387b), Yoshida et al. (4390)
Albumin	Yasuda et al. (4382a)
Soybean globulin	Ohgaki et al. (2849b), Yoshida et al. (4389a)
Calf thymus Egg white Serum albumin	Nagao et al. (2667b)
Casein, collagen Gluten, histone Insulin, lysozyme Ovalbumin, zein Tobacco protein	Matsumoto et al. (2491c)
Polypeptides	Johnson et al. (1968)
Carnosine Glycyl glycine[a] Glycyl glutamic acid Glycyl proline Glycyl tryptophan Leucyl glycyl phenylalanine Tryptophanyl alanine Tryptophanyl glycine Tryptophanyl tryptophan Tryptophanyl tyrosine	Matsumoto et al. (2491c)
Amino acid pyrolysates	Kato et al. (2048, 2049), Kosuge et al. (2178a), Masuda et al. (2486), Nebert et al. (2688a)
Phenylalanine	Sugimura et al. (3829)
Lysine	Wakabayashi et al. (4102a)
Tryptophan	Hosaka et al. (1835a), Matsukura et al. (2491a), Negishi and Hayatsu (2689a), Sugimura et al. (3829), Takayama et al. (3862d), Yamazoe et al. (4370a), Yoshida and Matsumoto (4390)
Glutamic acid	Ohgaki et al. (2849b), Sugimura (3828a), Takeda et al. (3863a), Takayama et al. (3862b), Yamamoto et al. (4365a)
Histidine	Smith et al. (3722a)
Histidine, 3-methyl-	

(*continued*)

TABLE 17.26 (continued)
***N*-Heterocyclic Amines: Mutagenicity of Beverages, Heated Foods, and Heated Food Components**

Food or Food Component	References
Alanine[b], arginine Asparagine, citrulline Cysteine, cystine Glutamic acid Glutamine, histidine Lysine, methionine Ornithine Phenylalanine, serine Threonine, tryptophan Tyrosine, valine	Matsumoto et al. (2491b)
Beverages	
Coffee, roasted	Aeschbacher and Würzner (38a), Kuratsune (2237)[c], Nagao et al. (2667d, 2667e), Sugimura (3828d)
Coffee, instant	Aeschbacher and Würzner (38a), Fujita et al. (1256a), Kosugi et al. (2178b)
Tea	Nagao et al. (2667e), Sugimura (3838d)
Brandy	Sugimura (3828d)
Sake	Takase and Murakami (3862a)
CSC	DeMarini (930–933), Matsumoto et al. (2492), Sugimura (3828d), Yoshida and Matsumoto (4388)

[a] No mutagens detected in glycylglycine pyrolysate.
[b] The pyrolysates from the various amino acids studied showed mutagenicities (Ames test) in the following sequence (revertant/mg of pyrolysate), the amino acid (tryptophan) yielding the highest mutagenic pyrolysate listed first: tryptophan, serine, glutamic acid, ornithine, lysine, arginine, citrulline, threonine, alanine, cystine, glutamine, methionine, cysteine, tyrosine, phenylalanine, histidine, asparagine, valine.
[c] This was a PAH study, with emphasis on the generation of B[*a*]P.

TABLE 17.27
Mutagenicity of Common Beverages *vs.* CSC

Agent	Exposure Level	*ST* Strain	S-9 Mix	Revertants
Cigarette	One, inhaled	TA98	Yes	4,000
Coffee	200 mL	TA100	No	180,000
Tea[a]	200 mL	TA100	No	Mutagenic
Brandy	50 mL	TA100	No	10,500

ST, *S. typhimurium*.
[a] Japanese green tea.

TABLE 17.28
Benzo[*a*]pyrene Equivalency of Extracts of Charred Fish and Meat

Analyte	Sample Wt., g	B[*a*]P Equivalency, ng	Cigarette Equivalency Based on B[*a*]P[a]
Sardine	100 (3.5)[b]	35,800	2,983
Mackerel	60 (2.1)	68,200	5,683
Beefsteak	190 (6.7)	85,500	7,125

[a] Calculation based on assumption of MSS yield of 12 ng/cig of B[*a*]P.
[b] Number in parentheses is weight in ounces.

three amino acids and many of the compounds listed in Table 17.29. It also lists, with appropriate citations, the amino-acid-derived compounds reported in tobacco smoke and citations to the studies demonstrating their mutagenicity and tumorigenicity. Additional references to the tobacco smoke components may be found in the chapters on the aza-arenes (Section 17.5) and the three amino acids (Section 4.2).

Table 17.30 summarizes the chronology of the studies pertinent to the *N*-heterocyclic amines in tobacco smoke and in commonly consumed cooked foodstuffs. Included in Table 17.30 are events pertinent to the studies of 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), 9*H*-pyrido[3,4-*b*]indole (norharman), and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman). Although none is an *N*-heterocyclic amine, their pyrogenesis from specific amino acids was the background for the subsequent studies on *N*-heterocyclic amines, each of which is derived from an amino acid.

Table 17.31 lists, with appropriate citations, the *N*-heterocyclic amines reported in tobacco and tobacco smoke. While Table 17.31 lists the citations pertinent to the nine highly mutagenic *N*-heterocyclic amines, as noted previously, citations pertinent to tobacco smoke components related to them are available in several other chapters (Section 4.2; Section 17.5).

TABLE 17.29
Components Related to *N*-Heterocyclic Amines in Tobacco Smoke: Identification and Biological Properties

Compound	References to		
	Identification in Smoke	Mutagenicity[a]	Tumorigenicity[b]
Glutamic acid derived			
Glutamic acid	Buyske et al. (526), Izawa et al. (1910), Izawa and Taki (1914)		
Butanoic acid, 2-amino-	Hecht et al. (1580)		
Butanoic acid, 4-amino-	Izawa et al. (910), Izawa and Taki (1914)		
2-Pyridinamine	Heckman and Best (1587), Saint-Jalm and Morée-Testa (3386)		
2-Pyridinamine, 3-methyl-	Lippiello et al. (2378a)		
2-Pyridinamine, 6-methyl-	Lippiello et al. (2378a), Sanders et al. (3410)		
Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino- {Glu-P-2}	Clapp (751), Clapp et al. (755, 756), Massey (2484a)	Yamamoto et al. (4365a), Sugimura (3828c), Lee et al. (2327c)	Ohgaki et al. (2849a, 2849b), Takayama et al. (3862c), Sugimura (3828c)
Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-6-methyl- {Glu-P-1}	Clapp (751), Clapp et al. (755, 756), Massey (2484a)	Yamamoto et al. (4365a), Sugimura (3828c), Lee et al. (2327c)	Ohgaki et al. (2849a, 2849b), Takayama et al. (3862c), Sugimura (3828c)
Tryptophan-derived			
Tryptophan		+	
9*H*-Pyrido[3,4-*b*]indole {norharman}	Poindexter and Carpenter (2972)	Levitt et al. (2355a), Nagao et al. (2667g)	USPHS (4010)
9*H*-Pyrido[3,4-*b*]indole, 1-butyl-	Heckman and Best (1587)		
9*H*-Pyrido[3,4-*b*]indole, 1-ethyl-	Schumacher et al. (3553)		
9*H*-Pyrido[3,4-*b*]indole, 1-methyl- {harman}	Poindexter and Carpenter (2972)	Levitt et al. (2355a), Nagao et al. (2667g)	USPHS (4010)
9*H*-Pyrido[3,4-*b*]indole, 1-methyl-1,2,3,4-tetrahydro-	Schumacher et al. (3553)		
9*H*-Pyrido[3,4-*b*]indole, 1-propenyl-	Heckman and Best (1587)		
5*H*-Pyrido[4,3-*b*]indole, 3-amino-1,4-dimethyl- {Trp-P-1}	Yamashita et al. (4367, 4368)	Sugimura et al. (3828c, 3829, 3829a), Lee et al. (2327c)	Matsukura et al. (2491a), Hosaka et al. (1835a), Takayama et al. (3862d), Sugimura (3828c)
5*H*-Pyrido[4,3-*b*]indole, 3-amino-1-methyl- {Trp-P-2}	Yamashita et al. (4367, 4368)	Sugimura et al. (3829, 3829a), Sugimura (3828c), Lee et al. (2327c)	Matsukura et al. (2491a), Hosaka et al. (1835a), Takayama et al. (3862d), Sugimura (3828c)
1*H*-Pyrido[2,3-*b*]indole	Heckman and Best (1587)		
9*H*-Pyrido[2,3-*b*]indole, 2-ethyl-	Schumacher et al. (3553)		
9*H*-Pyrido[2,3-*b*]indole, 2-methyl-	Heckman and Best (1587)		
9*H*-Pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-	Heckman and Best (1587)		
9*H*-Pyrido[2,3-*b*]indole, 2-pentyl-	Heckman and Best (1587)		
9*H*-Pyrido[2,3-*b*]indole, 2-amino-{AαC}	Yoshida and Matsumoto (4388), Matsumoto et al. (2492), Yamashita et al. (4367, 4368)	Yoshida and Matsumoto (4388), Matsumoto et al. (2492), DeMarini (933), Sugimura (3828c)	Ohgaki et al. (2849b), Sugimura (3828c)
9*H*-Pyrido[2,3-*b*]indole, 2-amino-3-methyl- {MeAαC}	Yoshida and Matsumoto (4388), Matsumoto et al. (2492), Yamashita et al. (4367, 4368)	Yoshida and Matsumoto (4388), Matsumoto et al. (2492), DeMarini (933), Sugimura (3828c)	Ohgaki et al. (2849b), Sugimura (3828c)

(*continued*)

TABLE 17.29 (continued)
Components Related to *N*-Heterocyclic Amines in Tobacco Smoke: Identification and Biological Properties

Compound	References to		
	Identification in Smoke	Mutagenicity[a]	Tumorigenicity[b]
Imidazo[4,5-*f*]quinoline, 2-amino-3,4-dimethyl- {MeIQ}	Bao et al. (179a), Levasseur et al. (2354a), Massey (2484a), Rodgman (3255, 3257, 3265), Rodgman and Green (3300), Smith et al. (3714)	Ohgaki et al. (2849), Lee et al. (2327c)	Ohgaki et al. (2849)
Imidazo[4,5-*f*]quinoline, 2-amino-3-methyl- {IQ}	Yamashita et al. (4367, 4368)	Yoshita et al. (4389a), Ohgaki et al. (2849a), Lee et al. (2327c)	Ohgaki et al. (2849a), Takayama et al. (3862b, 3862c), Tanaka et al. (3865c)
Indole, 2,3-dimethyl-	Rodgman and Cook (3279), Izard et al. (1898), Schmeltz et al. (3506)		
Indole-3-acetonitrile	Izard et al. (1898)		
Proline derived			
Proline	Izawa et al. (1910), Izawa and Taki (1914)		
5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione {pyrocoll}	Mold et al. (2592), Rodgman and Cook (3279), Schmeltz et al. (3505), Testa and Testa (3886)		
5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione, methyl- {methylpyrocoll}	Izard et al. (1898)		
5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione, 1,2a,3,5a,8,10a-hexahydro-	Schumacher et al. (3553)		
5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione, 1,2a,3,5a,8,10a-hexahydro-3-methyl-	Schumacher et al. (3553)		
5*H*,10*H*-Dipyrrolo[1,2-*a*: 1′,2′-*d*] pyrazine-5,10-dione, octahydro-	Schumacher et al. (3553)		

[a] Mutagenic (*S. typhimurium*).
[b] Tumorigenic to mammalian skin.

TABLE 17.30
Chronology of *N*-Heterocyclic Amine Studies

Year	Event
1959	The only fused-ring *N*-heterocyclic compound listed by Johnstone and Plimmer (1971) as a component of tobacco smoke was the bicyclic compound quinoline
1960	Mold et al. (2592) reported the isolation and identification of the tricyclic *N*-heterocyclic 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) from CSC and its relationship to its precursor in tobacco, the amino acid proline
1961/1962	Poindexter and Carpenter (2972) reported the isolation and identification of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) from CSC. They reported that the yield of the total harmans in burley and flue-cured MSSs was between 15 and 20 µg/g of tobacco smoked, values which were 40–50 times that of the harmans in the unsmoked tobacco. Since the weight of tobacco in cigarettes sold at that time approximated 1 g, the yield of these two compounds was about 15–20 µg/cig. Poindexter and Carpenter concluded from experiments with radiolabeled tryptophan that the harmans (found to be radiolabeled in the smoke) were generated pyrogenetically from a reaction between aldehydes (formaldehyde for norharman, acetaldehyde for harman) and the tryptophan in tobacco
1962	Rodgman and Cook (3279) confirmed the presence in CSC of 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) and also reported the identification of indole, carbazole, and several alkylated indoles and carbazoles. Rodgman and Cook (3279) also reviewed the previously reported biological studies on indole, 3-methylindole (skatole), and carbazole: none of the three were reported to be tumorigenic
1964	Schmeltz et al. (3505) reported 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), 9*H*-pyrido[3,4-*b*]indole (norharman), and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) as tobacco smoke components. Testa and Testa (3886) also identified 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) as components of CSC
1964	The Advisory Committee to the U.S. Surgeon General (3999) briefly discussed only four fused-ring *N*-heterocyclic compounds in tobacco smoke, quinoline and the two dibenzacridines (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine) and the dibenzocarbazole (7*H*-dibenzo[*c,g*]carbazole) reported by Van Duuren et al. (4027)
1968	In his review of tobacco smoke composition, Stedman (3797) discussed the identification of tumorigenic *N*-heterocyclic compounds (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]carbazole) reported by Van Duuren et al. (4027) as well as the following *N*-heterocyclic compounds: 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) reported by Mold et al. (2592) and 9*H*-pyrido[3,4-*b*]indole (norharman), 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), and 9*H*-pyrido[2,3-*b*]indole reported by Poindexter and Carpenter (2972)
1971/1972	Wakeham (4103) noted the reported presence of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) in cigarette smoke and discussed their formation from a reaction product of tryptophan and an aldehyde. As noted by Rodgman (3253a), the structure of the aldehyde reacting with tryptophan ultimately dictates the structure of alkylated norharmans found (see Table 17.29) in CSC
1974	In addition to 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), Izard et al. (1899) reported the identification of methyl-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (methylpyrocoll) in CSC
1974/1975/1977	In a 1974 in-house report, a 1975 TCRC presentation, and a 1977 publication on their study of the water-soluble portion of CSC, Schumacher et al. (3553) reported the identifications of 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (octahydropyrocoll), and 2-ethyl-9*H*-pyrido[2,3-*b*]indole
1977	Sugimura et al. (3829a) reported the isolation and identification of the *N*-heterocyclic amines 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) from tryptophan pyrolysates
1977	In separate studies, Levitt et al. (2355a) and Nagao et al. (2667b) demonstrated the mutagenicity of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) in the Ames test
1978	Yamamoto et al. (4365a) reported the isolation and identification of 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) and 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2) from glutamic acid pyrolysates
1978/1981	Heckman and Best (1587) reported the identification of nearly 270 previously unidentified and over 150 previously identified *N*-containing components in CSC. These included several components structurally similar to the *N*-heterocyclic amines: 9*H*-pyrido[2,3-*b*]indole, 2-methyl-9*H*-pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-9*H*-pyrido[2,3-*b*]indole, 2-pentyl-9*H*-pyrido[2,3-*b*]indole, 1-butyl-9*H*-pyrido[3,4-*b*]indole, 9*H*-1-propenyl-pyrido[3,4-*b*]indole, and a partially characterized norharman isomer
1979	In the 1979 Surgeon General's report (4005), the aza-arenes dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]carbazole, quinoline, and alkylated quinolines in CSC were discussed but not the presence or properties of the *N*-heterocyclic amines identified in tobacco smoke
1980/1981	Yoshida and Matsumoto (4388) and Matsumoto et al. (2492) reported the identification of 2-amino-9*H*-pyrido[2,3-*b*]indole (AαC) and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC) in CSC
1981	Matsukura et al. (2491a) demonstrated the tumorigenicity in mice of 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) Hosaka et al. (1835a) demonstrated the tumorigenicity in rats of 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2)

(*continued*)

TABLE 17.30 (continued)
Chronology of *N*-Heterocyclic Amine Studies

Year	Event
1982	In the 1982 report of the Surgeon General (4010), 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) were classified as "toxic and tumorigenic agents of cigarette smoke" in amounts of 3.2–8.1 and 1.1–3.1 μg/cig, respectively, in cigarette MSS. None of the other *N*-heterocyclic amines present in tobacco smoke were discussed
1982/1984	Snook and Chortyk (3739) reported the MSS yield of 9*H*-pyrido[3,4-*b*]indole (norharman) to be 1.2–13.4 μg/cig; that for 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) to be 0.3–3.8 μg/cig. They found a linear relationship between the yield of cigarette MSS "tar" and the yields of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman). In contrast to the 1962 findings of Poindexter and Carpenter, Snook and Chortyk reported that the MSS yields of these two compounds were not influenced by the tobacco type
1983	Demarini (933) reviewed the studies on the mutagenicity of CSC. He discussed the studies of Yoshida and Matsumoto (4388) and Matsumoto et al. (2492) on the mutagens 2-amino-9*H*-pyrido[2,3-*b*]indole (AαC) (80 ng/cig) and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC) (7 ng/cig)
1984	None of the authors contributing to the second edition of the *American Chemical Society's Monograph*, edited by Searle (3568), on chemical carcinogens mentioned the tumorigenic and mutagenic *N*-heterocyclic amines reported in cigarette smoke and/or numerous cooked foods. In fact, the only class of tumorigens in cigarette MSS discussed in the 1400-page treatise was the *N*-nitrosamines. No tumorigenic PAH was mentioned as a component of cigarette MSS
1984	Ohgaki et al. (2849) demonstrated the tumorigenicity in mice, and Takayama et al. (3862b) demonstrated the tumorigenicity in rats of 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) and 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2) Takayama et al. (3862c) demonstrated the tumorigenicity in rats of the tobacco smoke component 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ)
1984/1985	Ohgaki et al. (2849a, 2849b) demonstrated the tumorigenicity in mice of 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ) and 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ), found in broiled fish, fried beef, beef extract, and CSC
1985	Takayama et al. (3862d) demonstrated the tumorigenicity in rats of 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) Tanaka et al. (3865b) demonstrated the tumorigenicity of 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ)
1985	In an in-house presentation, Rodgman (3253a) discussed the already identified and other possible theoretical relationships between tryptophan and the substituted norharmans, the tryptophan pyrolysis products 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2), the 2-amino-9*H*-pyrido[2,3-*b*]indoles (AαC and MeAαC), indole-3-acetonitrile, and the alkyl- and dialkylindoles He also discussed the theoretical relationships among glutamic acid, its possible degradation products, 2- and 4-aminobutanoic acid, 2-aminopyridine, 2-amino-3- and 6-methylpyridine, and the possible reactions between these substituted aminopyridines to form 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1), 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2), and two similar products not yet identified
1985/1986	In its 1985 review, published in 1986, of the various problems from exposure to numerous components in tobacco smoke, the IARC (1870) did not designate the *N*-heterocyclic amines as a problem. IARC did list several tryptophan-derived tobacco smoke isolates including 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman). The per cigarette MSS yields of these two components were listed as 9.5–14.1 and 2.5–5.8 μg/cig, respectively. No mention was made of the *N*-heterocyclic amines in CSC or the degree of evidence for their carcinogenicity in animals and humans The identification of several *N*-heterocyclic amines was reported in 1985 and 1986 by Yamashita et al. (4367, 4368)
1985/1986	Yamashita et al. (4367, 4368) identified and quantitated the per cigarette yields of the following *N*-heterocyclic amines in CSC: 2-Amino-3-methylimidazo[4,5-*f*]quinoline (IQ) 0.3 ng/cig 3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) 0.3 ng/cig 3-Amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) 0.2 ng/cig 2-Amino-9*H*-pyrido[2,3-*b*]indole (AαC) 16.9 ng/cig 2-Amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC) 1.6 ng/cig
1986	Hoffmann and Wynder (1808) in their list of tobacco and tobacco smoke tumorigens did not list any *N*-heterocyclic amine
1986	Sugimura (3828c) reviewed the isolation and identification of the *N*-heterocyclic amines, their high mutagenicity in the Ames test (*S. typhimurium*) of several of them, their tumorigenicity, and their various sources—including CSC for many. However, Sugimura did write the following about the importance of the "cooked food" mutagens as human carcinogens: "Taking various factors into consideration, it is probably impractical and not realistic to make risk estimations from the carcinogenicity data on rodents given a single carcinogen. However, for a simple extrapolation of animal data for risk estimation, TD_{50} values, which are the doses needed to develop cancers in 50% of animals fed on carcinogens [IQ, Trp-P-1, Trp-P-2, Glu-P-1, Glu-P-2, AαC, and MeAαC] for their life time, have been calculated based on mouse experiments… If we assume the average TD_{50} value of heterocyclic amines should be about 8mg/kg/day, we can roughly estimate the risk of these carcinogenic heterocyclic amines for human beings. The intake of heterocyclic amines was calculated from available data on their quantities in foods. Apparently the human intake is about 0.0002% times the TD_{50} obtained from animal data. This means that heterocyclic amines may not be so serious for human cancer development"

TABLE 17.30 (continued)
Chronology of *N*-Heterocyclic Amine Studies

Year	Event
	Sugimura added: "On the other hand, it is also true that human beings are being exposed to many heterocyclic amines and many other carcinogens with tumor promoters and/or suppressing factors for carcinogenesis. At this moment, it is honest to state that no solid information on the estimation of risk of heterocyclic amines has been obtained in any direction, either positive or negative"
1990	Felton and Knize (1177d) reviewed the results of numerous studies on the mutagenicity and tumorigenicity of the *N*-heterocyclic amines
1990	Manabe et al. (2448) identified the *N*-heterocyclic amine 1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine (PhIP) in CSC
1991	By their addition to tobacco, Clapp (751) reported the contribution of various individual amino acids (asparagine, aspartic acid, arginine, glutamine, glutamic acid, histidine, proline, lysine, tryptophan, phenylalanine, creatine, creatinine) to the Ames test mutagenicity of cigarette MSS
1993	Lee et al. (2327c) reported that the CSC from cigarette MSS significantly inhibited the mutagenicity of several *N*-heterocyclic amines as measured in the Ames assay with *S. typhimurium* strain TA 98 in presence of the S-9 mix. The *N*-heterocyclic amines tested included the following: 2-Amino-3-methylimidazo[4,5-*f*]quinoline (IQ) 2-Amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ) 2-Amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) 2-Aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2) 3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) 3-Amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) The mutagenic activities of these mutagens were suppressed as much as 80% by addition of 50–100 µg of CSC per plate
1993	In their list of toxicants and tumorigens in tobacco and MSS, Hoffmann et al. (1773) did not include any *N*-heterocyclic amines
1994	In its list of toxicants and tumorigens in MSS, OSHA (2825) did not include any *N*-heterocyclic amines
1997	Hoffmann and Hoffmann (1740) issued a revised list of tumorigenic components in tobacco and tobacco smoke. Their revision of the Hoffmann–Hecht (1727) list included, in addition to several vapor-phase components, the following eight *N*-heterocyclic amines: 2-Amino-3-methylimidazo[4,5-*f*]quinoline (IQ) 2-Amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ) 2-Amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1) 2-Aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2) 3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) 3-Amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) 2-Amino-9*H*-pyrido[2,3-*b*]indole (AαC) 2-Amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC)
1998	In a letter to the editors of Beiträge zur Tabakforschung International, Hoffmann and Hoffmann (1741) listed eight *N*-heterocyclic amines as biologically active agents in the MSS of nonfiltered cigarettes. They also included the three aza-arenes reported as MSS components by Van Duuren et al. in 1960
1999/2000	Clapp et al. (755,756) reported that reduction of the level of protein in flue-cured tobaccos by 70% resulted in a reduction of 80% in the mutagenicity of the MSS "tar" (strain TA98 *S. typhimurium*) and 50% (strain TA100). Reduction of the protein level in burley tobacco by 50% resulted in reductions in mutagenicity of its MSS "tar" of 81% and 54%, with strain TA98 and TA100, respectively
2001	Hoffmann and Hoffmann (1743) and Hoffmann et al. (1744) listed eight *N*-heterocyclic amines as biologically active agents in the MSS of nonfiltered cigarettes. In both publications, the three aza-arenes reported as MSS components by Van Duuren et al. in 1960 were listed
2002/2003	In a presentation and publication, Rodgman and Green (3300) discussed the deficiencies of many of the lists of toxicants in cigarette MSS
2003	Rodgman (3265) outlined the major problems with the lists published by Hoffmann and colleagues (1740, 1741, 1743, 1744) and others
2005	Kinae et al. (2095a) reported that *N*-heterocyclic amines [2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ), 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ), 1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine (PhIP)] were produced in an incubated solution of *D*-glucose and several amino acids at much lower temperatures and longer time periods than those encountered in the cooking of various foodstuffs (beef, poultry, fish). Several *N*-heterocyclic amines not found in CSC were also generated. The generation of the *N*-heterocyclic amines, as measured by the Ames test (*S. typhimurium* TA98), increased in proportion to the conditions imposed: 37°C (90 d), 50°C (30 d), 128°C (2 h)

TABLE 17.31
N-Heterocyclic Amines in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

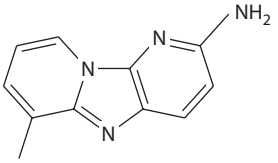
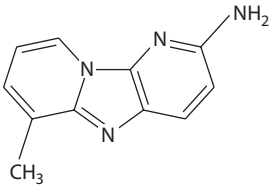
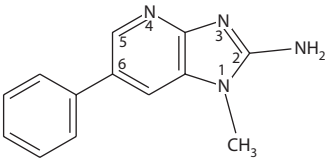
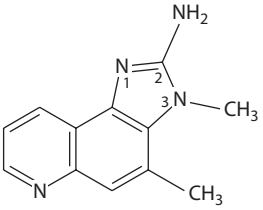
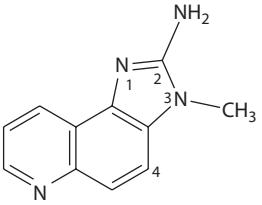
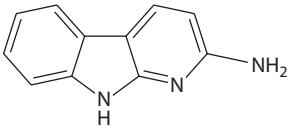
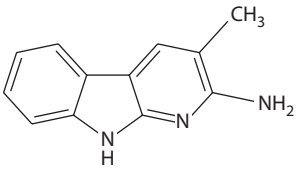
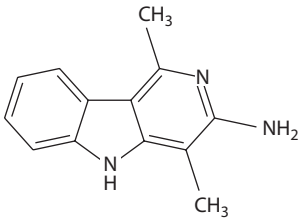
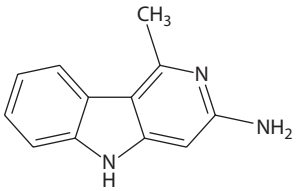
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
1.	67730-10-3	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine {Glu-P-2} 	751, 755, 756, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 5002, 5512, 5811b, 5869a		
2.	67730-11-4	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 6-methyl- {Glu-P-1} 	751, 755, 756, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 5002, 5512, 5811b, 5869a		
3.	105650-23-5	1*H*-Imidazo[4,5-*b*]pyridin-2-amine, 1-methyl-6-phenyl- {PhIP} 	1740, 1741, 1743, 1744, 2095a, 2448, 2484a, 2601, 3265, 3300, 3714, 5002, 5512, 5811b		
4.	77094-11-2	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3,4-dimethyl- {MeIQ} 	179a, 2095a, 2327c, 2354a, 2484a, 3255, 3257, 3265, 3300, 3714, 5002		
5.	76180-96-6	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3-methyl- {IQ} 	158a, 179a, 751, 755, 756, 1740, 1741, 1743, 1744, 2095a, 2327c, 2354a, 2484a, 2601, 3255, 3257, 3265, 3300, 3714, 3865c, 4367, 4368, 5002, 5512, 5811b, 5869a		
6.	26148-68-5	1*H*-Pyrido[2,3-*b*]indol-2-amine {AαC} 	179a, 179b, 751, 755, 756, 933, 1740, 1741, 1743, 1744, 2354a, 2449, 2450, 2484a, 2492, 3265, 3300, 3714, 4367, 4368, 4388, 4389, 4390, 5002, 5512, 5869a		
7.	68006-83-7	1*H*-Pyrido[2,3-*b*]indol -2-amine, 3-methyl- {MeAαC} 	179a, 179b, 751, 755, 756, 933, 1740, 1741, 1743, 1744, 2354a, 2449, 2450, 2484a, 2492, 3265, 3300, 3714, 4367,4368, 4388, 4389, 4390, 5002, 5512, 5811b, 5869a, 17F01		

TABLE 17.31 (continued)
***N*-Heterocyclic Amines in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke**

	CAS No.	Name (per CA Collective Index)	References		
			Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
8.	62450-06-0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1,4-dimethyl- {Trp-P-1} 	751, 755, 756, 1373, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4367, 4368, 5002, 5512, 5869a		
9.	62450-07-1	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1-methyl- {Trp-P-2} 	751, 755, 756, 1373, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4367, 4368, 5002, 5512, 5869a		

18 Miscellaneous Components

18.1 SULFUR-CONTAINING COMPONENTS

Sulfur is a well-known constituent of tobacco and is essential for growth of the plant. In 1990, Tso (3973) reviewed the chemistry, biology, and physiological aspects of sulfur in tobacco. It is absorbed by the plant as sulfate, some of which undergoes reduction during assimilation and becomes incorporated into amino acid components of proteins (18A11). The sulfur content of tobacco varies by tobacco type and has been reported (3973) to range from 0.4% for flue-cured varieties to 1.1% for the Maryland tobacco (4246). Sulfur-containing (*S*-containing) compounds in or on tobacco can also come from added flavors and casings such as cocoa, as a contaminant of the leaf or of flavors and casings, or from agrochemicals (fertilizers, pesticides, herbicides insecticides, etc.) applied to the tobacco. Endogenous *S*-containing compounds of tobacco include numerous proteins, peptides, nucleotides, several amino acids (methionine, cysteine, cystine, taurine, homocysteine), and B vitamins (thiamine and biotin). Sulfur is also available as various inorganic sulfates or sulfides found in tobacco.

Sulfur is found in many casings and flavors used on tobacco. Solid flavorants or casing materials used on tobacco such as cocoa and licorice are natural products, and just like tobacco, they contain *S*-containing amino acids and proteinaceous substances. Some flavor additives used on tobacco products are *S*-containing compounds. In 1994, the tobacco rod of a cigarette produced by any of the six major manufacturers could have had any combination of 599 different ingredients (1053), 460 of which were individual compounds as described by Rodgman (3266). Of the 460, Rodgman listed 212 identified as untreated tobacco components, 245 identified in its smoke, and 168 in both tobacco and smoke. Those numbers have changed slightly since several of the 460 components have recently been identified in tobaccos by Leffingwell and Alford (2339a) and Peng et al. (2917a). Within the compounds listed by Doull et al. (1053) are nine *S*-containing compounds, e.g., methyl sulfide, *d,l*-methionine, 5-methyl-2-thiophenecarboxaldehyde, 3-methylthiopropionaldehyde, and methional.

Tobacco contains residual levels of the *S*-containing agrochemical compounds that are used to treat tobacco, e.g., Benfuracarb®, Oryzalin®, Thiofide®, Malathion®, Pebulate®, Cyolane®, Thiodicarb®, Trapex®, and Zineb®.

Cigarette mainstream smoke (MSS) contains a wide variety of *S*-containing compounds, e.g., *S*-containing amino acids, residues of herbicides, pesticides, insecticides, and growth promoters [Malathion, Captan®, Thiodan®; α- and β-Endosulfan®, Disulfoton®, Guthion®; and Chlorpyriphos®)], certain organic sulfates and sulfides, and decomposition products of *S*-containing agrochemicals. MSS components possess a wide variety of *S*-containing functionalities (thiol, alkylthio, mercapto, isothiocyanatoalkyl, thiazolyl, phosphinothioyl, alkyldithio, phosphoramidothio, phosphonodithio, thiacycloalkyl, thiadiazinyl, thienyl, thiocarbamato, sulfide, sulfonate, sulfonyl, sulfuroxides, and trisulfide). MSS also contains several polycyclic compounds that contain sulfur (18A14), e.g., benzothiophenes, dibenzothiophenes, and nonbenzenoid aromatic heterocycles, e.g., benzodioxathiepins.

The sulfur compounds in cigarette MSS reside in both the volatile and semivolatile fractions of MSS. Some *S*-containing compounds are also present in the particulate phase of MSS. The largest amount of research on *S*-containing compounds in MSS has been on those in the vapor phase of MSS. The low-molecular-weight *S*-containing compounds are volatile and highly odorous at ppm and ppb concentrations. Their odor characteristics have been reported by a GC–port sniffing technique [Alford and Houpt (18A01), Ayya (18A03)].

Because of the odiferous nature of many of the vapor-phase *S*-containing compounds in MSS, their presence has often been considered undesirable. However, it must be kept in mind that smoke is a complex mixture and the contribution of any single component depending on its concentration can actually add to the overall characteristic of tobacco smoke. Certain *S*-containing compounds are excellent tobacco flavors such as butyl sulfide (floral), furfuryl mercaptan (coffee), and allyl disulfide (garlic, nutty) and provide positive smoke taste characteristics, although their aroma is considered harsh or garlic (2341). *S*-containing compounds in tobacco are also possible precursors to Maillard reaction flavors. *S*-containing compounds can participate in Amadori rearrangement and Strecker degradation (18A03). The unpleasantness of a single odorant should never be a valid reason to ignore or to reduce their effects in a complex mixture like tobacco smoke.

Ayya (18A03) in 1994 posed the question of whether any of the *S*-containing compounds of tobacco smoke might be important pharmacologically if present in sufficiently high concentration. There are a number of *S*-containing compounds that are pharmacologically active [Rezanka et al. (18A12)], but none is found in tobacco smoke at concentrations that are of any concern. In terms of any of the *S*-containing compounds in tobacco or tobacco smoke being biologically active, the International Agency for Research on Cancer (IARC) has only tested sulfur dioxide and various sulfites, bisulfites, and metabisulfites. In their 1992 monograph (18A05), IARC stated:

> There is inadequate evidence for the carcinogenicity in humans of sulfur dioxide, sulfites, bisulfites and metabisulfites. There is limited evidence for the carcinogenicity in experimental animals of sulfur dioxide. There is inadequate evidence for the carcinogenicity in experimental animals

of sulfites, bisulfites and metabisulfites. Overall evaluation: sulfur dioxide, sulfites, bisulfites and metabisulfites are not classifiable as to their carcinogenicity to humans (Group 3).

IARC provides a classification for its overall evaluations of carcinogenicity to humans (18A04). It classifies individual compounds and mixtures into five categories based on scientific data on humans and animals. The classification is as follows:

- Group 1: Carcinogenic to humans
- Group 2A: Probably carcinogenic to humans
- Group 2B: Possibly carcinogenic to humans
- Group 3: Not classifiable as to carcinogenicity to humans
- Group 4: Probably not carcinogenic to humans

There are no known *S*-containing compounds in tobacco or tobacco smoke in groups 1, 2A, or 2B. There are only six compounds that are found in group 3 (Malathion, ethylenethiourea, Parathion®, Parathion-methyl®, sulfur dioxide, and ethylene sulfide). The evidence for the carcinogenicity in humans of all these compounds was classified as inadequate (18A04).

Periodically during the past five decades, various reviews and catalogs on the composition of tobacco and tobacco smoke have been published. Some have listed *S*-containing compounds in tobacco and tobacco smoke, while others have not. In 1936, Bruckner (451) listed 120 known components in tobacco and tobacco smoke. Of the identified compounds that Bruckner listed, only one contained sulfur (sulfate). In 1954, Kosak (2170) categorized about 50 components in tobacco smoke whose identities were certain. Under his heading of *Inorganic Components*, Kosak listed hydrogen sulfide and thiocyanic acid (?). The question mark indicated that Kosak did not consider the evidence in the literature to be definitive proof of the identity of the component. Latimer (2270) in 1955 listed 231 compounds identified from tobacco and tobacco smoke. Cystine, methionine, thiamine, and sulfur were present in tobacco, and thiocyanic acid, carbonyl sulfide, and methyl mercaptan were identified in tobacco smoke. Johnstone and Plimmer in 1959 (1971) listed 950 compounds in tobacco and tobacco smoke. In their review, they listed only two sulfur compounds as identified in tobacco, cystine and methionine. Obi and Nakano conducted studies on sulfur in tobacco and tobacco smoke, in 1962 (2822). They determined that the sulfur content in Japanese tobacco was 0.3%–3%, of which 30%–60% is organic sulfur. In a review of compounds identified in tobacco and tobacco smoke, Philip Morris, Inc., in 1963 (2939) listed 17 *S*-containing compounds. Stedman (3797) in 1968 listed 950 identified compounds in tobacco and tobacco smoke; of these, only 10 compounds were *S*-containing and all were from tobacco smoke. Izawa (1900) in 1961 reported on 440 identified tobacco and tobacco smoke components; of these, only two *S*-containing compounds in tobacco were mentioned (cystine, methionine). Roberts et al. in 1975 (3224) listed 2783 compounds identified in tobacco and tobacco smoke. In their report, they listed 41 *S*-containing compounds identified in tobacco smoke. There were no *S*-containing compounds reported in tobacco. In 1980, Ishiguro and Sugawara (1884) listed 1889 identified tobacco smoke components in their monograph; 46 *S*-containing compounds were listed. IARC, in 1986, (1871) listed only three *S*-containing agrochemicals in tobacco. Elmenhorst and Schultz in 1986 (1140) listed 13 *S*-containing compounds in their publication. Roberts in 1988 (3215) tabulated that there were 5868 identified compounds in tobacco and tobacco smoke. By functional groups, 3044 compounds had been identified in tobacco, 3996 had been identified in smoke, and 1172 were identified in both tobacco and tobacco smoke. Under the function group heading *Sulfur Compounds*, three compounds had been identified in tobacco, 37 were identified in tobacco smoke, and two compounds were found in both tobacco and tobacco smoke. In 1994, Ayya (18A03) summarized the previous work on *S*-containing compounds in tobacco smoke. He listed 32 sulfur compounds that had previously been identified in tobacco smoke. In his report, he cited work at Brown and Williams Tobacco Company on the odor characterization of low-molecular-weight *S*-containing compounds employing a gas chromatograph with a sniffing port.

As mentioned previously, several reviews on tobacco and tobacco smoke have not included or have omitted the *S*-containing compounds in tobacco and tobacco smoke. These include the reports by Bentley and Berry in 1959 and 1960 (282, 283), Berry (296) in 1963, and the reports by Sakuma et al. (3394, 3397, 3398) in 1983 and 1984. Bentley and Berry reported in 1959 that "Sulphur compounds have been found in smoke [Izawa et al. (1905)] but these have not been identified."

Whether there was a lack of analytical instrumentation and/or methodology for the determination of *S*-containing compounds in tobacco and smoke or a lack of concern for these types of compounds cannot be said. But it is interesting that even by 1994 (18A03), only about 40 *S*-containing compounds were identified as components of tobacco and tobacco smoke.

From 1966 through 1974, several notable studies were conducted on *S*-containing compounds in tobacco smoke. In 1966, Philippe (2940) reported on the identification of thiocyanogen, thiocyanic acid, hydrogen sulfide, carbonyl sulfide, methylthionitrite, dimethyl sulfide, carbon disulfide, and thiophene in MSS. In that same year, ethyl mercaptan has been qualitatively detected by Grob (1419).

Williams and McRae (4246) examined the fate of *S*-containing compounds in tobacco during cigarette smoking in 1967. The nonfiltered cigarettes in their experiments contained approximately 0.5% sulfur. They determined that 61.4% of the total sulfur content of the cigarette was found in the cigarette ash and 33.2% was found in the cigarette butt. They reported that the sulfur content of the whole MSS was 39 μg per cigarette, which was equivalent to 0.5% of the total sulfur in the cigarette. In total, they could account for over 95% of the total sulfur content measured in the cigarettes used in their experiments.

Groenen and Van Gemert (1429) in 1971 and Horton and Guerin (1831) in 1974 reported on the identification of *S*-containing compounds in the vapor phase of MSS. Both investigator groups employed flame photometric detection (FPD) gas chromatography (GC) for the determination of sulfur compounds in smoke (1831). Groenen and Van Gemert identified 37 compounds, while Horton and Guerin identified 28 *S*-containing compounds. Typical cigarette yields reported by Horton and Guerin were approximately 85 µg of H_2S, 35 µg of COS, 2 µg of CS_2, and 3 µg of SO_2 per cigarette when smoked under standard conditions. Horton and Guerin reported that the vapor phase of MSS contained *at least* 28 sulfur components but that the quantitative distribution of these components was highly sensitive to sampling methodologies. Quantitation is an obvious issue as Williams and McRae (4246) only could account for 39 µg of sulfur per cigarette in whole MSS.

Generally, sulfur compounds in tobacco samples can be converted by wet oxidation to sulfate. The sulfate is then reduced to H_2S which is separated by distillation and determined as methylene blue by the method of Johnson and Nishita (18A06). Protein sulfur can also be determined by the oxidation of sulfur to sulfur dioxide and titration with 0.1 N I_2 with starch as an indicator (18A02). These classic methods serve as determinations of total sulfur in a sample. Similar wet methods for the analysis of sulfur compounds in tobacco now employ autoanalyzers and robotics [Mottershead (18A10)]. Total sulfur in the sample can also be analyzed by x-ray emission spectroscopy [Keen et al. (18A07)], atomic absorption spectrometry [SAH and Miller (18A13)], atomic emission spectroscopy (AES) and inductively coupled plasma ICP-AES [Littlefield et al. (18A08)], or a variety of other instrumental methods. For example, ESR has also been used for the analysis of the presence of sulfur in tobacco (18A09). Specific *S*-containing amino acids in tobacco, e.g., methionine, cysteine, and cystine, are generally analyzed by GC, GC-MS, or liquid chromatographic techniques such as HPLC and LC-MS. Sulfur in proteins, nucleotides, and peptides is normally analyzed by digestion of samples into free amino acids and then determination of the amino acids by GC or LC.

FPD-GC (1429, 1831) and flame ionization detection (FID) GC (1419) have been used for the determination of sulfur compounds in tobacco smoke. Although these methods are still used today, GC–mass spectrometry is normally the preferred method for the determination and quantification of *S*-containing components in MSS.

Table 18.1 lists the *S*-containing components in tobacco, tobacco smoke, and tobacco substitute smoke. A total of 289 *S*-containing components have been identified in tobacco and/or tobacco smoke. Of these compounds, 139 were identified in tobacco smoke, 194 were identified in tobacco, and 44 were identified in both tobacco and tobacco smoke. It is interesting to note that over 80 of the 289 *S*-containing components in tobacco and/or its smoke are compounds that are used or have been used in tobacco agronomy.

18.2 HALOGENATED COMPONENTS

All of the halogens [chlorine (Cl), bromine (Br), fluorine (F), and iodine (I)] are minor constituents of tobacco and are essential for growth of the plant. In 1990, Tso (3973) reviewed the chemistry, biology, and physiological aspects of each halogen in tobacco. Soil contains low levels of all of the halogens in the form of salts (halides). Low levels of these halogenated salts generally promote growth in the plants and improve quality and yield. At high levels of absorption, all halides can cause toxicity (3979). The various halides are absorbed by the plant roots and are important in certain oxidative, enzymatic, and plant regulatory processes (3973). The content of Cl, Br, F, and I in tobacco varies by tobacco type, soil, and climatic conditions. Typical ranges of Cl, Br, F, and I reported in tobacco are 0.07%–3%, 100–200 ppm, 4–40 ppm, and 0.55–1.75 ppm, respectively (3979). Other sources of halogens in tobacco come from trace amounts of halides in fertilizers and from agrochemical treatments of tobacco.

Over the last 70 years, several review articles on the constituents of tobacco and tobacco smoke have been published. In 1936, Bruckner (451) discussed the biochemistry of tobacco. In his book, he briefly mentioned that tobacco contained *chloride*. Kosak (2170) in 1954 categorized about 50 components in tobacco smoke whose identities were certain. Under his heading of *Inorganic Components*, Kosak listed "chlorides" (?). The question mark indicated that Kosak did not consider the evidence in the literature to be definitive proof of the identity of the component. Latimer (2270) in 1955 listed 231 compounds identified from tobacco and tobacco smoke. At that time, methyl chloride was the only halogenated compound identified in tobacco smoke. Johnstone and Plimmer in 1959 (1971) listed 950 compounds in tobacco and tobacco smoke. In their review, they listed only one halogenated compound as identified in tobacco, 1,1,-dichloro-2-2(4,4′-dichlorodiphenyl)ethane (TDE or DDD), and two in tobacco smoke, methyl chloride (specifically) and certain other unnamed volatile chlorides. Bentley and Berry in 1959 and 1960 (282, 283) and Berry (296) in 1963 failed to report any halogenated compounds in tobacco or tobacco smoke. Izawa (1900) in 1961 reported 440 identified compounds in tobacco and tobacco smoke. In his report, he listed only methyl chloride as being identified in tobacco smoke.

In a review of compounds identified in tobacco and tobacco smoke, Philip Morris, Inc., in 1963 (2939) listed seven halogenated compounds: Cl, bromomethane, chloromethane, chloroethane, bromoethane, Endrin®, and TDE. Stedman (3797) in 1968 listed 950 identified compounds in tobacco and tobacco smoke; of these, only 17 compounds were halogen containing. Cl, F, and I were identified in tobacco, along with tobacco residues of methylene bromide, 1,1,1-trichloro-2-(4,4′-dichlorodiphenyl)ethane (DDT), Dieldrin®, Dyrene®, Endrin, TDE, Telodrin®, Thiodan®, Toxaphene®, Trichlorfon®, and Diclone®. *o*-Chloroaniline, ethyl chloride, and agrochemical residues from TDE, Endrin, chloro-2,2-bis-(4′-chlorophenyl) ethylene (TDEE), Telodrin, Thoidan, and Dyrene were reported in tobacco smoke. Roberts et al. in 1975 (3224) listed 2783 components identified in tobacco and tobacco smoke.

TABLE 18.1
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

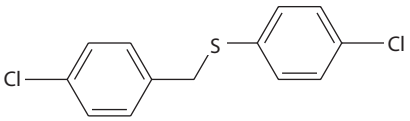
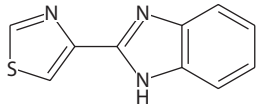
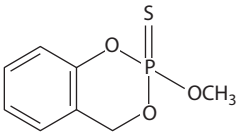
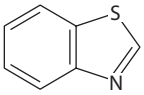
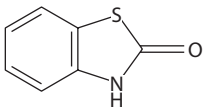
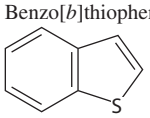
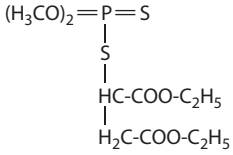
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	16752-77-5	Acetamidic acid, thio-, *N*-[(methylcarbamoyl)oxy]-, methyl ester {Methomyl®}		1219, 1219b, 1219c, 1333, 2650b, 3633, 3977, 4271a	
2.	26190-61-4	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-		2371a, 4249	
3.	53274-45-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-,(*E*)-		2371a, 4249, 4778	
4.	52049-48-6	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-,(*Z*)-		2371a, 4249, 4778	
5.	9012-52-6	Adenosyltransferase, methionine		429b, 922d, 4249	
6.	9012-39-9	Adenylyltransferase, sulfate		429b, 922d, 3973, 4249, 4853, 5811b	
7.	13100-82-8	Alanine, 3-sulfo-		3797, 3983b, 4249	
8.	82560-54-1	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy) carbonyl)methylamino) thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}		3633	
9.	12135-76-1	Ammonium sulfide		1053, 3266	
10.	103-17-3	Benzene, 1-chloro-4-(((4-chlorophenyl)methyl) thio)- {Chlorobenside®} 		3633	
11.	622-78-6	Benzene, (isothiocyanatomethyl)-		4249	
12.	2257-09-2	Benzene, (2-isothiocyanatoethyl)-		4249	
13.	116-29-0	Benzene, 1,2,4-trichloro-5-((4-chlorophenyl) sulfonyl)- {Tetradifon®}		3633	
14.	140-56-7	Benzenediazosulfonate, dimethylamino-, sodium salt {Fenaminosulf®}		3633	
15.	19044-88-3	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro- {Oryzalin®}		4271a	
16.	108-98-5	Benzenethiol {phenyl mercaptan} C_6H_5–SH	329, 2761, 4249, 5811b	937, 4249	
17.	148-79-8	1*H*-Benzimidazole, 2-(4-thiazolyl)- {Thiabendazole®} 	568b, 2207, 4249	568b, 2207, 3633, 4249	
18.	3811-49-2	4*H*-1,3,2-Benzodioxaphosphorin-2-sulfide, 2-methoxy- {Salithion®} 		3381, 3633, 4271a	
19.	26225-79-6	7-Benzofuranol, 2,3-dihydro-3,3-dimethyl-2-ethoxy-, methanesulfonate {Ethofumesate®}		3633, 4271a	
20.	239-35-0	Benzo[*b*]naphtho[2,1-*d*]thiophene	1409, 5811b		
21.	95-16-9	Benzothiazole {benzosulfonazole} 	2761, 4249, 4570a	404, 937, 984, 2336, 2917a, 2995, 3491, 4249, 5811b	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
22.	120-78-5	Benzothiazole, 2,2′-dithiobis- {Thiofide®}		3476	
23.	615-22-5	Benzothiazole, 2-methylthio-		404, 4249	
24.	934-34-9	2(3*H*)-Benzothiazolone 		404, 2917a, 4249	
25.	1128-67-2	2(3*H*)-Benzothiazolone, 3-methyl-, hydrazone	4249		
26.	95-15-8	Benzo[*b*]thiophene 	3514, 4249, 5811b		
27.		Benzo[*b*]thiophene, C_2-alkyl-	3514, 4248, 4249		
28.		Benzo[*b*]thiophene, C_3-alkyl-	4248		
29.	31393-23-4	Benzo[*b*]thiophene, methyl- {four isomers reported}	3514, 4248, 4249		
30.	14315-11-8	Benzo[*b*]thiophene, 4-methyl-	4249, 5811b		
31.	628-29-5	Butane, 1-(methylthio)- {butyl methyl sulfide} $H_3C\text{-}S\text{-}(CH_2)_3\text{-}CH_3$	568b, 1429, 4249		
32.	1613-46-3	Butane, 1-(propylthio)- $H_3C\text{-}(CH_2)_2\text{-}S\text{-}(CH_2)_3\text{-}CH_3$	568b, 1429, 4249, 5811b		
33.	544-40-1	Butane, 1,1′-thiobis- {dibutyl sulfide} $H_3C\text{-}(CH_2)_3\text{-}S\text{-}(CH_2)_3\text{-}CH_3$	1429, 4249, 5811b		
34.	121-75-5	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester {Malathion®} 	1618, 1619, 1884, 3634, 4249, 5811b, 21A19	1219b, 1219c, 1618, 2058a, 2650b, 3633, 3634, 3767a, 3973, 4249, 4271a, 21A19	
35.	2432-51-1	Butanethioic acid, *S*-methyl ester	5770		
36.	109-79-5	1-Butanethiol {butyl mercaptan} $H_3C\text{-}(CH_2)_3\text{-}SH$	568b, 1429, 4249, 5811b		
37.	541-31-1	1-Butanethiol, 3-methyl- $(H_3C)_2{=}CH\text{-}(CH_2)_2\text{-}SH$	1429, 4249, 5811b		
38.	513-53-1	2-Butanethiol $H_3C\text{-}CH_2\text{-}CH(SH)\text{-}CH_3$	568b, 1429, 4249		
39.	454-41-1	Butanoic acid, 2-amino-4-(methylsulfinyl)-		172, 429b, 4249	
40.	1118-85-0 3226-65-1	Butanoic acid, 2-amino-4-(methylsulfonyl)- {methionine sulfone, methionine S-oxide} $H_3C\text{-}SO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		120, 172, 1305a, 1351, 2337, 3491, 3729, 3797, 3974a, 4224, 4249, 5811b	
41.	583-92-6	Butanoic acid, 4-(methylthio)-2-oxo- $H_3C\text{-}S\text{-}(CH_2)_2\text{-}CO\text{-}COOH$		429b, 4249, 4699	
42.	462-10-2	Butanoic acid, 4,4′-dithiobis[2-amino- {homocystine} $[S\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH]_2$		2337, 3491, 3729, 3797, 3974a, 4224, 4226, 4249	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

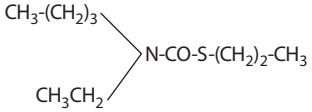
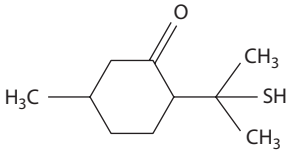
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
43.	68697-66-5	1-Butanone, 3-(methylthio)-1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-		3215, 4249, 4967	
44.		1-Butanone, 3-(methylthio)-1-(2,6,6-trimethylcyclohexenyl)-		3215, 4249, 4967	
45.	34047-39-7	2-Butanone, 4-(methylthio)-	3410, 4249, 4570a	937, 938, 1248, 2386, 4249	
46.	29736-33-2	2-Buten-1-ol, 2-methyl-4-[[2-(methylthio)-1*H*-purin-6-yl]amino]-,(*E*)-		4249, 4703	
47.	137-42-8	Carbamic acid, *N*-methyldithio-, monosodium salt {Metham-sodium®}		3633, 3646a, 4271a	
48.	594-07-0	Carbamodithioic acid		2574, 4249	
49.	9006-42-2	Carbamodithioic acid, 1,2-ethylene(bis-, polymer with ammonia complex of zinc ethylenebisdithiocarbamate {Metiram®}		429b, 3633, 4249, 4271a, 5525	
50.	1114-71-2	Carbamothioic acid, butylethyl-, *S*-propyl ester {Pebulate®} 		1219b, 1219c, 2913a, 3633, 4271a	
51.	759-94-4	Carbamothioic acid, dipropyl-, *S*-ethyl ester {EPTC®}		3633	
52.	1929-77-7	Carbamothioic acid, dipropyl-, *S*-propyl ester {Vernolate®}		2650a	
53.	2303-17-5	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester {Triallate®}		2650a	
54.	75-15-0	Carbon disulfide CS_2	237, 722, 1140, 1373, 1420, 1422, 1741,1831, 2310, 2313a, 2799a, 2939, 2940, 2945, 3255, 3257, 3265, 3300, 3302, 3729, 3797, 4249, 4319, 4332, 5039, 5811b, 5869a	5079, 5189, 21A05	
55.	463-58-1	Carbon oxide sulfide {carbonyl sulfide} COS	126b, 621, 722, 1140, 1445, 1674, 1828, 1831, 1832, 2025, 2079, 2142, 2170, 2270, 2293, 2310, 2634, 2799a, 2866, 2939, 2940, 2942, 3059, 3105, 3106, 3255, 3300, 3302, 3308, 3516, 3583, 3584, 3729, 3797, 3817a, 3897, 3939, 4135, 4249, 4319, 4360, 4395, 5039, 5811b, 5835		
56.	2944-05-0	Carbon sulfide CS	1140, 1429, 4249, 5811b		
57.	1333-22-8	Copper oxysulfate $Cu_4(OH)_6(SO_4)$		5811	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
58.	38462-22-5	Cyclohexanone, 2-(1-mercapto-1-methylethyl)-5-methyl- 		172a, 174b, 1053, 3266	
59.	74051-80-2	2-Cyclohexen-1-one, 2-[1-(ethoximino) butyl]-5-[2-(ethylthio)-propyl]-3-hydroxy- {Sethoxydim®}		3633	
60.	498-40-8	Cysteic acid $HO\text{-}SO_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$		622, 1351, 2337, 3491, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079	
61.	52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto-(R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1274, 3265, 3266, 4249	120, 158, 172, 342, 722, 927, 1053, 1128b, 1305a, 1351, 1918, 2049, 2337, 2939, 3266, 3491, 3729, 3797, 3974a, 3978, 4224, 4249, 4398c, 5079, 5189, 5376, 5811b, 5874, 5881	
62.	636-58-8	*L*-Cysteine, *N*-*L*-γ-glutamyl-		4249	
63.	24645-67-8	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-} $\{S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH\}_2$		116, 120, 172, 622, 722, 749, 752–754, 1063–1066, 1068–1074, 1127b, 1329, 1330, 1332, 1351, 2049, 2079, 2270, 2337, 2453, 2597a, 2939, 3491, 3499, 3705, 3729, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4249, 4398c, 5079, 5189, 5376, 5603, 5881, 5907	
64.	56-89-3 13028-62-1	*L*-Cystine		5811, 5811b	
65.	9036-20-8	Decarboxylase, adenosylmethionine		429b, 920a, 4249	
66.	9026-38-4	Dehydrogenase, glutathione (ascorbate)		429b, 922a, 4249, 4834	
67.	149309-58-0	Deoxyribonucleic acid (tobacco thioredoxin h2 gene plus 5′- and 3′-flanking region fragment)		452, 950b, 4249	
68.	140114-22-3	Deoxyribonucleic acid (tobacco thioredoxin messenger RNA complementary plus 5′- and 3′-flanking region fragment)		950b, 2934a, 4249	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

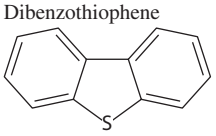
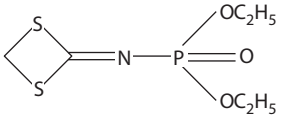
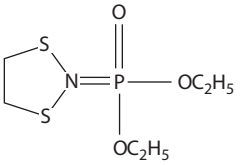
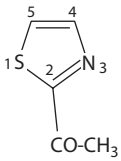
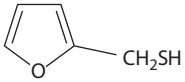
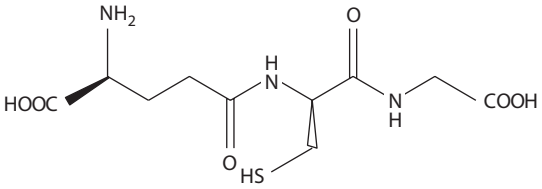
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
69.	148037-15-4	Deoxyribonucleic acid, (*Arabidopsis thaliana* thioredoxin h messenger RNA complementary plus 5′- and 3′-flanking region fragment)		950b, 2254a, 4249	
70.	132-65-0	Dibenzothiophene 	2596a, 3514, 3741, 4249, 5811b	3547	
71.	70021-47-5	Dibenzothiophene, dimethyl- {at least four isomers detected}		3547, 4249	
72.	30995-64-3	Dibenzothiophene, methyl- {at least four isomers detected}	3514	3547, 4249	
73.	5905-46-4	Disulfide, 1-propenyl propyl	1429, 4249		
74.	110-81-6	Disulfide, diethyl $H_3C\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_3$	1429, 4249, 5811b		
75.	624-92-0	Disulfide, dimethyl $H_3C\text{-}S\text{-}S\text{-}CH_3$	348, 1140, 2940, 3797, 4249, 4570a, 5039, 5770, 5811b	984, 3550, 4249	
76.	20333-39-5	Disulfide, ethyl methyl	1429, 4249, 5811b		
77.	5905-47-5	Disulfide, methyl 1-propenyl	1429, 4249		
78.	2179-58-0	Disulfide, methyl 2-propen-1-yl-	5811, 5811a		
79.	2179-59-1	Disulfide, propyl 2-propen-1-yl-	5811, 5811a		
80.	2179-60-4	Disulfide, methyl propyl	1429, 4249, 5811b		
81.	21548-32-3	1,3-Dithietan-2-ylidenephosphoramidic acid, diethyl ester {Fosthietan®} 		3633	
82.	947-02-4	Dithiolan-2-ylidenephosphoramidic acid, diethyl ester {Cyolane®, Phosfolan®} 		3380	
83.	2439-01-2	1,3-Dithiolo[4,5-*b*]quinoxalin-2-one, 6-methyl- {Quinomethionate®}		3633	
84.	9007-57-2	Edestin		429c, 2079	
85.	624-89-5	Ethane, (methylthio)-	1429, 4249		
86.	352-93-2	Ethane, 1,1′-thiobis- $C_2H_5\text{-}S\text{-}C_2H_5$	1590, 1831, 3854, 4249, 5811b		
87.	107-35-7	Ethanesulfonic acid, 2-amino- {taurine} $H_2N\text{-}(CH_2)_2\text{-}SO_3H$		622, 1351, 2337, 3491, 3974a, 4224, 4226, 4249	
88.	75-08-1	Ethanethiol {ethyl mercaptan} $C_2H_5\text{–}SH$	37, 38, 568b, 1140, 1828, 2079, 3854, 4249, 4425, 5811b		
89.	23135-22-0	Ethanimidothioic acid, 2-(dimethylamino)-*N*-[[(methylamino) carbonyl]oxy]-2-oxo-, methyl ester {Oxamyl®} $(H_3C)_2{=}N\text{-}CO\text{-}C(S\text{-}CH_3){=}N\text{-}OOC\text{-}NH\text{-}CH_3$		1280, 3633, 3634, 3646a, 3973, 4249, 4271a, 4891	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
90.	59669-26-0	Ethanimidothioic acid, *N′,N′*-(thiobis((methylimino) carbonyloxy))bis-, dimethyl ester {Thiodicarb®}		3633	
91.		Ethanone, 1-(2,3-dihydrothiophen-2-yl)-	568b, 4249		
92.	24295-03-2	Ethanone, 1-(2-thiazolyl)- {2-acetylthiazole} 		172a, 174b, 1053, 3266, 3370, 4249	
93.	88-15-3	Ethanone, 1-(2-thienyl)- {2-acetylthiophene}		937, 4249	
94.	38205-66-2	Ethanone, 1-(4-thiazolyl)- {4-acetylthiazole}	568b, 1587, 3266, 4249, 5811b		
95.	98-02-2	2-Furanmethanethiol 		1053, 3266, 4249	
96.	19246-18-5	Glycine, *N-L*-cysteinyl-		429b	
97.	70-18-8	Glycine, *N*-(*N-L*-γ-glutamyl-*L*-cysteinyl)- {glutathione} 		120, 1351, 1668, 2337, 2939, 3491, 3797, 3974a, 4249, 5079, 5220, 5572, 5811b	
98.	111-31-9	1-Hexanethiol	1429, 4249, 5811b		
99.	7783-06-4	Hydrogen sulfide H_2S	199, 239, 782, 916, 957, 1067, 1128, 1140, 1202, 1240, 1276, 1283, 1419, 1437, 1445, 1466, 1469, 1495, 1526, 1741, 1744, 1828, 1832, 1842, 2067, 2079, 2170, 2252, 2270, 2293, 2310, 2313a, 2342, 2343, 2502, 2524, 2607, 2621, 2782, 2799a, 2804, 2939, 2940, 3121a, 3187, 3300, 3302, 3308, 3493, 3524, 3525, 3797, 3817a, 3880, 3882, 3897, 3933, 3973, 4052, 4056, 4063, 4187, 4202, 4215, 4249, 4319, 4332, 4360, 5034, 5039, 5042, 5079, 5140, 5189, 5512, 5811b, 5835, 5869a	2607, 4249, 4795, 5079, 5323	4052, 4056, 4249
100.	96-45-7	2-Imidazolidinethione {ethylenethiourea}	124, 568b, 3265, 3300, 3714, 4249, 4596, 5811b, 5869a		

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

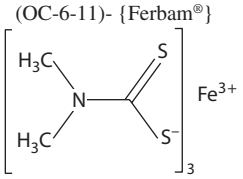
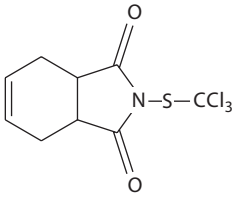
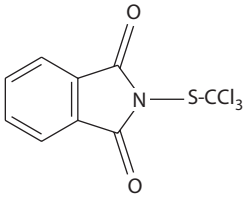
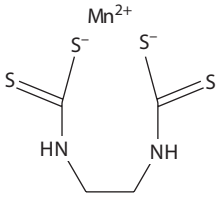
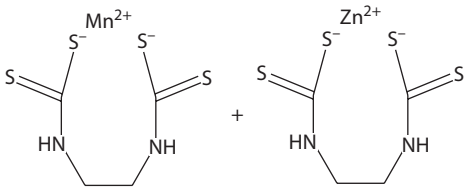
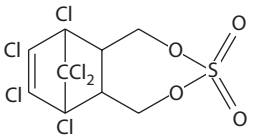
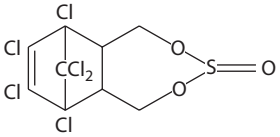
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
101.	14484-64-1	Iron, tris(dimethylcarbamodithioato-S,S′)-, (OC-6-11)- {Ferbam®} 		186, 3481, 3491, 3513, 3633, 4249, 4271a	
102.	133-06-2	1*H*-Isoindole-1,3(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]- {Captan®} 	3302, 4249, 21A19	1219c, 1884, 3633, 21A19	
103.	133-07-3	1*H*-Isoindole-1,3(2*H*)-dione, 2-[(trichloromethyl)thio]- {Folpan®} 		3633	
104.	139681-66-6	*L*-Isoleucine, *N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-valyl)-*L*-phenylalanyl]-*L*-leucyl]-		4249	
105.	556-61-6	Isothiocyanic acid, methyl- {Trapex®} $H_3C\text{-}N{=}S$	4570a	3633, 3646a, 3973, 4271a	
106.	288-16-4	Isothiazole 	568b, 1075, 1370, 4249		
107.	139681-65-5	*L*-Leucine, *N*-[*N*-[*N*-[*N*-[*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-phenylalanyl)-*L*-seryl]-*L*-leucyl]-*L*-leucyl]-*L*-methionyl]-*L*-valyl]-*L*-valyl]-		4249	
108.	12427-38-2	Manganese, [[1,2-ethanediylbis[carbamodithioato]](2-)]- {Maneb®} 		3491, 3513, 3633, 3661a, 4249, 4271a, 5811b, 21A19	
109.	8018-01-7	Manganese [[1,2-ethanediylbis[carbamodithioato]](2-)] + zinc, [[1,2-ethanediylbis-[carbamodithioato]](2-)] {Mancozeb®} 		2892a, 3633, 4271a, 5811b	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
110.	67-68-5	Methane, sulfinylbis- $(H_3C)_2{=}S{=}O$		4249	
111.	75-18-3	Methane, thiobis- {methyl sulfide} $(H_3C)_2{=}S$	1140, 1590, 2767, 2823, 2940, 3266, 3302, 3308, 3797, 3854, 4249, 4570a, 5811b	984, 1053, 2339a, 2611, 3266, 4249	
112.	74-93-1	Methanethiol {methyl mercaptan} $H_3C{-}SH$	112, 1140, 1419, 1634, 1828, 2079, 2090a, 2270, 2940, 3302, 3797, 3854, 3897, 4249, 4360, 4570a, 5034, 5039, 5811b	5811b	
113.	1031-07-8	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3,3-dioxide {Thiodan® sulfate, Endosulfan sulfate®} 	644, 1619, 3634, 4249, 21A19	644, 1028, 1219, 1219a, 1458, 1619, 2650a, 3188a, 3633, 3634, 3770, 3915, 4249, 21A19	
114.	115-29-7	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide {Thiodan®, Thiosulfan®, Endosulfan®} 	419, 644, 1457, 1619, 3302, 3634, 4249	419, 644, 1028, 1219, 1219a, 1219b, 1219c, 1457, 1458, 1619, 2650a, 2650b, 3188a, 3633, 3634, 3770, 3973, 4249, 4271a, 4858, 5811b	
115.	33213-65-9	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aα,6β,9β,9aα)- {β-Endosulfan®}	644, 3634, 4249	644, 2650a, 3188a, 3633, 3634, 3770, 4249, 5811b	
116.	959-98-8	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aβ,6α,9α,9aβ)- {α-Endosulfan®}	3634, 4249	2650a, 3633, 3634, 3770, 4249, 5811b	
117.	7005-18-7	Methionine		116, 120, 3705, 4249, 5907	
118.	63-68-3	*L*-Methionine $H_3C{-}S{-}(CH_2)_2{-}CH(NH_2){-}COOH$		116, 120, 158, 172, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1127b, 1305a, 1329, 1330, 1332, 1351, 1493, 2049, 2270, 2337, 2359, 2532, 2597a, 2795, 2939, 3186, 3188, 3266, 3491, 3499, 3705, 3729, 3797, 3973, 3974a, 3978, 4226, 4249, 4398c, 5079, 5376, 5811b, 5907	
119.	20236-97-9	*D*-Methionine, *N*-(carboxyacetyl)-		4249, 4699	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

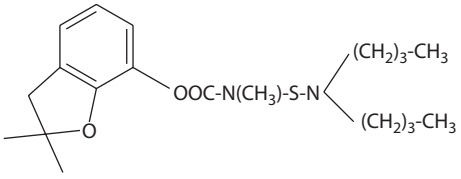
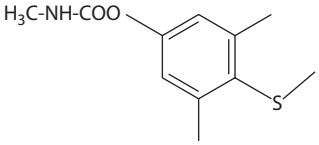
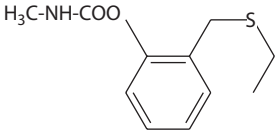
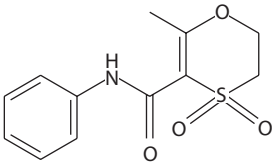
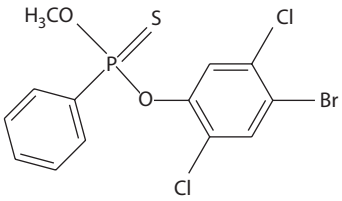
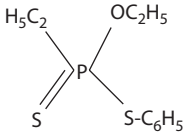
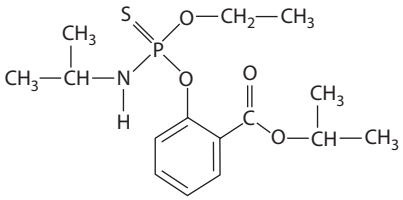
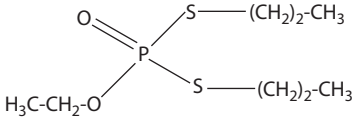
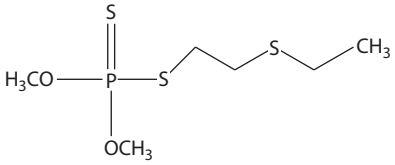
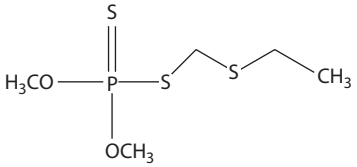
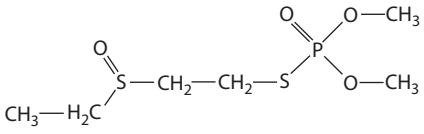
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
120.	55285-14-8	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl [(di-*N*-butylamino)thio] ester {Carbosulfan®} 		3633	
121.	2032-65-7	Methylcarbamic acid, 3,5-dimethyl-4-(methylthio)phenyl ester {Methiocarb®} 		3633, 4271a	
122.	29973-13-5	Methylcarbamic acid, 2-((ethylthio)methyl)phenyl- {Ethiofencarb®} 		3633, 4271a	
123.	1822-74-8	Methyl ethenyl sulfide H_3C-S-CH═CH_2-	3973, 4249		
124.	9012-40-2	Methyltransferase, homocysteine		429b, 4249	
125.	9027-77-4	Methyltransferase, methionine *S*-		429b, 4249	
126.	5259-88-1	1,4-Oxathiin-3-carboxamide 4,4-dioxide, 5,6-dihydro-2-methyl-*N*-phenyl- {Oxycarboxin®} 		2650b	
127.	110-66-7	1-Pentanethiol H_3C-$(CH_2)_4$-SH	1429, 4249, 5811b		
128.	66735-69-1	3-Pentanone, 1-(methylthio)-	4570a		
129.	9013-66-5	Peroxidase, glutathione		2954, 4249	
130.	21609-90-5	Phenylphosphonothioic acid, *O*-(4-bromo-2,5-dichlorophenyl)-, *O*-methyl ester {Leptophos®, Phosvel®} 	21A19	3381, 3634, 21A19	
131.	98886-44-3	Phosphonodithioic acid, *O*-ethyl *S*-(1-methylpropyl) (2-oxo-3-thiazolidinyl)- {Fosthiazate®}		3633	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
132.	944-22-9	Phosphonodithioic acid, ethyl-, *O*-ethyl *S*-phenyl ester {Fonofos®} 		3633, 4271a	
133.	22224-92-6	Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylthio)phenyl ester {Fenamiphos®}		2856a, 3381, 3633, 3646a, 3973, 4249, 4271a, 5811b	
134.	30560-19-1	Phosphoramidothioic acid, *N*-acetyl-, *O,S*-dimethyl ester {Acephate®}		1219a, 1219b, 1219c, 2058a, 2650b, 3633, 3634, 3973, 4271a	
135.	10265-92-6	Phosphoramidothioic acid, *O,S*-dimethyl ester {Methamidophos®}		2058a, 3633, 4271a, 5811b	
136.	25311-71-1	Phosphoramidothioic acid, *O*-ethyl *O*-2 (1-methylethyl) carbonylphenyl-, (1-methylethyl) ester {Isofenphos®} 		3633, 21A61	
137.	13194-48-4	Phosphorodithioic acid, *O*-ethyl-*S,S*, dipropyl ester {Ethoprophos®} 		2345, 3381, 3633, 3634, 3646a, 3767a, 3973, 4271a	
138.	2497-06-5	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylsulfonyl)ethyl] ester (Thiodemeton sulfone®)		4249	
139.	298-04-4	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester {Disulfoton®} 	1127	1127, 2058a, 2345, 3633, 3973, 4249, 4271a, 5811b, 21A19	
140.	298-02-2	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)methyl] ester {Phorate®} 		2058a, 3381, 3633, 4271a	
141.	301-12-2	Phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(ethylsulfinyl)ethyl] ester {Oxydemeton methyl®} 		3633, 21A22	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

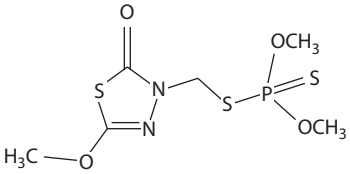
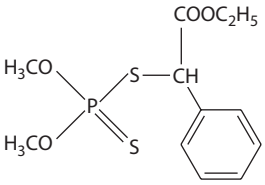
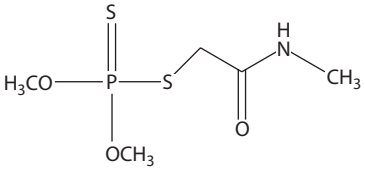
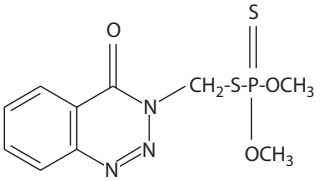
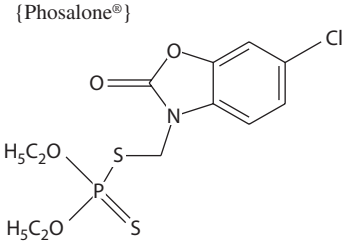
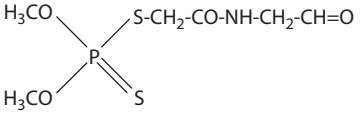
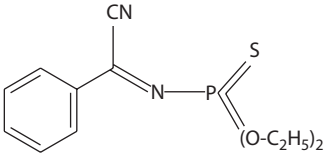
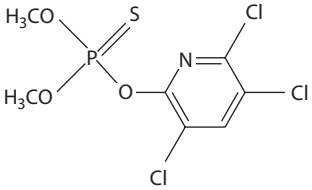
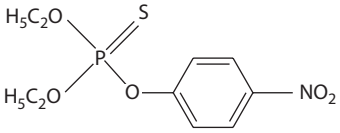
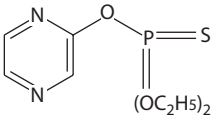
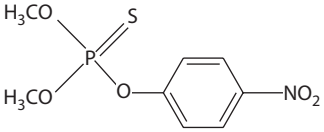
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
142.	640-15-3	Phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Thiometon®}		4271a	
143.	950-37-8	Phosphorodithioic acid, *O,O*-dimethyl-*S*-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl ester {Methidathion®} 		2058a, 3633, 3973, 4271a	
144.	2597-03-7	Phosphorodithioic acid, *O,O*-dimethyl *S*-(α-ethoxycarbonylbenzyl) ester {Fenthoate®, Phenthoate®} 		3381	
145.	60-51-5	Phosphorodithioic acid, *O,O*-dimethyl-*S*-[2-(methylamino)-2-oxoethyl] ester {Dimethoate®} 	5553b, 5811b	3380, 3633, 3797, 3973, 4271a, 5811b	
146.	2642-71-9	Phosphorodithioic acid, *O,O*-diethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Azinphos ethyl®}		3633, 4271a	
147.	86-50-0	Phosphorodithioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Guthion®, Azinphos-Methyl®} 	417, 419, 1457, 3302, 4249, 21A19	419, 1219a, 1219c, 1457, 2650b, 3381, 3973, 4249, 4271a, 21A19	
148.	2310-17-0	Phosphorodithioic acid, *S*-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl) methyl] *O,O*-diethyl ester {Phosalone®} 		3381, 4271a	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
149.	2540-82-1	Phosphorodithioic acid, *S*-[2-(formylmethylamino)-2-oxoethyl] *O,O*-dimethyl ester {Formothion®} 		2058a, 2650b, 3380, 3633, 4271a	
150.	41198-08-7	Phosphorothioic acid, *O*-(4-bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl ester {Profenophos®}		2058a	
151.	38527-91-2	Phosphorothioicacid, 2-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester {Ethaphos®}	5811, 5811a, 5811b		
152.	14816-18-3	Phosphorothioic acid, *O,O*-diethyl *O*-(α-cyanobenzylideneamino)- {Phoxim®} 		1492a, 4271a	
153.	2921-88-2	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyriphos®, Dursban®} 	717, 1333, 21A19	717, 1219a, 1219b, 1219c,1333, 2058a, 3381, 3633, 3919, 3977, 4249, 21A19	
154.	13071-79-9	Phosphorodithioic acid, *O,O*-diethyl *S*-[(1,1-dimethylethyl)thio] methyl ester {Terbuphos®}		2650b, 3633	
155.	115-90-2	Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylsulfinyl)phenyl] ester {Fensulfothion®}		2650b, 3633, 3973, 4249, 4271a	
156.	56-38-2	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®} 	21A19	2058a, 3381, 3633, 3634, 3973, 4249, 4271a, 5079, 5439, 5811b, 21A19	
157.	297-97-2	Phosphorothioic acid, *O,O*-diethyl *O*-pyrazinyl ester {Zinophos®, Thionazine®} 		3633, 4249, 4271a	
158.	298-00-0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-nitrophenyl) ester {Parathion-methyl®} 	5811b	2058a, 3381, 3633, 3973, 4271a	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

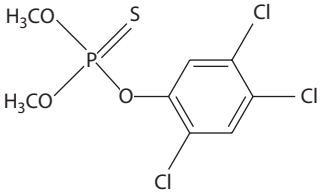
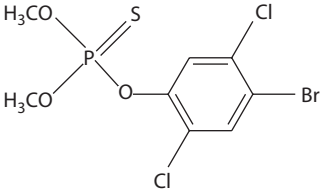
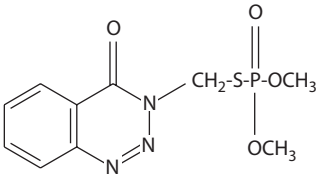
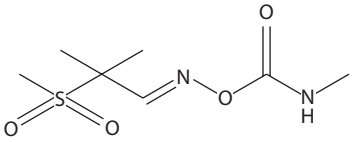
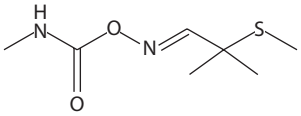
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
159.	299-84-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester {Fenchlorphos®, Phenchlorphos®} 		3381, 3633	
160.	2104-96-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-bromo-2,5-dichlorophenyl) ester {Bromophos®} 		3381, 3633, 4271a	
161.	333-41-5	Phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester {Diazinon®}	5811b	1219b, 1219c, 2058a, 2650b, 3633, 3973, 4249, 4271a	
162.	24017-47-8	Phosphorothioic acid, *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) ester {Triazophos®}		2650a	
163.	919-86-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Demeton-S-methyl®}		2058a, 3633, 4271a	
164.	961-22-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl) methyl] ester 	419, 3302, 4249	419, 4249	
165.	20300-00-9	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfinyl]ethyl] ester {Vamidothion sulfoxide®}		3992a, 4249	
166.	2275-23-2	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester {Vamidothion®}		822a, 2650a, 3633, 4249	
167.	70898-34-9	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfonyl]ethyl] ester {Vamidothion sulfone®}		4249, 4917	
168.	122-14-5	Phosphorothioic acid, *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester {Fenitrothion®}		3633, 3973, 4249, 4271a, 4917	
169.	55-38-9	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-methylthio)-3-methylphenyl ester {Fenthion®}		3633, 4271a	
170.	29232-93-7	Phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-dimethyl ester {Pirimiphos-methyl®}		4249	
171.	40626-35-5	Phosphorothioic acid, *O*-ethyl *O*-phenyl *S*-propylester {Heterophos®}	5811, 5811a, 5811b		
172.	1646-87-3	Propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino) carbonyl]oxime {Aldicarb Sulfoxide®}		1280, 2650a, 4249, 4271a, 5811b	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
173.	1646-88-4	Propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino) carbonyl]oxime {Aldoxycarb®} 		1280, 3585d, 4249, 5811b	
174.	116-06-3	Propanal, 2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl] oxime {Aldicarb®} 		1280, 1451, 2650a, 3585d, 3633, 3634, 3646a, 3973, 4249, 4271a, 5811b	
175.	3268-49-3	Propanal, 3-(methylthio)- {methional}	568b, 1365, 3255, 3266, 3854, 4249, 5770	174b, 568b, 1053, 3266, 4249	
176.	4110-50-3	Propane, 1-(ethylthio)- $H_3C\text{-}(CH_2)_2\text{-}S\text{-}CH_2\text{-}CH_3$	1429, 4249, 5811b		
177.	3877-15-4	Propane, 1-(methylthio)- $H_3C\text{-}(CH_2)_2\text{-}S\text{-}CH_3$	1429, 4249, 5811b		
178.	111-47-7	Propane, 1,1′-thiobis- {dipropyl sulfide} $[H_3C\text{-}(CH_2)_2]_2{=}S$	568b, 1429, 4249, 5811b		
179.	592-65-4	Propane, 1,1′-thiobis[2-methyl- {diisobutyl sulfide} $[(H_3C)_2{=}CH)_2]_2{=}S$	1429, 4249, 5811b		
180.	111-97-7	Propanenitrile, 3,3′-thiobis-	568b, 1587, 4249, 5811b		
181.	107-03-9	1-Propanethiol {propyl mercaptan}	3854, 4249, 5811b		
182.	513-44-0	1-Propanethiol, 2-methyl- {isobutyl mercaptan}	568b, 1429, 4249, 5811b		
183.	75-33-2	2-Propanethiol {isopropyl mercaptan}	1429, 4249, 5811b		
184.	13532-18-8	Propanoic acid, 3-(methylthio)-, methyl ester $H_3C\text{-}S\text{-}(CH_2)_2\text{-}COO\text{-}CH_3$		172a, 174b, 1053, 3266, 4249	
185.	10152-76-8	1-Propene, 3-(methylthio)- $H_3C\text{-}S\text{-}CH_2\text{-}CH{=}CH_2$	568b, 1429, 3973, 4249, 5811b		
186.	27817-67-0	1-Propene, 3-(propylthio)-	568b, 4249, 5811b		
187.	592-88-1	1-Propene, 3,3′-thiobis-	1429, 4249, 5811b		
188.	2028-39-9	1-Propene-3-thiol	568b, 4249		
189.	870-23-5	2-Propene-1-thiol	1429, 4249, 5811b		
190.		Protease, sulfhydryl		4249, 4287	
191.	67952-65-2	Pyrazine, 3 (5 or 6)-methyl-2-methylthio-		1053, 3266, 4249	
192.	65-30-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate (2:1)		3633, 3634, 3874c, 4249	
193.	6505-86-8	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate		3633, 3634, 3874c, 4249	
194.	9038-53-3	Pyrophosphatase, thiamin		429b, 4249, 4462	
195.	9001-48-3	Reductase, glutathione		429b, 2954, 3093c, 4249, 4834, 5811b	
196.	142785-07-7	*L*-Serine, *L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		4249	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

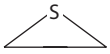
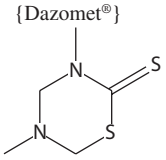
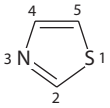
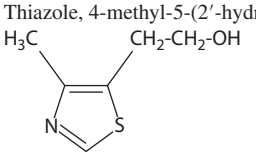
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
197.	146440-48-4	*L*-Serine, *L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		4249	
198.	14808-79-8	Sulfate	1445, 2931, 4249, 5811b	385, 1545, 1895, 2154, 2338, 2356, 2543, 2545, 2627, 2761, 2762, 2765, 2766, 3160, 4249, 5053, 5079, 5189, 5195, 5811b	
199.	18496-25-8	Sulfide	2621, 2627, 4249, 5811b	20A89	
200.		Sulfonium		2823, 5777	
201.	14265-45-3	Sulfite	4249, 20A88	1243a, 4249	
202.	7704-34-9	Sulfur	50, 641, 1240, 1933b, 2270, 2524a, 3302, 4229, 4230, 4249, 5811b	116, 193, 1127b, 1240, 2079, 2270, 2283, 2338, 2393, 3476, 3633, 3797, 3973, 3974b, 4249, 5079, 5113, 5189, 5220, 5282, 5378, 5448, 5811b, 5670, 5715	50, 4249
203.	7446-09-5	Sulfur dioxide	213, 270, 891a, 1140, 1445, 1828, 1832, 2083, 2084, 3255, 3257, 3300, 3302, 3306, 3729, 3817a, 3880, 3882, 3973, 4005–4007, 4052, 4056, 4249, 4332, 5042	4908a, 5811b	4052, 4056, 4249
204.	2551-62-4	Sulfur hexafluoride SF_6		4860, 18B17	
205.	7446-11-9	Sulfur trioxide	1240, 1941, 4249	1941,4249	
206.	7664-93-9	Sulfuric acid		3476, 3633	
207.	7783-20-2	Sulfuric acid, ammonium salt		5811	
208.	7778-18-9	Sulfuric acid, calcium salt		5811, 5811b	
209.	7758-98-7	Sulfuric acid, copper salt		3633	
210.	10377-48-7	Sulfuric acid, dilithium salt		5811b	
211.	7778-80-5	Sulfuric acid, dipotassium salt		3973, 4249, 5811b	
212.	7757-82-6	Sulfuric acid, disodium salt		3973, 4249, 5811b	
213.	7487-88-9	Sulfuric acid, magnesium salt		5811, 5811b	
214.	7488-54-2	Sulfuric acid, rubidium salt		5811	
215.	7733-02-0	Sulfuric acid, zinc salt		5811	
216.	7757-83-7	Sulfurous acid, disodium salt		3973, 4249	
217.	7773-03-7	Sulfurous acid, monopotassium salt		3973, 4249	
218.	420-12-2	Thiacyclopropane {ethylene sulfide} 		3973	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
219.	533-74-4	1,3,5-Thiadiazine, 2-thio-3,5-dimethyl-tetrahydro- {Dazomet®} 		3633, 3646a, 3973	
220.	288-47-1	Thiazole 	568b, 1371, 1590, 3266, 4248, 4249	568b, 1053, 2359, 3266	
221.		Thiazole, methyl-5-propyl-	4570a		
222.	37645-61-7	Thiazole, 2-butyl-	4570a		
223.	15679-09-1	Thiazole, 2-ethyl-	568b, 1590, 2049, 4249, 4570a		
224.	15679-12-6	Thiazole, 2-ethyl-4-methyl-	5811		
225.	19961-53-6	Thiazole, 2-ethyl-5-methyl-	568b, 1587, 4249, 4570a		
226.	3581-87-1	Thiazole, 2-methyl-	312, 568b, 4249, 4570a		
227.	17626-75-4	Thiazole, 2-propyl-	5811		
228.	15679-11-5	Thiazole, 2-methyl-4-(1,1-dimethylethyl)-	5811		
229.	15679-10-4	Thiazole, 2-(1-methylethyl)-	4570a		
230.	18277-27-5	Thiazole, 2-(1-methylpropyl)-	4570a		
231.	18640-74-9	Thiazole, 2-(2-methylpropyl)-	4570a		
232.		Thiazole, 2-(3-methylbutyl)-	4570a		
233.	32272-49-4	Thiazole, 2,4-diethyl-	4570a		
234.	52414-89-8	Thiazole, 2,4-diethyl-5-methyl-	5811		
235.	541-58-2	Thiazole, 2,4-dimethyl-	312, 568b, 1371, 4249		
236.	13623-11-5	Thiazole, 2,4,5-trimethyl-	568b, 1587, 1587a, 4249, 5811b		
237.	41981-71-9	Thiazole, 2,5-diethyl-4-methyl-	4570a		
238.	4175-66-0	Thiazole, 2,5-dimethyl-	568b, 4249, 4570a, 4570a		
239.	32272-48-3	Thiazole, 4-ethyl-2-methyl-	568b, 1587, 1587a, 4249, 5811b		
240.	52414-91-2	Thiazole, 4-ethyl-5-methyl-	568b, 1587, 1587a, 4249, 5811b		
241.	87116-68-5	Thiazole, 4-ethyl-5-methyl-2-(1-methylethyl)-	5811		
242.	693-95-8	Thiazole, 4-methyl-	568b, 1360, 1371, 1375a, 1590, 2761, 2762, 2777, 4249		1360, 1375a, 4249
243.	656-53-1	Thiazole, 4-methyl-5-(2-acetoxyethyl)-	5811		
244.	137-00-8	Thiazole, 4-methyl-5-(2′-hydroxyethyl)- 		174b, 3266	

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

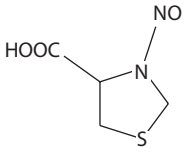
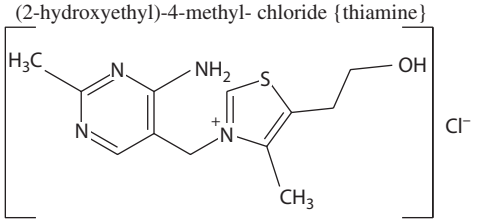
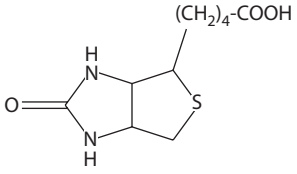
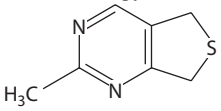
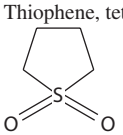
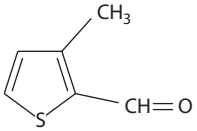
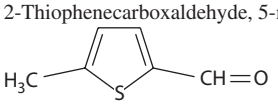
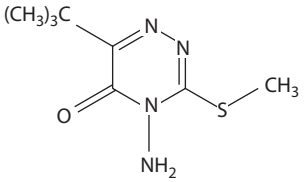
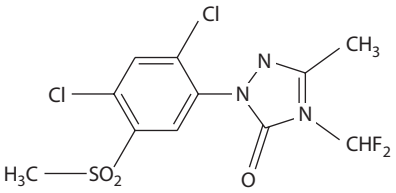
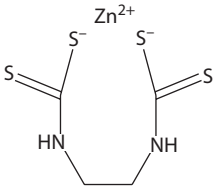
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
245.	15679-13-7	Thiazole, 4-methyl-2-(1-methylethyl)-	5811		
246.		Thiazole, 4-(2-methylpropyl)-	4570a		
247.	41981-60-6	Thiazole, 4-propyl-	568b, 1587, 1587a, 4249, 5811b		
248.	2346-00-1	Thiazole, 4,5-dihydro-2-methyl-	5811		
249.	3581-91-7	Thiazole, 4,5-dimethyl-	568b, 1587, 1587a, 1590, 4249, 5811b	568b, 2336	
250.	873-64-3	Thiazole, 4,5-dimethyl-2-ethyl-	5811		
251.	53498-30-9	Thiazole, 4,5-dimethyl-2-(1-methylethyl)-	5811		
252.	53498-32-1	Thiazole, 4,5-dimethyl-2-(2-methylpropyl)-	5811		
253.	1759-28-0	Thiazole, 5-ethenyl-4-methyl-	5811	1053, 3266	
254.	17626-73-2	Thiazole, 5-ethyl-	568b, 1587, 1587a, 4249, 5811b		
255.	38205-61-7	Thiazole, 5-ethyl-2,4-dimethyl-	568b, 2773, 4249		
256.	19961-52-5	Thiazole, 5-ethyl-2-methyl-	568b, 1587, 4249		
257.	31883-01-9	Thiazole, 5-ethyl-4-methyl-	568b, 1587, 1587a, 4249, 5811b		
258.	3581-89-3	Thiazole, 5-methyl-	568b, 1370, 4249		
259.	72611-71-3	Thiazole, 5-methyl-2-(2-methylpropyl)-	5811		
260.	88381-44-6	4-Thiazolidinecarboxylic acid, 3-nitroso- {*N*-nitrosothioproline} 		486, 3300, 5811b	
261.	154-87-0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, *P*,*P*′-dioxide		4051a, 4249, 4798	
262.	59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride {thiamine} 		120, 1941, 2270, 4249, 5079, 17B10	
263.	67-03-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride, monohydrochloride {thiamine hydrochloride}		1053, 3266, 4249	
264.	58-85-5	1*H*-Thieno[3,4-*d*]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3aS-(3aα,4β,6aα)]- 		2408a, 4249, 4789	

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
265.	36267-71-7	Thieno(3,4-*d*)pyrimidine, 5,7-dihydro-2-methyl- 		1053, 3266, 17B22	
266.	302-04-5	Thiocyanate	1445, 4249	20A56	
267.	463-56-9	Thiocyanic acid	1140, 1971, 2170, 2270, 2607, 2724, 2939, 2940, 3302, 3491, 3525, 3797, 4249, 4319, 4332, 5079, 5770, 5811b	2607, 3525, 5079	
268.	556-64-9	Thiocyanic acid, methyl ester	1587, 4249, 5039, 5811b		
269.	505-14-6 15941-77-2	Thiocyanogen $(SCN)_2$	1140, 1971, 2724, 2939, 2940, 3302, 3491, 3797, 3931, 4249, 5079, 5811b		
270.	137-26-8	Thioformamide, 1,1′-dithiobis(*N,N*-dimethyl {Thiram®}		3633, 5811b	
271.	22223-61-6	Thionitrous acid (HNOS), *S*-methyl ester	1140, 1420, 2724, 2939, 2940, 2945, 3491, 4249, 4319, 5811b		
272.	110-02-1	Thiophene 	329, 348, 1140, 1153, 1412–1414, 1416, 1422, 1590, 1831, 2767, 2782, 2804, 2940, 3302, 3308, 3514, 3557, 3797, 4249, 4319, 5770, 5811b	1849, 4249	
273.	638-00-6	Thiophene, 2,4-dimethyl-	1429, 1590, 4249, 5811b		
274.	872-55-9	Thiophene, 2-ethyl-	5811		
275.	25154-40-9	Thiophene, methyl-	1153, 1154, 4249, 5811b	1849, 4249	
276.	554-14-3	Thiophene, 2-methyl-	568b, 1590, 4249		
277.	616-44-4	Thiophene, 3-methyl-	5811		
278.	126-33-0	Thiophene, tetrahydro-, 1,1-dioxide {Sulfolan®} 	568b, 1360, 1375a, 2761, 2762, 3553, 4249, 5811b		1360, 1375a, 4249
279.	98-03-3	2-Thiophenecarboxaldehyde	568b, 1360, 1375a, 2761, 4249	568b, 1590, 3547, 4249	1360, 1375a, 4249

(*continued*)

TABLE 18.1 (continued)
Sulfur-Containing Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
280.	5834-16-2	2-Thiophenecarboxaldehyde, 3-methyl- 	568b, 2761, 2765, 2766, 3553, 4249, 5811b	568b, 937, 2389, 2544, 4249, 5811b	
281.	13679-70-4	2-Thiophenecarboxaldehyde, 5-methyl- 	568b, 1590, 2761, 2762, 2765, 2766, 2777, 3266, 4249, 4570a	568b, 937, 1053, 1590, 3266, 4249	
282.	149956-84-3	Thioredoxin h2 (tobacco)		1280a, 4249	
283.	7772-98-7	Thiosulfuric acid, disodium salt		5811	
284.	50812-37-8	Transferase, glutathione *S*-		429b, 922d, 4249	
285.	21087-64-9	1,2,4-Triazin-5(4*H*)-one, 4-amino-6-tert-butyl-3-(methylthio)- {Metribuzin®} 		2913a, 4249	
286.	122836-35-5	1*H*-1,2,4-Triazol-1-yl)phenyl)methane-sulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)phenyl)-; Sulfentrazone®} 		2913a	
287.	3658-80-8	Trisulfide, dimethyl $H_3C\text{-}S\text{-}S\text{-}S\text{-}CH_3$	1429, 4249, 4570a, 5770, 5811b		
288.	12122-67-7	Zinc, [[1,2-ethanediylbis[carbamodithioato]](2-)]- {Zineb®} 		3481, 3491, 3513, 3633, 4249, 4271a, 4645, 5629, 5811b, 21A19	
289.	18920-65-5	Zinc, bis(thiocarbamato)-		3481, 3513, 4249, 5629	

In their report, they listed 30 chloro compounds, two bromo-containing compounds, two fluoro-containing compounds, and one iodo-containing compound. Thirty-one halogenated compounds were identified in tobacco smoke, 12 were identified in tobacco, and several were found in both tobacco and tobacco smoke. In 1980, while noting that the number of confirmed components exceeded 2500, Ishiguro and Sugawara (1884) listed 1889 identified tobacco smoke components in their monograph; 17 were halogenated. In their review, Ishiguro and Sugawara stated:

> All of the halogenated compounds found in smoke are chlorinated compounds. These probably originate from the chloride ions [3797] in the tobacco or from residual chlorinated organic additives. The chlorine atom in methyl chloride originates [712] mainly from inorganic chlorides.

They listed Cl, Br, I, and F as identified components in tobacco smoke. In their review, Ishiguro and Sugawara also examined several agrochemicals and their decomposition products transferred to smoke. The distribution of the chlorinated organic chemicals was examined in detail. It was clear to them that chlorinated organic agricultural chemicals produced the chlorinated compounds mentioned in their review during smoking. They stated:

> At present, the use of chlorinated organic insecticides has been banned in many countries, and their residues in tobacco have been decreasing every year. Organophosphorus types and synthetic organic compounds which are less likely to persist have become the mainstay of agricultural chemicals for tobacco cultivation, displacing the chlorinated organic types.

Unfortunately, their prediction was not totally correct as a great variety of chlorinated organic agrochemicals are still being discovered and used today in parts of the world. However, since 1969, the use of chlorinated pesticides has been banned in the cultivation of tobacco in the United States. As a result, DDT and TDE in tobacco and in cigarette smoke have drastically decreased. In the tobacco of a cigarette made in 1965, 13.4 ppm DDT and 20.2 ppm TDE were measured, and in the tobacco of the leading cigarette brand made in 1993, only 0.02 ppm DDT and 0.013 ppm TDE were detected, a decrease of more than 98% (999). The small amounts of residual DDT and TDE in more recently produced cigarettes appear to originate from imported tobaccos used for blended cigarettes (1714). It is interesting to note the following: Despite the fact that DDT was banned from agronomic use on tobacco in the United States in 1969, Chopra and his colleagues between 1969 and 1973 conducted exceptionally detailed studies on the degradation products generated during the smoking process from the *p,p′*-DDT in *p,p′*-DDT-treated cigarettes (703, 707–709, 711–714). Examination of the citations in the catalog (Table 18.4) of chloro compounds identified in the smoke from DDT-containing tobacco indicates that Chopra and his colleagues identified 10 chloro compounds, including transferred DDT.

New types of chlorinated organic agrochemicals though are still being developed. Their popularity and efficiency have not been displaced by organophosphorus types of agrochemicals or other synthetic organic compounds. Sakuma et al. (3394, 3397, 3398) in 1983 and 1984 reported on the identification of numerous compounds in tobacco smoke. In their reports, no halogenated compounds were reported. IARC, in 1986 (1871), listed only four halogen-containing compounds in tobacco and tobacco smoke in their report on the evaluation of the carcinogenic risk of chemicals to humans: vinyl chloride and the agricultural chemicals, DDT, Captan®, and Endrin. Of these compounds, only vinyl chloride and DDT showed sufficient evidence of carcinogenicity in experimental animals according to the IARC criteria. Most recently in 2005, Eberhardt (21A19) prepared an extensive review of pesticides used on tobacco, the transfer rates of pesticides to MSS and sidestream smoke (SSS), and decomposition products of pesticide residues identified in MSS. In his review, much data previously presented by Ishiguro and Sugawara (1884) were presented and updated.

The vast majority of the halogenated compounds presented in this chapter are covered in other chapters of this book, e.g., Chapters 4, 9, 10, 19, 20, and 21. One particular group of halogenated compounds only reviewed in this chapter is the dioxins. Dioxins are polychlorinated heterocycles. The three forms found in tobacco and tobacco smoke are polychlorodibenzo-*p*-dioxins (PCDDs), polychlorodibenzofurans (PCDFs), and polychlorinated biphenyls (PCBs). Another group of compounds that is not reviewed elsewhere in the book is the Freon® compounds. Green et al. (1375b) recently reviewed the various chemicals used in the expansion of tobacco and their effect on cigarette MSS properties. In their review, Green et al. (1375b) discussed the use of various Freon compounds for tobacco expansion. Rix, in 1989, analyzed expanded tobacco for the expansion agent Freon 123 (4859). Additionally, sulfur hexafluoride and perfluoropropane have been investigated as alternate tobacco expanding agents (4860, 18B17). As a result, these classes of compounds will not be discussed further in this chapter, and the reader is directed to the review by Green et al. (1375b) and references from R.J. Reynolds Tobacco Company (4859, 4860, 18B05, 18B06 18B08, 18B16, 18B17).

In 2002, Rodgman and Green (3300) reviewed the literature on tobacco smoke toxicants. In their review, they discussed the PCDDs and PCDFs identified in tobacco and tobacco smoke. Rodgman and Green noted that among the smoke toxicants conspicuous in their absence from all toxicant lists except that of Fowles and Bates (1217) are the PCDDs and PCDFs. The presence of dioxins in cigarette smoke was first reported in 1980 by Crummett (854). There are at least five other publications in which the presence of dioxins (PCDDs and PCDFs) in cigarette tobacco or its MSS (3300) is reported. These include publications by Muto and Takizawa (2664), Ball et al. (177), Matsueda et al. (2490, 2491), and Löfroth and Zebühr (2391).

The smoke yield data of Muto and Takizawa (2664) were obtained from a single smoking puff that entirely consumed the cigarette and are clearly not appropriate for comparisons of MSS yields obtained by FTC or Coresta methods. The MSS and SSS data of Löfroth and Zebühr (2391) were obtained from only one Swedish cigarette brand. The PCDD and PCDF data reported by Matsueda et al. (2491) were for the amount of these compounds contained in the cigarette tobacco rather than the smoke. The smoke yield data for the Ball et al. (177) and Matsueda et al. (2490) experiments were similar. The Ball et al. data were collected and analyzed by a well-validated method, and the laboratory where the analyses were performed, i.e., ERGO Forschungsgesellschaft mbH, Hamburg, has been accredited by the World Health Organization (WHO) for dioxin analysis (177). The analytical data of Ball et al. (177) represent results from the 10 top selling brands in Germany during the fourth quarter of 1989. The ERGO scientists chose to present individual data on each of the tested cigarettes. It should be noted that the most toxic isomer, 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD), was not detected in any of the samples, and additionally, not every isomer present was quantifiable in each product tested. The total amount of total PCDDs and PCDFs was 7.50 and 2.98 pg/cig, respectively (see Table 2 of 3300). In 1998, Radovanović and Mišić (18B15) examined the MSS of Yugoslavian cigarettes for PCBs. They identified 10 PCBs. The level of PCBs identified ranged from less than 1 to 78.1 ng/g of smoke condensate (18B15). Generally, the levels of PCBs in MSS are considerably less than the PCDDs and PCDFs (3715).

Dioxins are not typical herbicides used on tobacco. So where do they come from and why are they so important?

2,4-Dichlorophenoxyacetic acid (2,4-D) was introduced in 1944 as the first of the phenoxy herbicides, phenoxyacetic acid derivatives, or hormone weed killers. The phenoxy herbicides have complex mechanisms of action resembling those of auxins (growth hormones). They affect cellular division, activate phosphate metabolism, and modify nucleic acid metabolism. These herbicides are highly selective for broadleaf weeds and are translocated throughout the plant. 2,4-D provided most of the impetus in the commercial search for other organic herbicides in the 1940s. Several compounds belonged to this group, of which 2,4-D and 2,4,5-trichlorophenoxyacetic acid (2,4,5-T) are the most familiar. Other important compounds in this group are 4-(2,4-dichlorophenoxy)butyric acid (2,4-DB), 2-methyl-4-chlorophenoxy-acetic acid (MCPA), and 2-(2,4,5-trichlorophenoxy)propionic acid (Silvex® or Fenoprop®) [Ware and Whitacre (18B18)].

2,4-D, MCPA, and 2,4,5-T have been used worldwide for years in very large volume. The latter product, 2,4,5-T, used mainly to control woody perennials, became the subject of extended investigation, particularly because of its use in Vietnam in combination with 2,4-D as Agent Orange. Certain samples were found to contain small amounts of a highly toxic impurity, TCDD, commonly referred to as tetrachlorodioxin, or dioxin. Although alterations in manufacturing procedures reduced the dioxin content to minimal levels, 2,4,5-T registrations were canceled, and the product was voluntarily removed by the manufacturers in 1985 (18B18).

2,4-D has been and continues to be one of the most useful herbicides ever developed. More than 33 million pounds manufactured in the United States are used each year in 35 ester and salt forms. In agriculture, it is used on cereal, grain crops, and sugarcane for the control of broadleaf weeds and on rights-of-way, turf and lawns, and in forest conservation programs. The manufacturing process for 2,4-D used in the United States does not result in any level of tetrachlorodioxin contamination. Other members of the phenoxys in wide use are 2-(2,4-dichlorophenoxy)propionic acid (Dichlorprop® or 2,4-DP), 4-(4-chloro-2-methylphenoxy)butanoic acid (MCPB), and 2-(4-chloro-2-methylphenoxy)propanoic acid (Mecoprop® or MCPP) (18B18). None of these compounds [2,4-DB, 2,4-DP, MCPB, MCPA, MCPP, 2-(2,4,5-trichlorophenoxy)propionic acid] have been found in tobacco or tobacco smoke.

Of the three forms of dioxins found in tobacco and tobacco smoke, the PCDDs, PCDFs, and PCBs are a group of chemical compounds which are among the most toxic and hazardous pollutants in the environment. The PCDDs, PCDFs, and PCBs compounds, collectively referred to as dioxins, are impurities associated with certain end products resulting from the treatment of chlorinated benzenes at elevated temperature and pressure under alkaline conditions. The most notable contaminant of the group is TCDD which can be formed along with other dioxin compounds during the manufacture of several commercially important products such as the herbicide 2,4,5-T, the fungicide pentachlorophenol, and the germicide Hexachlorophene® (18B19). Numerous investigators have found PCDDs, PCDFs, and PCBs in tobacco as well as tobacco smoke [1457, Gichner et al. (18B14), Djordjevic et al. (1000, 1006), Radovanović and Mišić (18B15)].

Suspicions of the possible long-term health hazards of dioxins arose after it was found that 2,4,5-T was teratogenic in rat and mouse [Courtney et al. (18B10)]. Shortly thereafter, it was discovered that the 2,4,5-T sample used in this study contained about 30 ppm TCDD (18B10). It was primarily the report by Courtney et al. (18B10) implicating TCDD as a contaminant of 2,4,5-T that led to its further evaluation for teratogenicity [Courtney and Moore (18B11)] and its eventual testing for mutagenicity. These and other similar reports published during the late 1960s and early 1970s also stimulated toxicological studies on other dioxin derivatives as well as studies dealing with issues such as environmental contamination and movement and analytical detection of these compounds. Numerous detailed reviews summarizing work in these areas have been published. The latest and perhaps the most comprehensive review was prepared by the World Health Organization in 2002 (18B07).

Additionally, IARC has prepared a monograph on dioxins (7A03), and Wassom et al. (18B19) reviewed the genetic toxicology of PCDDs.

Dioxins are produced inadvertently as a by-product of chemical production or during combustion and are widespread pollutants in the environment. They are ubiquitous. The biggest source of PCDDs, PCDFs, and PCBs is the large-scale burning of municipal and medical waste. Other sources include

- The production of iron and steel
- Backyard burning of household waste, especially plastics
- Fuel burning, including diesel fuel and fuel for agricultural purposes and home heating
- Wood burning, especially if the wood has been chemically treated
- Electrical power generation
- Tobacco smoke

Dioxins can also be produced from natural processes, such as forest fires, explosions, and volcanic eruptions. Most dioxins are introduced to the environment through the air. The airborne chemical can attach to small particles that can travel long distances in the atmosphere. PCDDs, PCDFs, and PCBs are found in very small amounts in the environment, including in the air, water, and soil. As a result, they are also present in some foods. They can also present a health risk at elevated dosages. As for tobacco smoke, the dosage of dioxins from cigarettes is extremely low. Exposure estimates suggest that the smoking of 20 cigarettes/day contributes approximately 2%–4% of the total daily exposure to dioxins for a 70 kg adult (177). The major source of exposure to PCDDs, PCDFs, and PCBS is the diet [Canady et al. (18B07)].

Rodgman and Green (3300) noted in their review of MSS toxicants that certain dioxins are antitumorigens. Slaga and DiGiovanni (3685) summarized the studies in which dioxins were shown to interfere with the enzyme pathways responsible for tumorigenesis of several of the most potent polycyclic aromatic hydrocarbons (PAHs). The dioxins were not listed as MSS toxicants in previous tabulations of MSS toxicants reviewed by Rodgman (3255, 3255a, 3257, 3265) and Rodgman and Green (3300). In fact, only one MSS toxicant list issued since 1990, that of Fowles and Bates (1217), has included the dioxins even though their presence in MSS was known in 1980 (854). Dioxins are antitumorigenic to DMB[*a*]A (7,12-dimethylbenz[*a*]anthracene), MC (3-methylcholanthrene, more recently named 1,2-dihydro-3-methylbenz[j]aceanthrylene), B[*a*]P (benzo[*a*]pyrene), 7-MB[*a*]A (7-methylbenz[*a*]anthracene), 12-MB[*a*]A (12-methylbenz[*a*]anthracene), 5-MeC (5-methylchrysene), and DB[*a,h*]A (dibenz[*a,h*]anthracene) [Berry et al. (18B04), Cohen et al. (18B09), DiGiovanni et al. (976), DiGiovanni et al. (18B12)].

The IARC classification of carcinogenicity (18A04) places 25 halogen-containing compounds in tobacco or tobacco smoke in groups 1, 2A, 2B, and 3. Table 18.2 lists the individual halogen-containing chemicals (agents) and families of chemicals (groups of agents) identified in tobacco and tobacco smoke. IARC lists TCDD and vinyl chloride as group 1 human carcinogens. Trichloroethylene, epichlorohydrin [(chloromethyl)oxirane], ethylene dibromide, and PCBs are listed by IARC as group 2A (probably carcinogenic to humans). Ten halogen-containing compounds are listed in group 2B (possibly carcinogenic to humans): Chlordane®, *p*-chloroaniline, chloroform, chlorophenoxy herbicides, chlorothalonil (2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile), DDT (*p,p′*-DDT), dichloromethane (methylene chloride), 1,3-dichloropropene, Heptachlor®, and hexachlorobenzene. Nine halogen-containing compounds are listed in group 3 (not classifiable as to carcinogenicity to humans): chloroethane, *m*-dichlorobenzene, *o*-dichlorobenzene, 1,2-dichloropropane, Hexachlorophene®, Methoxychlor®, methyl iodide, polychlorinated dibenzofurans, and 1,1,1-trichloroethane.

There are numerous analytical methodologies to identify and quantify halogenated compounds in tobacco and smoke. The method of analysis will vary among the halogenated compounds and particularly the pesticide types. Sources of methods include the *FDA Pesticide Analytical Manuals* (PAMs) I and II (18B13), the *FDA Index of Residue Analytical Methods* (RAM) (18B13), the methods in the *Journal of the Association of Official Analytical Chemists* (18B02, 18B03), and methods found in journal articles. Generally, the preferred methods of analysis involve gas chromatography (GC), liquid chromatography (LC), or GC–mass spectrometry (MS) techniques. Flame ionization detectors (FIDs) are normally used for quantitative analysis of halogen-containing organics, while electron capture detectors (ECDs) are preferred for quantitative determination of PCDDs, PCDFs, PCBs, and other pesticides [Radovanović and Mišić (18B15)].

There are 266 identified halogenated compounds in tobacco and/or tobacco smoke. As seen in Table 18.3, the vast majority (215 compounds) contain chlorine only. Thirteen compounds contain bromine only, four containing iodine only, and 14 contain fluorine only. Twenty are multihalogen-containing components. Over 85% of all the halogenated compounds found in tobacco and tobacco smoke are either halogenated agrochemicals, impurities found in the agrochemicals (PCDDs, PCDFs, PCBs), or decomposition products from the agrochemicals. Table 18.4 lists the 266 halogenated compounds identified in tobacco and/or tobacco smoke. In a few cases, a halogenated component has been identified in tobacco substitute smoke. Table 18.4 is divided by halogen type (chloro, bromo, iodo, and fluoro compounds) and includes several halogenated compounds with two or more halogens (mixed halogenated compounds).

TABLE 18.2
Halogenated Components Identified in Tobacco and Tobacco Smoke (18A04)

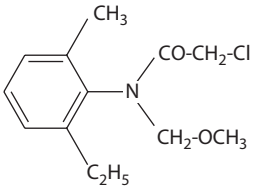
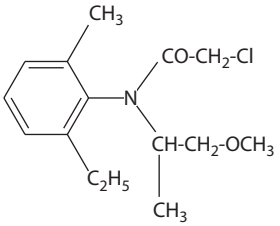
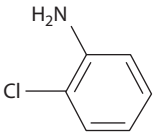
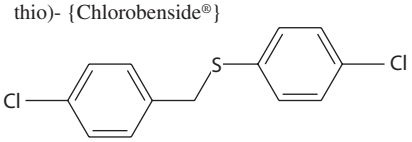
IARC Group Classification	IARC Chemical Came (Number of Compounds)	CAS No.	IARC Volume; Date	Comment by IARC
Group 1	2,3,7,8-Tetrachlorodibenzo-*para*-dioxin	1746-01-6	Vol. 69; 1997	Overall evaluation upgraded from 2A to 1 with supporting evidence from other relevant data
	Vinyl chloride	75-01-4	Vol. 19, Suppl. 7, Vol. 97; in preparation	
Group 2A	Trichloroethylene	79-01-6	Vol. 63; 1995	
	Epichlorohydrin	106-89-8	Vol. 11, Suppl. 7, Vol. 71; 1999	Overall evaluation upgraded from 2B to 2A with supporting evidence from other relevant data
	Ethylene dibromide	106-93-4	Vol. 15, Suppl. 7, Vol. 71; 1999	Overall evaluation upgraded from 2B to 2A with supporting evidence from other relevant data
	PCBs (11)	1336-36-3	Vol. 18, Suppl. 7; 1987	
Group 2B	Chlordane	57-74-9	Vol. 79; 2001	
	p-Chloroaniline	106-47-8	Vol. 57; 1993	
	Chloroform	67-66-3	Vol. 73; 1999	
	Chlorophenoxy herbicides (5)		Vol. 41, Suppl. 7; 1987	
	Chlorothalonil	1897-45-6	Vol. 73; 1999	
	DDT [*p*,*p*′-DDT]	50-29-3	Vol. 53; 1991	
	Dichloromethane [methylene chloride]	75-09-2	Vol. 71; 1999	
	1,3-Dichloropropene	542-75-6	Vol. 41, Suppl.7, Vol. 71; 1999	
	Heptachlor	76-44-8	Vol. 79; 2001	
	Hexachlorobenzene	118-74-1	Vol. 79; 2001	
Group 3	Chloroethane	75-00-3	Vol. 52, Vol. 71; 1999	
	m-Dichlorobenzene	541-73-1	Vol. 73; 1999	
	o-Dichlorobenzene	95-50-1	Vol. 73; 1999	
	1,2-Dichloropropane	78-87-5	Vol. 41, Suppl. 7, Vol. 71; 1999	
	Hexachlorophene	70-30-4	Vol. 20, Suppl. 7; 1987	
	Methoxychlor	72-43-5	Vol. 20, Suppl. 7; 1987	
	Methyl iodide	74-88-4	Vol. 41, Suppl. 7, Vol. 71; 1999	
	Polychlorinated dibenzofurans (18)		Vol. 69; 1997	
	1,1,1-Trichloroethane	71-55-6	Vol. 20, Suppl. 7, Vol. 71; 1999	

Agents, groups of agents, mixtures, and exposure circumstances (associated with tobacco) evaluated in IARC Monographs Volumes 1–95. This list contains all agents evaluated as of November–December 2006 that are considered: carcinogenic to humans (group 1), probably carcinogenic to humans (group 2A), and possibly carcinogenic to humans (group 2B). For details of the evaluation, the relevant monograph should be consulted; see http://monographs.iarc.fr/ENG/Classification/crthgr01.php. Those agents listed have been identified in tobacco or tobacco smoke.

TABLE 18.3
Distribution of Halogenated Components Identified in Tobacco and Tobacco Smoke

Halogen	Total No. Compounds	Smoke	Tobacco	Tobacco and Smoke	Agrochemical/ Decomposition Product	Other
Chloro	215	129	141	55	171	21
Bromo	13	8	11	6	7	5
Iodo	4	2	4	2	2	2
Fluoro	14	4	13	3	9	5
Mixed halogens	20	10	19	9	11	9
Total	266	153	188	75	200	42

TABLE 18.4
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Chloro Compounds					
1.	15972-60-8	Acetamide, 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)- {Alachlor®} 		2650a, 2913a, 3633, 4271a	
2.	51218-45-2	Acetamide, 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)- {Metolachlor®} 		2650b, 4271a	
3.	79-43-6	Acetic acid, dichloro- Cl_2CH-COOH		1948, 3821a, 4249	
4.	94-75-7	Acetic acid, 2,4-dichlorophenoxy- {2,4-D}		3633, 5015, 5521, 5811b	
5.	93-76-5	Acetic acid, 2,4,5-trichlorophenoxy- {2,4,5-T®}		3633, 5015	
6.		Ammonium chloride	5013		
7.	53516-76-0	Ammonium chloride, alkyldimethylbenzyl- {Benzalkonium chloride®}		3633	
8.	95-51-2	Benzenamine, 2-chloro- 	3491, 4249, 5811b	3797, 4249, 5811b	
9.	106-47-8	Benzenamine, 4-chloro-	822, 4249		
10.	95-76-1	Benzenamine, 3,4-dichloro-	822, 4249	4271a	
11.	99-30-9	Benzenamine, 2,6-dichloro-4-nitro- {Dicloran®}		3633	
12.	108-90-7	Benzene, chloro- C_6H_5-Cl	707, 1884, 2570, 4249, 5811b		
13.	104-83-6	Benzene, 1-chloro-4-(chloromethyl)-	5811, 5811a, 5811b		
14.	22349-74-2	Benzene, 1-chloro-4-(2-chloro-1-phenylethenyl)-	703, 4249		
15.	103-17-3	Benzene, 1-chloro-4-(((4-chlorophenyl)methyl) thio)- {Chlorobenside®} 		3633	
16.	3424-82-6	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethenyl]-	476, 644, 1767, 2550, 4249		

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

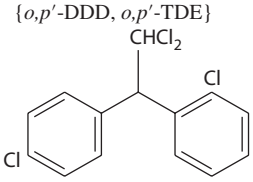
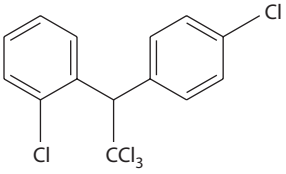
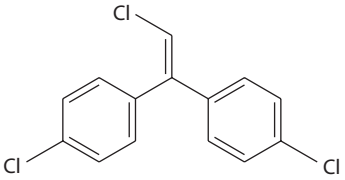
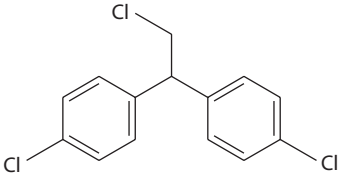
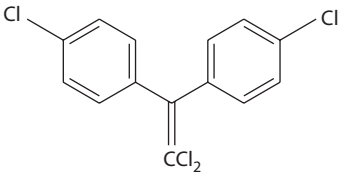
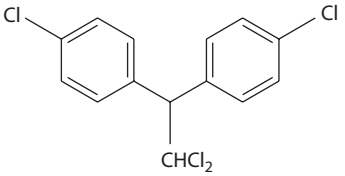
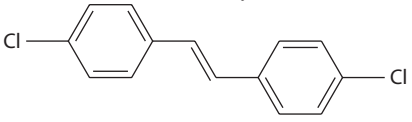
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
17.	53-19-0	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDD, *o,p′*-TDE} 	416, 518, 658, 758, 759, 1000, 1006, 1756, 1767, 1767a, 1781, 1884, 2550, 2596, 2697, 2767, 3493, 3634, 4249, 5811b, 21A19	518, 644, 713, 714, 758, 759, 1000, 1006, 1029, 1030, 1219, 1333, 1460, 1740, 1767, 2697, 3198, 3348–3350, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3977, 4249, 4271a, 5079, 5439, 5811b, 21A19	
18.	4329-12-8	Benzene, 1-chloro-3-[2,2-dichloro-1-(4-chlorophenyl) ethyl]- {*m,p′*-DDD}	1000, 1006, 1756, 1767, 1767a, 1781, 2767, 3493, 4249, 4342, 5811b, 21A19	1000, 1006, 1740, 3767a, 3770, 4249, 4271a, 5079, 5439, 21A19	
19.	789-02-6	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl) ethyl]- {*o,p′*-DDT} 	517, 518, 758, 759, 1000, 1006, 1333, 1373, 1756, 1767, 1767a, 1781, 2697, 3257, 3493, 3685, 4005–4007, 4249, 4342, 5811b, 21A19	517, 518, 644, 722, 758, 759, 1000, 1006, 1029, 1030, 1219, 1219a, 1219b, 1333, 1460, 1740, 1767, 2697, 3138, 3633, 3637, 3767a, 3770, 3915, 3977, 3973, 3977, 3984, 4249, 4271a, 5079, 5439, 5811b, 21A19	
20.	4541-89-3	Benzene, 1,1′-(chloroethenylidene)bis-	2767, 4249		
21.	1022-22-6	Benzene, 1,1′-(chloroethenylidene)bis[4-chloro-] {DDM} 	707, 708, 713, 714, 758, 1000, 1006, 1767, 1781, 2767, 3557, 4005–4007, 4249, 5811b	708, 722, 758, 759, 1000, 1006, 1740, 1767, 2389, 2544, 4249, 5811b	
22.	2642-80-0	Benzene, 1,1′-(2-chloroethylidene)bis[4-chloro-] {DDMS} 	707, 708, 713, 714, 758, 1000, 1006, 1767, 1781, 2767, 3557, 4005–4007, 4249	708, 722, 758, 759, 1000, 1006, 1740, 1767, 2389, 2544, 4249	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
23.	622-24-2	Benzene, 2-chloroethyl- C_6H_5-CH_2CH_2-Cl		984, 4249	
24.		Benzene, chloromethoxy- {chloroanisole}		268, 4249	
25.	27987-13-9	Benzene, chloromethyl- C_6H_5-CH_2-Cl	4249		
26.	95-50-1	Benzene, 1,2-dichloro-	1445, 4249, 5811b	984, 2339a, 4249	
27.	541-73-1	Benzene, 1,3-dichloro-	1445, 1822, 4249		
28.	106-46-7	Benzene, 1,4-dichloro-	1168, 1445, 4249		
29.	72-55-9	Benzene, 1,1′-(dichloroethenylidene)bis[4-chloro-] {*p,p′*-DDE} 	518, 707, 708, 713, 714, 758, 759, 1000, 1006, 1375, 1375b, 1740, 1741, 1743, 1744, 1767, 1781, 2697, 2767, 3265, 3300, 3557, 4005–4007, 4249, 5512, 5811b	518, 644, 708, 722, 758, 759, 1000, 1006, 1029, 1030, 1219, 1219a, 1460, 1740, 2389, 2544, 2697, 3188a, 3633, 3637, 3770, 3915, 3974b, 4249, 4271a, 5811b	
30.	27013-25-8	Benzene, 1,1′-(2,2-dichloroethylidene)bis[chloro-]	1000, 4249		
31.	72-54-8	Benzene, 1,1′-(2,2-dichloroethylidene)bis[4-chloro-] {*p,p′*-DDD, *p,p′*-TDE} 	415, 419, 518, 658, 707, 708, 713, 714, 758, 759, 1000, 1006, 1375, 1375b, 1457, 1756, 1767, 1781, 2550, 2596, 2697, 2767, 2939, 3634, 4005–4007, 4249, 5811b	415, 419, 518, 644, 707, 708, 713, 714, 722, 758, 759, 1000, 1006, 1028–1030, 1219, 1219a, 1333, 1457, 1460, 1740, 1756, 1767, 2318, 2389, 2544, 2697, 2939, 3188a, 3348–3350, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3977, 3984, 4249, 4271a	
32.	5121-74-4	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-] {DCS (dichlorostilbene)}	708, 1756, 1767, 3493, 4005–4007, 4010, 4011	722, 1460, 1756	
33.	1657-56-3	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-], (*E*)- {*trans*-DCS} 	707, 713, 714, 1756, 1781, 4249, 5811b	1756, 4249	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

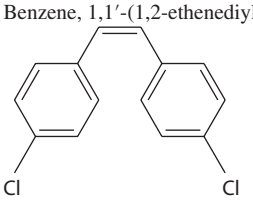
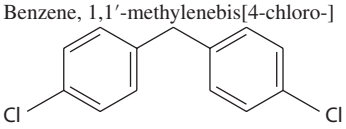
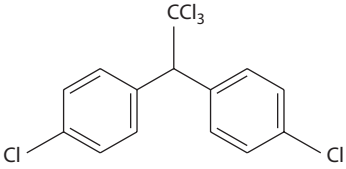
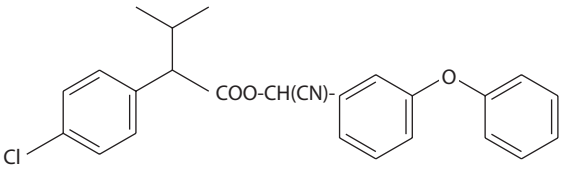
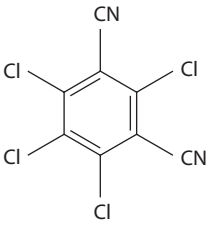
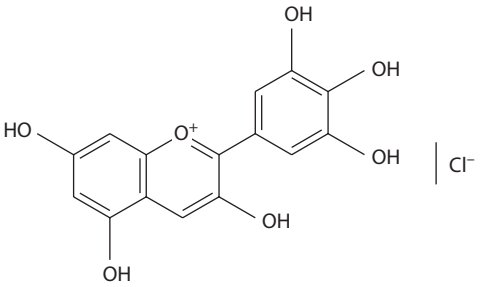
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
34.	2510-74-9	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-], (*Z*)- {*cis*-DCS} 	4249, 4342, 5811b		
35.	118-74-1	Benzene, hexachloro-		2389, 2544, 3152, 3188a, 3633, 3770, 4249, 4271a	
36.	101-76-8	Benzene, 1,1′-methylenebis[4-chloro-] 	707, 708, 713, 714, 1375, 1375b, 2767, 3557, 4249, 5811b		
37.	82-68-8	Benzene, nitropentachloro- {Quintocen®}		3770	
38.	938-22-7	Benzene, 1,2,3,5-tetrachloro-4-methoxy-		268, 4249	
39.	116-29-0	Benzene, 1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)- {Tetradifon®}		3633	
40.	50-29-3	Benzene, 1,1′-(2,2,2-trichloroethylidene)bis[4-chloro-] {*p,p′*-DDT} 	517, 518, 707–709, 711, 712, 714, 758, 759, 1333, 1373, 1740, 1741, 1743, 1744, 1756, 1767, 1767a, 1781, 1884, 2697, 2825, 3257, 3265, 3300, 3493, 3634, 3685, 4249, 4342, 5512, 5811b, 5869a	517, 518, 644, 707–709, 711–714, 758, 759, 1028–1030, 1219, 1219a, 1333, 1460, 1756, 1767, 2318, 2697, 3138, 3188a, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3973, 3974b, 3977, 4249, 4271a, 5079, 5439, 5811b	
41.	87-40-1	Benzene, 1,3,5-trichloro-2-methoxy-		268, 4249	
42.	51630-58-1	Benzeneacetic acid, 4-chloro- α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®} 	21A19	3585e, 21A19	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
43.	1897-45-6	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro {Chlorothalonil®} 		3585c, 3633	
44.	1861-32-1	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester {DCPA®}		2913a, 3633	
45.	1918-00-9	Benzoic acid, 3,6-dichloro-2-methoxy- {Dicamba®}	4857	3633, 3973, 4249, 4857, 5015, 5521, 5811b	
46.	528-58-5	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride		4249, 4681	
47.	22688-80-8	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-D-glucopyranosyl-D-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride		4249, 4681, 4710	
48.	528-53-0	1-Benzopyrylium, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-, chloride 		2855a, 4249, 4681	
49.	18719-76-1	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2-(3,4- dihydroxyphenyl)-5,7-dihydroxy-, chloride		928b, 4249, 4710	
50.	33978-17-5	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride		4681, 4249	
51.	8001-35-2	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated {Toxaphene®}		1028, 1029, 3633, 3770, 3973, 4249, 4271a, 5079, 5439	
52.	8001-50-1	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated + Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, polychlorinated {Strobane®, Dichloricide®}		3973	
53.	2051-60-7	1,1-Biphenyl, 2-chloro-	18B15		
54.	2051-24-3	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6,6′-decachloro- {1,1′-biphenyl, decachloro-}	636, 1979, 18B15	1979	
55.	2050-67-1	1,1′-Biphenyl, 3,3′-dichloro-	18B15		
56.	2050-68-2	1,1′-Biphenyl, 4,4′-dichloro-	5811, 5811a, 5811b		
57.	52712-05-7	1,1′-Biphenyl, 2,2′,3,4,5,5′, 6,-heptachloro-	18B15		
58.	38411-22-2	1,1′-Biphenyl, 2,2′,3,3′,6,6′-hexachloro-	18B15		

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

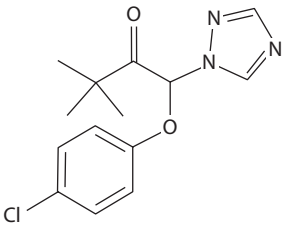
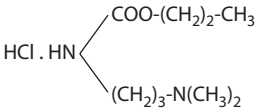
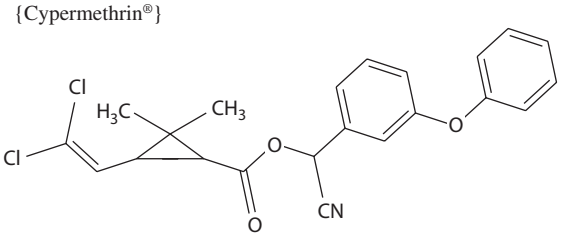
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
59.	40186-72-9	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6-nonachloro-	18B15		
60.	35694-08-7	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′-octachloro-	18B15		
61.	74472-39-2	1,1′-Biphenyl, 2,3′,4,5′,6-pentachloro-	18B15		
62.	71294-42-3	1,1′-Biphenyl, propyl-	2328, 4249		
63.	2437-79-8	1,1′-Biphenyl, 2,2′,4,4′-tetrachloro-	18B15		
64.	37680-65-2	1,1′-Biphenyl, 2,2′,5-trichloro-	18B15		
65.	43121-43-3	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl) {Triadimefon®} 		3633	
66.	10043-52-4	Calcium chloride		5811, 5811b	
67.	101-21-3	Carbamic acid, 3-chlorophenyl-, (1-methylethyl) ester {Chloropropham®}		4271a	
68.	25606-41-1	Carbamic acid, 3-(dimethylamino)propyl-, propyl ester, hydrochloride {Propamocarb hydrochloride®} 		3633	
69.	2303-17-5	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester amothioic acid, dipropyl-, *S*-propyl ester {Triallate®}		2650a	
70.	75-44-5	Carbon oxychloride {phosgene} $COCl_2$	1375b (0), 3254 (0), 3901a (0). 4249, 5046, 5059	2483a, 4249	
71.	56-23-5	Carbon tetrachloride	5811b	4249, 4271a	
72.	16887-00-6	Chloride	641, 1628, 1933, 1933b, 1934, 1939, 2170, 2524a, 2931, 3255, 4249, 5079, 5811b	193, 256, 385, 486, 677b, 963, 1063–1066, 1068–1074, 1189, 1333, 1373, 1895, 1933, 1934, 1939, 2079, 2154, 2283, 2313a, 2338, 2356, 2529, 2543, 2545, 2627, 2761, 2762, 2765, 2766, 2847, 3160, 3797, 3976, 4249, 4261, 4262, 4357, 5053, 5079, 5113, 5126, 5189, 5195, 5252, 5277, 5293, 5302, 5337, 5448,, 5642, 5811b	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
73.	7782-50-5	Chlorine	50, 1240, 2779, 3797, 4249, 5811b	1127b, 1240, 2779, 3973, 3974a, 3974b, 4108, 4249, 4512, 5654, 5688, 5811b	50, 4249
74.	14158-34-0	Chlorine, isotope of mass 38		3973, 20A115	
75.	1332-82-7	Cobalt chloride		5811	
76.	7447-39 4	Copper chloride (cupric chloride) $CuCl_2$		5811	
77.	1332-40-7 1332-65-6	Copper oxychloride {RAME}		3633	
78.	8012-69-9	Copper oxychloride sulfate $Cu_2Cl(OH)_3 + Cu_4(OH)_6(SO_4)$		3633	
79.	608-73-1	Cyclohexane, 1,2,3,4,5,6-hexachloro-	644, 2160, 2697, 4249	644, 2544, 2650b, 2697, 3492, 3663, 3634, 3770, 3973, 4249, 4436, 5079, 5439	
80.	319-84-6	Cyclohexane, 1,2,3,4,5,6-hexachloro- {α-Lindane®}	518, 644, 1000, 1006, 4249, 21A19	518, 644, 1000, 1006, 1219, 1219b, 1219c, 1740, 2650b, 3633, 3634, 3770, 3973, 4249, 21A19	
81.	319-85-7	Cyclohexane, 1,2,3,4,5,6-hexachloro- {β-Lindane®}	518, 1000, 1006, 4249	518, 1000, 1006, 1740, 2650b, 3633, 3770, 3973, 4249	
82.	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1α,2α,3β,4α,5α,6β)- {γ-Lindane®}	518, 644, 1000, 1006, 2697, 4249, 21A19	518, 644, 1000, 1006, 1740, 2389, 2544, 2650b, 2697, 3188a, 3633, 3634, 3770, 3973, 4249, 5811b, 21A19	
83.	319-86-8	Cyclohexane, 1,2,3,4,5,6-hexachloro- {δ-Lindane®}	518, 1000, 1006, 4249	518, 1000, 1006, 1740, 2650b, 3633, 3770, 3973, 4249	
84.	52315-07-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {Cypermethrin®} 	21A19	904, 1219b, 1219c, 3188a, 3585e, 3633, 4249, 4271a, 5568, 21A19	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

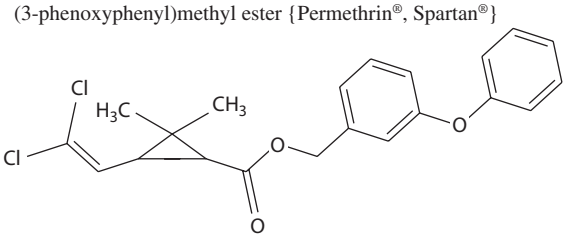
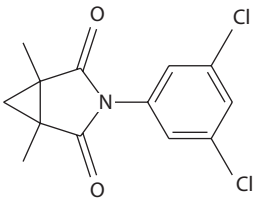
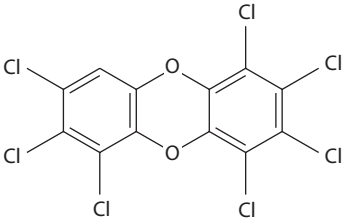
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
85.	67375-30-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {α-Cypermethrin}	21A19	3633, 21A19	
86.	52645-53-1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl)methyl ester {Permethrin®, Spartan®} 		904, 1219a, 1219b, 1219c, 2346, 2892a, 3188a, 3585e, 3633	
87.	32809-16-8	1,2-Cyclopropanedicarboximide, *N* (3,5-dichlorophenyl)-1,2-dimethyl {Procymidone®} 		3585c	
88.		Dibenzo[*b,e*][1,4]dioxin, polychloro-	854, 4249		
89.	35822-46-9	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,8-heptachloro- 	177, 1217, 2160, 2391, 2490, 2491, 3265, 3300, 4249	2160, 4249	
90.	58200-70-7	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,9-heptachloro-	177, 4249		
91.	39227-28-6	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,7,8-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
92.	57653-85-7	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,6,7,8-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
93.	19408-74-3	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8,9-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
94.	40321-76-4	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8-pentachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
95.	1746-01-6	Dibenzo[*b,e*][1,4]dioxin, 2,3,7,8-tetrachloro-	177, 1217, 2490, 2491,3265, 3300, 3685, 4249, 5869a	933, 4249	
96.	37871-00-4	Dibenzo[*b,e*][1,4]dioxin, heptachloro-	1217, 2391, 2490, 2491, 2664, 3265, 3300, 4249, 5811b		

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
97.	34465-46-8	Dibenzo[*b,e*][1,4]dioxin, hexachloro-	1217, 2391, 2490, 2491, 2664, 3265, 3300, 4249, 5811b		
98.	3268-87-9	Dibenzo[*b,e*][1,4]dioxin, octachloro-	177, 1217, 2391, 2490, 2491, 2664, 2897, 3300, 4249, 5811b		
99.	36088-22-9	Dibenzo[*b,e*][1,4]dioxin, pentachloro-	1217, 2391, 2490, 2491, 2664, 3265, 3300, 4249, 5811b		
100.	41903-57-5	Dibenzo[*b,e*][1,4]dioxin, tetrachloro-	1217, 2391, 2490, 2491, 2664, 3265, 3300, 4249, 5811b		
101.		Dibenzofuran, polychloro- {PCDFs}	177, 854, 1217, 2490, 2491,3265, 3300, 3715, 4249		
102.	67562-39-4	Dibenzofuran, 1,2,3,4,6,7,8-heptachloro-	177, 1217, 2160, 2391, 2490, 2491, 3265, 3300, 4249	2160	
103.	55673-89-7	Dibenzofuran, 1,2,3,4,7,8,9-heptachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
104.	70648-26-9	Dibenzofuran, 1,2,3,4,7,8-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
105.	91538-84-0	Dibenzofuran, 1,2,3,4,7,9-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
106.	67517-48-0	Dibenzofuran, 1,2,3,4,8-pentachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
107.	57117-44-9	Dibenzofuran, 1,2,3,6,7,8-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
108.	72918-21-9	Dibenzofuran, 1,2,3,7,8,9-hexachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
109.	57117-41-6	Dibenzofuran, 1,2,3,7,8-pentachloro-	177, 1217, 2391, 2490, 2491,3265, 3300, 4249		
110.	60851-34-5	Dibenzofuran, 2,3,4,6,7,8-hexachloro-	1217, 2391, 2490, 2491,3265, 3300, 4249		
111.	57117-31-4	Dibenzofuran, 2,3,4,7,8-pentachloro-	1217, 2391, 2490, 2491,3265, 3300, 4249		
112.	83704-32-9	Dibenzofuran, 2,3,4,8-tetrachloro-	1217, 2391, 2490, 2491,3265, 3300, 4249		
113.	51207-31-9	Dibenzofuran, 2,3,7,8-tetrachloro-	1217, 2391, 2490, 2491,3265, 3300, 4249		

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

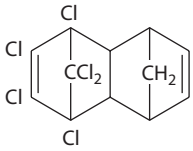
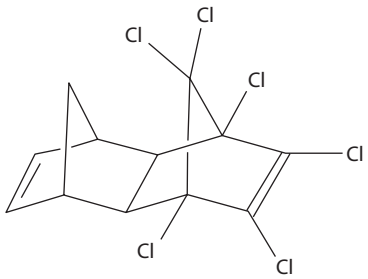
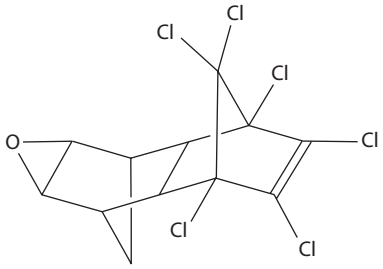
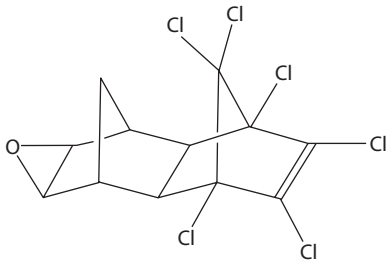
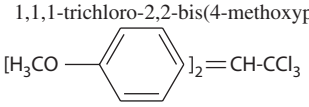
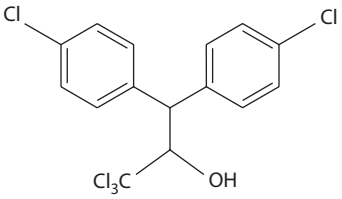
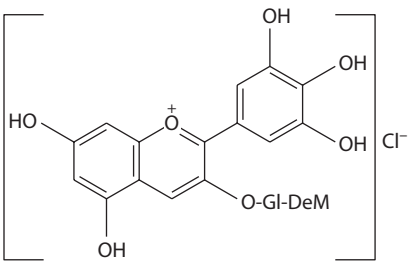
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
114.	38998-75-3	Dibenzofuran, heptachloro-	1217, 3265, 3300, 4249		
115.	55684-94-1	Dibenzofuran, hexachloro-	1217, 3265, 3300, 4249		
116.	39001-02-0	Dibenzofuran, octachloro-	1217, 3265, 3300, 4249		
117.	30402-15-4	Dibenzofuran, pentachloro-	1217, 3265, 3300, 4249		
118.	30402-14-3	Dibenzofuran, tetrachloro-	1217, 3265, 3300, 4249		
119.	309-00-2	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5α,8α,8aβ)- [endo, endo] {Aldrin®} 	518, 644, 2697, 3633, 4249	518, 644, 1333, 1457, 2389, 2544, 2650a, 2650b, 2697, 3138, 3188a, 3633, 3770, 3973, 3977, 4249, 4271a, 5811b	
120.	465-73-6	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5β,8β,8aβ)- [endo, exo] {Isodrin®} 		3770, 4249	
121.	60-57-1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aα,3β,6β,6aα,7β,7aα)- {Dieldrin®} 	518, 644, 1000, 1006, 2697, 4249, 21A19	518, 644, 1029, 1000, 1006, 1219, 1219a, 1219b, 1333, 1740, 2650a, 2650b, 2697, 3188a, 3633, 3767a, 3770, 3797,3915, 3973, 3977, 4249, 4271a, 5811b, 21A19	
122.	72-20-8	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aβ,3α,6α,6aβ,7β,7aα)- {Endrin®} 	415, 419, 518, 644, 1000, 1006, 1457, 2697, 3634, 4249, 21A19	415, 419, 518, 644, 1000, 1006, 1028, 1029, 1219, 1219a, 1333, 1457, 1740, 2318, 2389, 2544, 2650b, 2697, 2939, 3188a, 3633, 3634, 3637, 3767a, 3770, 3915, 3973, 3977, 4249, 4271a, 5811b, 21A19	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
123.	51-75-2	Ethanamine, 2-chloro-*N*-(2-chloroethyl)-*N*-methyl- $(Cl\text{-}CH_2\text{-}CH_2)_2{=}N\text{-}CH_3$	703, 4249		
124.	07-06-2	Ethane, 1,2-dichloro-	126, 4249, 5811b		
125.	75-00-3	Ethane, chloro- $C_2H_5\text{-}Cl$	126a, 1140, 1419, 1939, 4249, 5811b		
126.	67-72-1	Ethane, hexachloro-	5811, 5811b		
127.	71-55-6	Ethane, 1,1,1-trichloro- $CH_3\text{-}C{\equiv}Cl_3$	222–224, 4249		
128.	72-43-5	Ethane, 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)- {Methoxychlor®} 		3188a, 3663, 3770, 4249, 4271a	
129.	25323-89-1	Ethane, 1,2,2-trichloro-		4249, 4271a	
130.	107-07-3	Ethanol, 2-chloro- {chlorohydrin}	5811, 5811a	5811, 5811a	
131.	115-32-2	Ethanol, 2,2,2-trichloro-1,1-bis(4-chlorophenyl)- {Dicofol®} 		3633	
132.	75-01-4	Ethene, chloro- {vinyl chloride} $H_2C{=}CH\text{-}Cl$	203, 239, 603, 1037b, 1148, 1217, 1325, 1373, 1437, 1673, 1706, 1727, 1740, 1741, 1743, 1744, 1752, 1773, 1781, 1808, 1842, 1870, 1871, 2825, 3255, 3257, 3260, 3265, 3300, 3370, 3711, 4010, 4011, 4227, 4249, 4998, 5512, 5811b, 5869a		
133.	127-18-4	Ethene, tetrachloro- $Cl_2C{=}CCl_2$	126a, 222–224, 1168, 4249, 5811b		
134.	79-01-6	Ethene, trichloro- $Cl_2C{=}CHCl$	222–224, 1153, 1168, 4249, 5811b, 5869a		
135.	29732-48-7	Flavylium, 3-[[*O*-(6-deoxymannosyl)-D-glucosyl]oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride 		4249, 4527, 4710	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

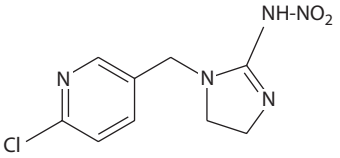
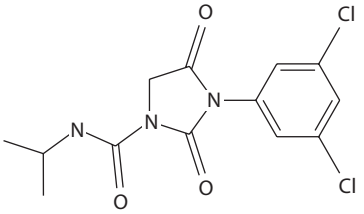
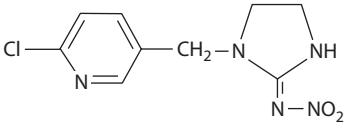
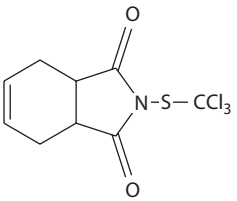
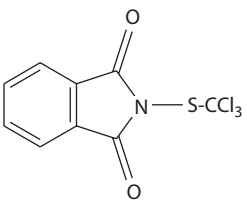
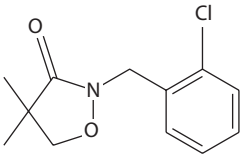
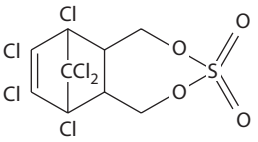
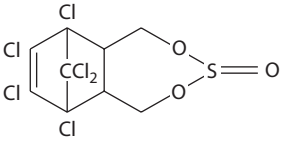
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
136.		Flavylium, 3-[[*O*-(6-deoxymannosyl)-D-glucosyl]oxy]-3′,4′,5,7-tetrahydroxy-, chloride		4249, 4527, 4644	
137.	3736-81-0	2-Furancarboxylic acid, 4-[(2,2-dichloroacetyl)-methylamino] phenyl ester	5811, 5811a, 5811b		
138.	629-06-1	Heptane, 1-chloro- $H_3C\text{-}(CH_2)_5\text{-}CH_2Cl$	199, 4249		
139.	33240-56-1	Hexane, 1-chloro-5-methyl-	200, 4249, 5811b		
140.	105827-78-9	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl) methyl)-4,5-dihydro-*N*-nitro- {Admire®} 		2892a, 4249	
141.	36734-19-7	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®} 		3585c, 3633, 3661a	
142.	138261-41-3	Imidazolidinimine, 1-((6-chloro-3-pyridinyl) methyl)-*N*-nitro- {Imidacloprid®} 	568b, 4249, 21A19	568b, 4249, 5064, 5568, 21A19	
143.	7705-08-0	Iron chloride (ferric chloride) $FeCl_3$		5811	
144.	133-06-2	1*H*-Isoindole-1,3(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]- {Captan®} 	1884, 3302, 4249, 21A19	1219c, 1884, 3633, 21A19	
145.	133-07-3	1*H*-Isoindole-1,3(2*H*)-dione, 2-[(trichloromethyl)thio]- {Folpan®} 		3633	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
146.	81777-89-1	3-Isoxazolidinone 2-[(2-chlorophenyl) methyl]-4,4-dimethyl- {Clomazone®} 		2913a, 3633	
147.	7791-18-6	Magnesium chloride		5811, 5811b	
148.	13446-35-0	Manganese chloride $MnCl_4$		2393, 4249	
149.	74-87-3	Methane, chloro- $H_3C\text{-}Cl$	112, 126b, 199, 172, 239, 298, 348, 604, 605, 621, 712, 1140, 1153, 1154, 1375a, 1377, 1437, 1440, 1939, 1962, 1966, 2060, 2079, 2142, 2270, 2634, 2782, 2939, 2940, 3059, 3106, 3255, 3302, 3308, 3493, 3583, 3584, 3692, 3882, 3901, 3939, 4005–4007, 4052, 4056, 4162, 4249, 4395, 5811b, 5869a	722, 1595, 4249	1375a, 1377, 3901, 4052, 4056, 4249
150.	782-08-1	Methane, chlorobis(4-chlorophenyl)-	5811b		
151.	75-09-2	Methane, dichloro- $H_2C{=}Cl_2$	222–224, 568b, 712, 1140, 4249, 5811b	568b, 984, 1595, 4249	
152.	76-06-2	Methane, nitrotrichloro- {Chloropicrin®}		3633, 3646a, 3973	
153.	67-66-3	Methane, trichloro- {chloroform} $H\text{-}CCl_3$	39, 568b, 712, 1939, 3300, 4249, 4570a, 5811b, 5869a	568b, 722, 4249	641, 4249
154.	1031-07-8	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3,3-dioxide {Thiodan® sulfate, Endosulfan® sulfate} 	644, 1619, 3634, 4249, 21A19	644, 1028, 1219, 1219a, 1458, 1619, 2650a, 3188a, 3633, 3634, 3770, 3915, 4249, 21A19	
155.	115-29-7	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide {Thiodan®, Thiosulfan®, Endosulfan®} 	419, 644, 1457, 1619, 3302, 3634, 4249, 4858	419, 644, 1028, 1219, 1219a, 1219b, 1219c, 1457, 1458, 1619, 2650a, 2650b, 3188a, 3633, 3634, 3770, 3973, 4249, 4271a, 4858, 5811b	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

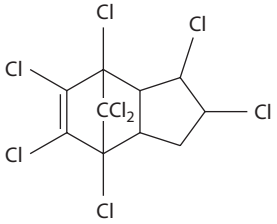
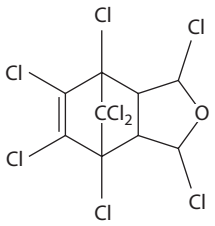
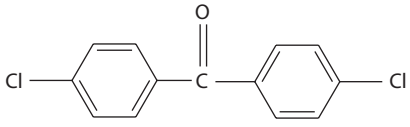
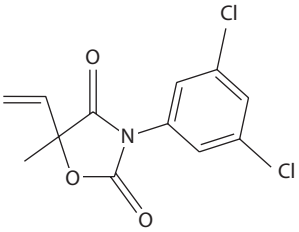
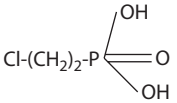
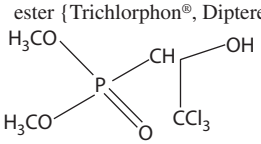
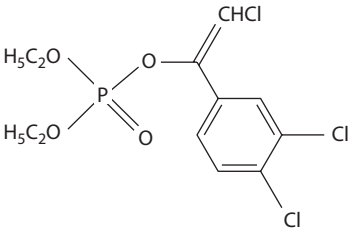
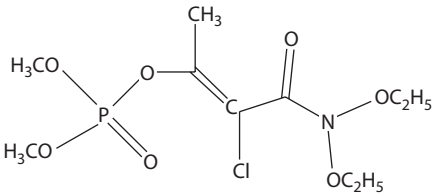
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
156.	33213-65-9	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aα,6β,9β,9aα)- {β-Endosulfan®}	644, 3634, 4249	644, 2650a, 3188a, 3633, 3634, 3770, 4249, 5811b	
157.	959-98-8	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aβ,6α,9α,9aβ)- {α-Endosulfan®}	3634, 4249	2650a, 3633, 3634, 3770, 4249, 5811b	
158.	76-44-8	4,7-Methano-1*H*-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- {Heptachlor®}	606, 2697, 4249, 21A19	2697, 3138, 3188a, 3633, 3770, 3973, 4249, 4271a, 21A19	
159.	5103-71-9	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- {α-Chlordane®} 		3138, 3633, 3634, 3770, 3973, 4249, 4271a	
160.	57-74-9 12789-03-6	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- {γ-Chlordane®}		2650b, 3138, 3188a, 3633, 3634, 3770, 4249, 5811	
161.	1024-57-3	2,5-Methano-2*H*-indeno[1,2-*b*]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)- {Heptachlor® epoxide}	606, 4249	1219, 1219a, 1219b, 3188a, 3633, 3770, 4249	
162.	297-78-9	4,7-Methanoisobenzofuran, 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro- {Telodrin®} 	937, 1457, 1458, 4249, 21A19	1457, 1458, 3797, 4249, 21A19	
163.	5293-97-0	Methanone, bis(2-chlorophenyl)-	2570, 4249	2389, 2544, 4249	
164.	90-98-2	Methanone, bis(4-chlorophenyl)- 	707, 708, 713, 714, 2570, 4249	4249, 5811b	
165.	5162-03-8	Methanone, (2-chlorophenyl)phenyl-		2917a, 4249	
166.	110488-70-5	Morpholine, 3-(3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl)- (Dimethomorph®, Acrobat®)		2892a, 3633, 4249	
167.	117-80-6	1,4-Naphthalenedione, 2,3-dichloro-	3797	2095, 3797, 4249, 4666a	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
168.	50471-44-8	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- {Vinclozolin®} 		2650a	
169.	106-89-8	Oxirane, (chloromethyl)-		642a, 4249, 4795	
170.	20851-90-5	Phenanthrene, 3,6-dichloro-	142, 1767, 2893, 4249		
171.	95-57-8	Phenol, 2-chloro-	568b, 1928, 1994, 1995, 3712, 4249, 5811b		
172.	70-30-4	Phenol, 2,2′-methylenebis[3,4,6-trichloro-]	2697, 4249		
173.	108-43-0	Phenol, 3-chloro-	278, 3712, 4249		
174.	16672-87-0	Phosphonic acid, 2-chloroethyl- {Ethephon®, Ethrel®} 		2913a, 3633, 3811a, 3973, 5811b	
175.	67255-31-6	Phosphonic acid, 2-chloroethyl-, hydrazine salt- {Hydrel®} H_2PO_3-CH_2CH_2-Cl. H_2N-NH_2		5811, 5811b	
176.	52-68-6	Phosphonic acid, 2,2,2-trichloromethyl-1-hydroxyethyl-, dimethyl ester {Trichlorphon®, Dipterex®} 	1333	1333, 2650a, 3380, 3633, 3973, 3977, 4271a	
177.	470-90-6	Phosphoric acid, 2-chloro-1-(2-dichlorophenyl)ethenyl-, diethyl ester {Chlorfenvivphos®} 		3381, 3633, 4271a	
178.	13171-21-6	Phosphoric acid, 2-chloro-3-(diethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Phosphamidon®} 		3380, 3633, 4271a	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

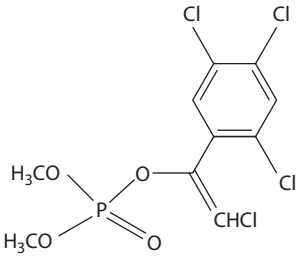
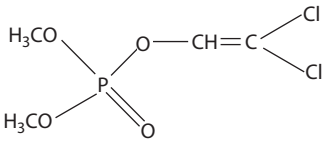
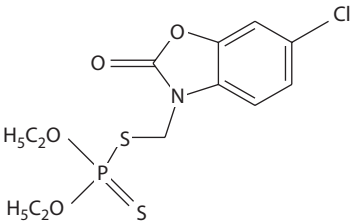
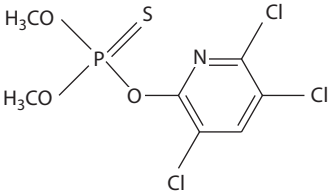
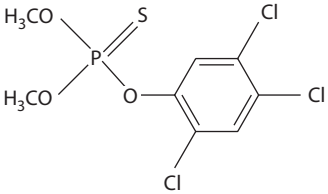
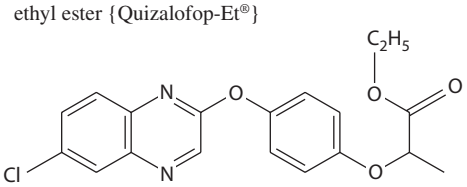
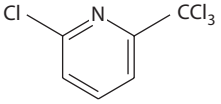
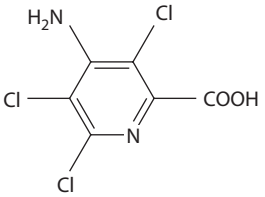
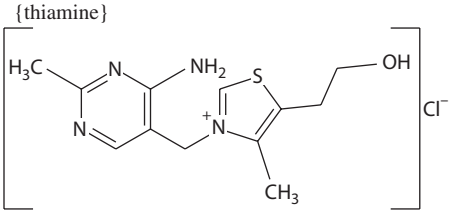
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
179.	22248-79-9	Phosphoric acid, 2-chloro-1-(2,4,5-trichlrophenyl)ethenyl-, dimethyl ester {Tetrachlorvinphos®} 		3381, 3633, 4271a	
180.	62-73-7	Phosphoric acid, 2,2,-dichloroethenyl-, dimethyl ester {Dichlorvos®} 		2058a, 3380, 3633, 4271a	
181.	2310-17-0	Phosphorodithioic acid, *S*-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl) methyl] *O,O*-diethyl ester {Phosalone®} 		3381, 4271a	
182.	38527-91-2	Phosphorothioicacid, 2-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester {Ethaphos®}	5811, 5811a, 5811b		
183.	2921-88-2	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyriphos®, Dursban®} 	717, 1333, 21A19	717, 1219a, 1219b, 1219c,1333, 2058a, 3381, 3633, 3919, 3977, 4249, 21A19	
184.	299-84-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester {Fenchlorphos®, Phenchlorphos®} 		3381, 3633	
185.	7647-10-1	Platinum chloride		5811	
186.	7447-40-7	Potassium chloride (KCl)	4249, 4558	3973, 4249, 4560, 4654, 5811b	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
187.	78-87-5	Propane, 1,2-dichloro-		3633, 3634, 3646a, 4249	
188.	142-28-9	Propane, 1,3-dichloro-		3633, 3634, 3646a, 4249	
189.	96-24-2	1,2-Propanediol, 3-chloro- $Cl\text{-}CH_2\text{-}CHOH\text{-}CH_2OH$	568b, 1375, 1375b, 1586, 2570, 2767, 3255, 3553, 3557, 4249, 5811b		
190.	76578-14-8	Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester {Quizalofop-Et®} 		3633	
191.	127-00-4	2-Propanol, 1-chloro-	3559, 4249		
192.	78-95-5	2-Propanone, 1-chloro- $H_3C\text{-}CO\text{-}CH_2\text{-}Cl$	2777, 4249, 5811b		
193.	26952-23-8	1-Propene, 1,2-dichloro- {Telone®}		4271a	
194.	542-75-6	1-Propene, 1,3-dichloro-		3633, 3634, 3646a, 3973, 4249, 5811b	
195.	20357-65-7	2*H*-Pyran-2-one, 6-chloro-	222–224, 4249		
196.	1929-82-4	Pyridine, 2-chloro-6-(trichloromethyl)- {Nitrapyrin®} 		3973, 4249	
197.	2820-51-1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, hydrochloride, (S)-		4249, 4849	
198.	1918-02-1	2-Pyridinecarboxylic acid, 4-amino-3,5,6-trichloro- {Picloram®} 		3973, 4249	
199.	58-56-0	3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride		429b, 4249, 4789	
200.	18028-53-0	2*H*-Pyrrolium, 3,4-dihydro-1-methyl-, chloride	4249, 4791		
201.	10361-82-7	Samarium chloride		5811	
202.	7647-14-5	Sodium chloride		174b, 1053, 3266, 3476, 4249, 5811b	
203.	154-87-0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydro xy-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, P,P′-dioxide		4051a, 4249, 4798	
204.	59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl) methyl]-5-(2-hydroxyethyl)-4-methyl-chloride {thiamine} 		120, 1941, 2270, 4249, 5079, 17B10	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

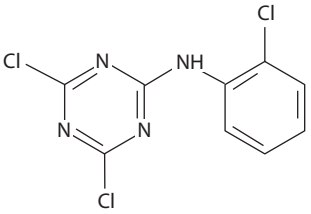
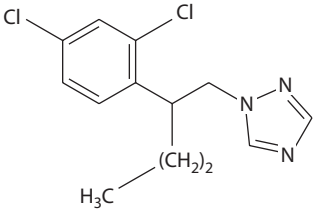
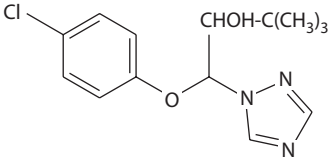
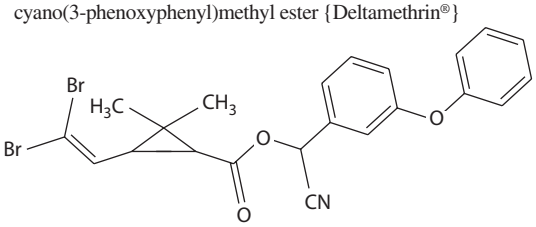
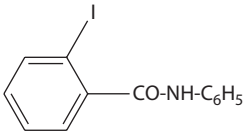
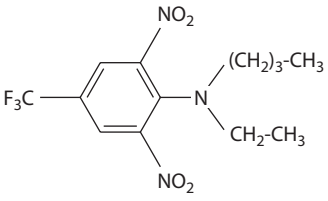
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
205.	67-03-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-chloride, monohydrochloride {thiamine hydrochloride}		1053, 3266, 4249	
206.	1344-13-4	Tin chloride (stannic chloride) $SnCl_4$		5811	
207.	101-05-3	1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-(2-chlorophenyl)- {Anilazine®, Dyrene®} 	1884	3633, 3661a, 3797, 4249, 4271a	
208.	66246-88-6	1,2,4-Triazole, 1-(2-(2,4-dichlorophenyl)pentyl)- {Penconazole®} 		3633, 4249	
209.	55219-65-3	1*H*-1,2,4-Triazol-1-ethanol, 8-(4-chlorophenoxy)-α-(1,1-dimethylethyl)- {Triadimenol®} 	;	928a	
210.	1746-81-2	Urea, *N′*-(4-chlorophenyl)-*N*-methoxy-*N*-methyl- {Linuron®, 30% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
211.	330-55-2	Urea, *N′*-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methyl- {Monolinuron®, 20% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
212.	150-68-5	Urea, 1,1-dimethyl-3-(4-chlorophenyl) {Monuron®}		3633, 4271a	
213.	330-54-1	Urea, 1,1-dimethyl-3-(3,4-dichlorophenyl) {Diuron®}		3973	
214.	11105-12-7	Vanadium chloride		5811	
215.	11126-30-0	Zirconium chloride		5811	
Bromo Compounds					
216.	162188-92-3	Acetic acid, bromo-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro[4.5] dec-7-yl ester, (±)-		4249	
217.	106-40-1	Benzenamine, 4-bromo-	822, 4249		
218.	24959-67-9	Bromide	486, 618, 641, 273, 1445, 1933, 1933b, 1934, 1939, 2524a, 3255, 4249, 5811b	15, 618, 1933, 1934, 1939, 3918, 4249, 4357, 4381, 5811b	
219.	7726-95-6	Bromine	50, 2667, 2779, 4249, 5811b	2667, 2779, 2913a, 3973, 4249, 5811b	50, 4249

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
220.	14686-69-2	Bromine, isotope of mass 82	20A73	3973, 4249, 4381, 20A115	
221.	155728-85-1	2-Butanol, 1-(4-bromophenoxy)-3-[(phenylmethyl)amino]-,(R*,R*)-		4249	
222.	52918-63-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl)methyl ester {Deltamethrin®} 	21A19	904, 1219b, 1219c, 3585e, 3633, 4271a, 21A19	
223.	106-93-4	Ethane, 1,2-dibromo- {ethylene dibromide, EDB®, Bromofume®} $Br\text{-}CH_2\text{-}CH_2\text{-}Br$		3188a, 3633, 3646a, 3973, 4249, 4271a, 5811b	
224.	74-83-9	Methane, bromo- {Brom-o-Gas®, Methogas®, ProFume®, Terr-o-Gas®, Zytox®}	1884, 3255	3633, 3646a, 3722b, 3973, 4249, 5811b	
225.	60918-97-0	1,3,4-Oxadiazol-2-amine, *N*-(4-bromophenyl)-5-(1-naphthalenylmethyl)-		4249	
226.	118-79-6	Phenol, 2,4,6-tribromo-		2650a, 4249	
227.	13808-64-5	1*H*-Pyrazole, 4-bromo-3-methyl-	568b, 4249		
228.	3060-89-7	Urea, *N′*-(4-bromophenyl)-*N′*-methoxy-*N′*-methyl- {Metobromuron®, Patoran®}	822, 4249	622, 3633, 4249, 4271a	
Iodo Compounds					
229.	15310-01-7	Benzamide, 2-iodo-*N*-phenyl- {Benodanil®} 		774a, 4271a, 4249, 4552	
230.	20461-54-5	Iodide		486	
231.	7553-56-2	Iodine	50, 641, 4249, 5811b	3797, 3973, 3974a, 4249, 4273, 5079, 5281, 5283, 5284, 5373, 5811b	50, 641, 4249
232.	74-88-4	Methane, iodo-	4249	5811b	
Fluoro Compounds					
233.	354-38-1	Acetamide, 2,2,2-trifluoro- $F_3C\text{-}CO\text{-}NH_2$	2882, 4249		
234.	1861-40-1	Benzenamine, *N*-butyl-2,6-dinitro-*N*-ethyl-4-(trifluoromethyl)- {Benefin®, Benfluralin®} 		2892a, 3633	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

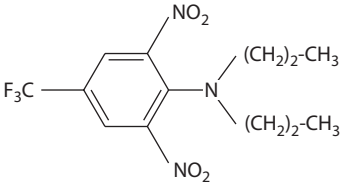
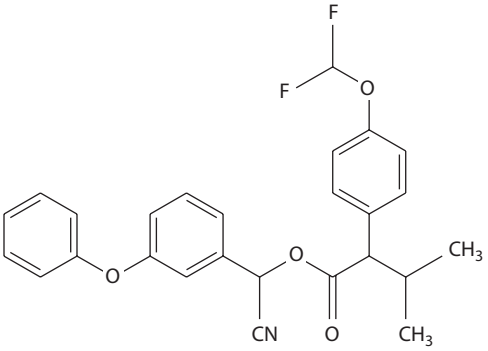
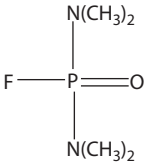
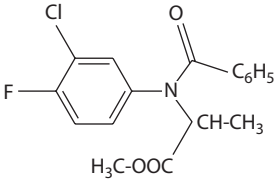
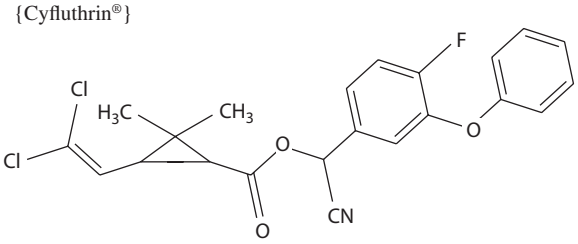
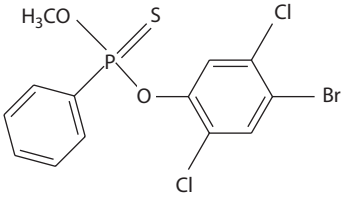
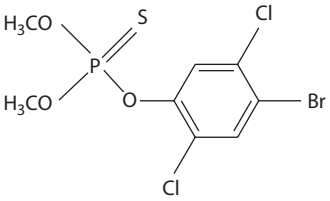
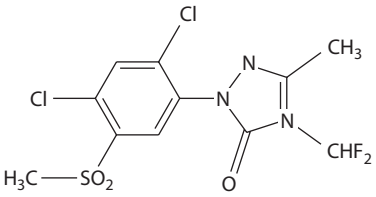
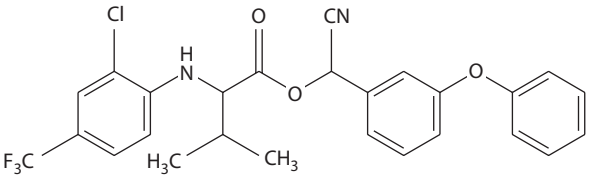
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
235.	1582-09-8	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)- (Trifluralin®) 		1219c, 2650a	
236.	15457-05-3	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)- {Fluorodifen®}		3633	
237.	70124-77-5	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Flucythrinate®} 		904	
238.	811-97-2	Ethane, 1,1,1,2-tetrafluoro- {Freon® 134a}	18B06	18B05, 18B06	
239.	16984-48-8	Fluoride	641, 3302, 4249	4092, 4249, 4629, 4807, 4951, 5811b, 20A24	
240.	7782-41-4	Fluorine	50, 3797, 4249, 5079, 5410, 5811b	3973, 3974a, 4249, 4692, 5811b	50, 4249
241.	115-26-4	Phosphine oxide, bis(dimethylamino)fluoro- {Dimefox®} 		2650b, 3633, 4271a	
242.	76-19-7	Propane, octafluoro- {Freon® 218, Perfluoropropane} $CF_3CF_2CF_3$		18B17	
243.	69806-50-4	Propanoic acid, 2-(4-(5-trifluoromethyl-2-pyridyloxy)phenoxy)-, butyl ester {Fluazifop-butyl®}		3633, 4271a	
244.	68258-35-5	Pyridine-2-^{13}C-3-^{14}C, 3-fluoro-5-(2-piperidinyl)-, (±)-		2331, 4249	
245.	34137-26-3	Pyridine, 5-fluoro-3-(1-methyl-2-pyrrolidinyl)-, (S)-		4736, 4249	
246.	2551-62-4	Sulfur hexafluoride SF_6		4860, 18B17	

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Compounds with Mixed Halogens					
247.	52756-25-9	DL-Alanine, *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-, methyl ester {Flamprop-methyl®} 		4271a	
248.	62924-70-3	Benzenemethanamine, 2-chloro-*N*-(2,6-dinitro-4-(trifluoromethyl)phenyl)-*N*-ethyl- 6-fluoro- {Flumetralin®}		2913a, 3633. 5568, 5811b	
249.	91465-08-6	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {λ-Cyhalothrin®}	21A19	2650b, 21A19	
250.	82657-04-3	Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-trifluoro-1-propenyl]-2,2-dimethyl-, (2-methyl[1,1′-biphenyl]-3-yl)methyl ester, (1R,3R)-rel- {Bifenthrin®, Biphenthrin®}		21A05	
251.	68359-37-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester {Cyfluthrin®} 		904, 3633	
252.	354-53-0	Ethane, 1-chloro-2-bromotetrafluoro- {Freon® 114b1}	18B06	18B06	
253.	75-88-7	Ethane, 1-chloro-2,2,2-trifluoro- {Freon® 133a}	18B06, 18B16	18B06	
254.	306-83-2	Ethane, 2,2-dichloro-1,1,1-trifluoro- {Freon® 123}	18B06, 18B08, 18B16	4859, 18B06, 18B08, 18B16	
255.	151-67-7	Ethane, 1,1,1-trifluoro-2-bromo-2-chloro- {Freon® 123b1, Halothane}	18B06, 18B16	18B06, 18B16	
256.	79-38-9	Ethene, chlorotrifluoro- {Freon® 1113}	18B06, 18B16	18B06	
257.	79-35-6	Ethene, 1,1-dichloro-2,2-difluoro- {Freon® 1112a}	18B06	18B06	
258.	75-71-8	Methane, dichlorodifluoro- {Freon® 12}	1495b, 3896, 4249		
259.	75-69-4	Methane, trichlorofluoro- {Freon® 11} $F\text{-}CCl_3$	770c, 1375b, 1495a, 3254, 3896, 3901a, 3903a, 4249	3254, 3896, 3901a, 3903a, 4249	
260.	21609-90-5 21A19	Phenylphosphonothioic acid, *O*-(4-bromo-2,5-dichlorophenyl)-, *O*-methyl ester {Phosvel®} 		3381, 3634, 21A19	

(*continued*)

TABLE 18.4 (continued)
Halogenated and Related Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
261.	300-76-5	Phosphate, 1,2-dibromo-2,2-dichloroethyl dimethyl {Naled®}		3633, 4271a	
262.	2104-96-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-bromo-2,5-dichlorophenyl) ester {Bromophos®} 		3381, 3633, 4271a	
263.	41198-08-7	Phosphorothioic acid, *O*-(4-bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl ester {Profenophos®}		2058a	
264.	96-12-8	Propane, 1,2-dibromo-3-chloro- {DBCP®}		3188a, 3633	
265.	122836-35-5	1*H*-1,2,4-Triazol-1-yl)phenyl)methane-sulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)phenyl)-; Sulfentrazone®} 		2913a	
266.	102851-06-9	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®} 		904, 2346, 3585e	

19 Fixed and Variable Gases

This chapter deals with gases found in tobacco and tobacco smoke. The gases discussed will be mainly inorganic gases. Two types of gases will be discussed, fixed gases and variable gases.

In the atmosphere, gases, the volume percentages of which do not change, are called fixed gases. Table 19.1 gives the volume percentages of these fixed gases. At altitudes below 100 km, nitrogen (N_2) makes up about 78% of all atmospheric gas by volume, and oxygen (O_2) makes up about 21%. The volume percentages of these fixed gases are constant with increasing altitudes, and the partial pressures of N_2 and O_2 are constant fractions of air pressure. Together, N_2 and O_2 make up 99% of all gases in the atmosphere by volume. Argon (Ar) at 0.93% makes up the bulk of the remaining 0.97%, with neon (Ne), helium (He), krypton (Kr), and xenon (Xe) present in trace quantities (19A04). As a result, the concentrations of fixed gases are the same not only in the atmosphere but in every material present on the Earth's surface where atmospheric gases reside.

Variable gases are gases with volume percentages that change with time and location. For example, water vapor in different areas of the world varies with climatic conditions and geography. Radon is a variable gas as it occurs in only specific areas of the world. The major variable gases are water vapor (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), ozone (O_3), sulfur dioxide (SO_2), nitric oxide (NO), nitrogen dioxide (NO_2), low-molecular-weight hydrocarbons, and simple aromatic chemicals. Much of the variability in the concentration of these gases in the atmosphere arises from the combustion of fossil fuels. Table 19.2 summarizes the volume percentages of some variable gases in a clean atmosphere and a polluted atmosphere, e.g., urban or industrial areas. Water vapor can vary tremendously and is primarily dependent on the environment. For example, water vapor in the atmosphere is always higher in areas near water and always lower in desert areas. As can be seen, some of the inorganic and organic gases change appreciably (CO, SO_2, NO, NO_2, organic gases) while others change minimally (CO_2, O_3), even in polluted atmospheres (19A04). For example, the concentration of CO_2 at point sources such as smoke stacks can be very elevated. O_3 concentrations during electrical storms can be elevated to the point that its characteristic odor is noticeable. As a result, they are termed variable gases.

Again, just as the fixed gases are present in nearly every material present on the Earth's surface, variable gases are also present in all materials that are porous and can be found on the surfaces of many other materials.

Tobacco contains all of the fixed gases that are present in the atmosphere. It also contains a variety of variable gases because it is grown in areas lacking a pristine atmosphere. Tobacco is often treated with agrochemicals (fertilizers, pesticides, herbicides, etc.). As such, these chemicals can decompose and create residues in/on the tobacco. Additionally, as tobacco is often cured in atmospheres that contain pollutants and/or combustion gases, e.g., NO, NO_2, SO_2, SO_3, the concentration of variable gases in the leaf can be elevated. Nitrogen and oxygen are the most plentiful fixed gases found in tobacco. Although the other fixed gases Ar, Ne, He, Kr, and Xe have not been identified in tobacco, there is no reason to believe that they are not present. The variable gases found in tobacco include ammonia (NH_3), bromine (Br_2), CO_2, CO, chlorine (Cl_2), fluorine (F_2), iodine (I_2), phosgene ($COCl_2$), hydrazine ($H_2N\text{-}NH_2$), hydrogen cyanide (HCN), isocyanic acid (H-N═C═O), nitrous oxide (N_2O), NO, NO_2, mixed nitrogen oxides (NO_x) [N_2O + NO + NO_2], phosphine (PH_3), radon (Rn and ^{222}Rn), and H_2O. Biochemically, some of these variable gases are produced by the plant to regulate growth processes, e.g., NO, NO_2, while others are formed, e.g., NH_3 via fertilization, or absorbed by the plant (H_2O) and used as energy sources. Some of the variable gases are found as plant residues from the atmosphere (Rn), while some are residues from water sources (halogens), agrochemicals ($COCl_2$, $H_2N\text{-}NH_2$, HCN, isocyanic acid, PH_3, etc.), or other environmental sources, e.g., SO_2.

The concentration of the fixed and variable gases in tobacco smoke is not directly related to the concentration of these gases in tobacco. As tobacco smoke is the result of combustion and pyrolysis of tobacco, the concentration and types of fixed and variable gases formed vary considerably.

Over the years, several scientific articles and reviews have been published that catalog the fixed and variable gases found in tobacco and tobacco smoke (172, 1140, 1067, 1140, 1971, 2068, 2170, 2799a, 3224, 3797, 4012, 4332, 19A05). One of the earliest articles that identified certain fixed and variable gases in tobacco smoke was published by Kosak (2170) in 1954. Kosak listed O_2, NH_3, CO, CO_2, HCN, other "cyanides" (?), hydrogen sulfide (H_2S), thiocyanic acid (?), "chlorides" (?), "nitrates" (?), and "unsaturated hydrocarbons." It should be noted

TABLE 19.1
Volume Percentages of Fixed Gases in the Earth's Atmosphere

Gas Name	Chemical Formula	Percent
Molecular nitrogen	N_2	78.08
Molecular oxygen	O_2	20.95
Argon	Ar	0.93
Helium	He	0.0015
Neon	Ne	0.0005
Krypton	Kr	0.0001
Xenon	Xe	0.000005

that the question marks associated with some of the compounds listed by Kosak indicate that Kosak did not consider the evidence in the literature to be definitive proof of the identity of the component. It is conceivable that the designation "chlorides" (?) and "nitrates" (?) could have indicated the presence of Cl_2, NO, NO_2, and other NO_x in tobacco smoke.

Johnstone and Plimmer (1971) reviewed the constituents of tobacco and tobacco smoke in 1959 and listed CO, CO_2, carbonyl sulfide (COS), NH_3, carbon disulfide (CS_2), cyanogen [$(CN)_2$], HCN, thiocyanogen [$(SCN)_2$], NO, and numerous small saturated and unsaturated hydrocarbons as components of the vapor phase of cigarette mainstream smoke (MSS).

Keith and Tesh reported in 1965 on the measurement of the total MSS issuing from a burning cigarette (2068). By utilizing a simple puffing mechanism which employed a cold trap packed with 5 Å molecular sieve pellets, they were able to quantitatively measure the total vapor mixture from a burning cigarette. This quantity when combined with the separately trapped particulate material provided a measure of the total effluent. It was found, contrary to previous thinking, that the vapor components of smoke comprised over 95% of the weight of material collected from a burning cigarette. By far, the greatest proportion of the collected weight of the total MSS vapor phase was contributed by the air entering the cigarette.

Wynder and Hoffmann in 1967 (4332) reviewed the known constituents of the particulate and vapor phase of MSS. Chapter VIII of their book provided historical information on our understanding of cigarette combustion processes and the composition of the vapor phase of tobacco smoke at that time. Wynder and Hoffmann cited the pioneering work of Jarrell and de la Burde (1924) and Keith and Tesh (2068) who reported in 1965 that the O_2 content in whole MSS is a function of air entering through the burning cone of the cigarette, part of which is consumed during combustion, and diluting air entering through the cigarette paper. The cigarette burning rate, dictated by the cigarette rod packing density, the tobacco type employed, and the cigarette paper air permeability affected O_2 consumption. Nitrogen and argon do not react with tobacco constituents during the burning as they are inert gases. Their concentrations were affected by the air entering through the burning cone, mainly the diluting air. Jarrell and de la Burde (1924) found that the burning zone of a cigarette represented a reducing atmosphere. The H_2 in the whole smoke was derived nearly exclusively from the

TABLE 19.2
Volume Percentages of Some Variable Gases (Inorganic and Organic) in the Atmosphere (19A04)

Gas Name	Chemical Formula	Clean Atmosphere (ppbv)	Polluted Atmosphere (ppbv)
Inorganic			
Water vapor	H_2O	$3{,}000–4.0 \times 10^7$	$5.0 \times 10^6–4.0 \times 10^7$[a]
Carbon dioxide	CO_2	365,000	365,000
Carbon monoxide	CO	40–200	2,000–10,000
Ozone	O_3	10–100	10–350
Sulfur dioxide	SO_2	0.02–1	1–30
Nitric oxide	NO	0.005–0.1	0.05–300
Nitrogen dioxide	NO_2	0.01–0.3	0.2–200
Organic			
Methane	CH_4	1,800	1,800–2,500
Ethane	C_2H_6	0–2.5	1–50
Ethene	C_2H_4	0–1	1–30
Formaldehyde	HCHO	0.1–1	1–200
Aromatics	C_6H_5R	—	1–30

R, hydrogen or alkyl functionality.

[a] 4.0×10^7 indicates that the volume percentage is negligible, on average.

burning of tobacco. During burning, certain tobacco components split off elementary hydrogen, which for the most part formed water with available oxygen. The presence of 8% H_2 (by volume) in the gas leaving the burning cone was indicative of the existence of a reducing atmosphere in the fire cone. The large concentrations of both CO and CO_2 relative to air indicated that several combustion and pyrolysis processes were occurring in the burning cigarette. The low ratio of CO_2 to CO indicated that incomplete combustion of tobacco was occurring. The ratio of CO_2 to CO is considered to be an index (3482) of the combustibility of tobacco. Generally, the ratio of CO_2 to CO is less than 3 in nonfiltered cigarettes.

In 1968, Stedman reviewed the chemical composition of tobacco and tobacco smoke (3797). The review noted that gaseous NH_3, I_2, and H_2O were identified constituents of tobacco. It also listed CO, CO_2, NH_3, CS_2, COS, Cl_2, F_2, H_2S, HSCN, and [$(SCN)_2$] as compounds present in the vapor phase of MSS.

In 1968, Elmenhorst and Schultz (1140) reported on the concentrations of various inorganic gaseous components in the vapor phase of MSS (Table 19.3).

In 1975, Roberts et al. (3224) reported on R.J. Reynolds Tobacco Company's (RJRT) literature study of tobacco and smoke components. RJRT had been collecting information from the literature and conducting extensive research on the identification of chemicals in tobacco and smoke since the early 1950s. As of 1975, RJRT had compiled a listing of 2783 components from tobacco, tobacco smoke, and other smoking products. Of these compounds, 1235 were tobacco isolates, 2266 were tobacco smoke components, and 356 have been identified from other smoking products. Approximately one-half of all the tobacco and smoke components were first isolated by RJRT research personnel. The lists were divided into functional group classes, including fixed and variable gases found in tobacco and smoke. Twenty-five gases had already been identified in tobacco and smoke by 1975. The number of fixed and variable gases identified in tobacco and tobacco smoke has not changed substantially since then.

Ishiguru and Sugawara in 1980 (1884) cataloged the components of tobacco smoke. In their review, they listed 1889 components of tobacco smoke [see Table 1 in (1884)]. They commented that the number could be about 2500, but they had omitted those components that were only partially identified. Among the components that they discussed were the fixed and variable gases in tobacco smoke.

In 1982, Dube and Green (1067) calculated the contribution of the fixed gases from 500 mg of unfiltered cigarette MSS. From 500 mg of whole smoke, 22.5 mg was the wet particulate matter, and 67.5 mg was vapor-phase compounds, of which ~10% (or 6.75 mg) was water vapor, ~80% (or 54 mg) was CO_2, and ~10% was organic compounds. The remaining 410 mg of whole smoke contained 310 mg of N_2, 65 mg of O_2, 20 mg of CO, an additional 5 mg of CO_2, 4 mg of Ar, and 1 mg H_2. Similar analyses were conducted by Keith and Tesh in 1965 (2068), Norman in 1977 (2799a), and Hoffmann and Hecht in 1990 [see Table 1 in (1727)]. Table 19.4 illustrates the data on fixed and variable gases in whole tobacco smoke that were provided by these investigators.

In 1999, Norman (19A05) and Baker (172) reviewed the literature on cigarette design and materials and smoke chemistry, respectively. Their works represent the most recent and comprehensive reviews on these subjects. Baker

TABLE 19.3
Fixed Gases in the Vapor Phase of MSS (1140)

Compound	Concentration/Cigarette
H_2	0.7–1.8 vol%
O_2	11–17 vol%
N_2	67–78 vol%
Ar	0.8 vol%
H_2O	6–9 mg

TABLE 19.4
Major Fixed and Variable Gases in Nonfiltered Whole Tobacco Smoke

	Keith and Tesh (2068)	Dube and Green (1067)	Norman (2799a)	Hoffmann and Hecht (1727)
Component	mg/cig (%)	mg/cig (%)	% only	mg/cig (%)
N_2	295 (67.2)	310 (62[a])	58	280–320 (56–64[b])
O_2	66.8 (13.3)	65 (13)	12	50–70 (11–14)
CO_2	68.1 (9.8)	59 (11.8)	13.0	45–65 (9–13)
CO	16.2 (3.7)	20 (4.0)	3.5	14–23 (2.8–4.6)
H_2O	5.8	6.75 (1.4)	1	7–12 (1.4–2.4)
Ar	5.0 (0.8)	4 (0.08)	0.5 (Ar + H_2)	5 (1.0)
H_2	0.7 (2.2)	1 (0.2)	—	0.5–1.0
Total weight (or %)	457.6 (97)	465.75 (93.2)	88	401.5–496 (81.7–99)

[a] Percent of total tobacco smoke generated based on 500 mg of whole smoke (1067).
[b] Number in parentheses represents % of individual compound identified in fixed gases from whole smoke (1727).

discussed the present fundamental knowledge of cigarette combustion and smoke formation including how the concentrations of fixed gases, e.g., O_2 and H_2, fluctuate during cigarette combustion and how variable gases, e.g., CO, CO_2, are formed. Norman discussed the complicated field of cigarette design and how each design variable (tobacco type, cigarette shape, weight, and size, cigarette paper properties, filter designs, etc.) affects cigarette performance and ultimately cigarette smoke yields (including fixed and variable gases).

19.1 ANALYTICAL METHODS

In 1996, Green and Rodgman (1373) summarized all the historical and currently used analytical methods for the identification of chemicals isolated from tobacco and tobacco smoke. Their review is so complete and so well documented that the reader is directed to read their review article to determine the analytical method best suited for the analysis of a particular chemical constituent in tobacco and smoke. All of the past and current methods for the determination of fixed and variable gases in tobacco and tobacco smoke can be found in their article and will not be included in this chapter. Only a few specific examples of analytical methods for the most important variable gases will be provided (1884).

Although there is no standard ISO or FTC method for the analysis of fixed gases in cigarette smoke, fixed gases are normally analyzed by mass spectrometry (MS), gas chromatography (GC), or GC-MS. Generally, the fixed gases, e.g., N_2, O_2, Ar, He, H_2, have been determined chromatographically with separation based on molecular size. A molecular sieve packing is normally used in a stainless steel packed column. Samples are introduced with either a gas tight syringe or a sampling valve with a fixed volume loop. Upon injection, the sample is swept through a gas chromatograph with carrier gas. After separation in the column, components are quantified based on the difference in thermal conductivity between the carrier gas and the component. For the analysis of H_2 and He, Ar is used as the carrier. He is used for all the other gases, such as N_2 and O_2. Detection limits using a thermal conductivity detector are typically 0.01% by volume (19A08). Gas samples can be analyzed by MS via a gas inlet port on the mass spectrometer. Methods for the determination of fixed gases in cigarette smoke have been reported by Routh (19A06) and Reynolds and Wheeler (3120). There are several methods for the analysis of the major variable gases from tobacco smoke, e.g., CO, CO_2, NO, NO_2, HCN, and NH_3. The current standard methods approved by International Organization for Standardization (ISO), Federal Trade Commission (FTC), and Cooperation Centre for Scientific Research Relative to Tobacco (CORESTA) for the determination of the variable gases are described by Counts et al. along with analytical results from a recent worldwide market sample of cigarette brands (19A02, 19A03).

19.1.1 Carbon Dioxide and Carbon Monoxide

CO_2 is a major vapor-phase MSS component exceeded only by N_2. Its concentration is about 10% of the weight of the whole tobacco smoke (4145), similar to that of O_2. The concentration of CO is next highest, being about 4% (4145). The ratio of CO_2 to CO is considered to be an index (3482) of the combustibility of tobacco. The currently approved methods for the determination of CO are ISO Standard Methods 3308, 3402, 4387, 8454, 10315, and 10362-1. In these methods, CO is determined by nondispersion infrared (NDIR) spectroscopy (19A02).

Historically, GC (474, 2123, 2662, 4145) and NDIR spectroscopic analysis (781, 782, 4251, 4252) have generally been the preferred methods for analysis of CO_2 and CO in MSS, but an electrochemical transducer (ECT) method (447) has also been used for the analysis of CO, in which the electrochemical reaction during oxidation by catalysis is converted to electrical signals. Sample treatments before GC or NDIR analyses such as oxidation (474, 4145) of CO to CO_2 with iodine pentoxide, reduction (2123, 2124) of CO to CH_4 with a Ni catalyst, and separation (2634) by lowering the column temperature to –70°C have also been studied. GC (2662) with 5 Å molecular sieves as the packing materials has also been employed. The levels of both CO_2 and CO in smoke increase (4251) as the number of puffs increases. The amounts of these combustion gases produced in the early puffs of a cigarette are lower than those analyzed at the end of a cigarette during smoking (4251, 4252). The relationship to the length of the cigarette is such that the concentrations of these components in the vapor phase decrease (3881, 3883) with increasing length, and this can be explained by the reduction in the amount of tobacco burned and diffusion of CO from the wrapper during smoking (19A05). Tobacco quality is an important factor in terms of the amount of CO and CO_2 produced during cigarette combustion. The amount of CO produced (474, 3088) is greater for low- to medium-grade tobaccos, and the amount of CO_2 increases (474) as tobacco quality becomes higher. Experiments with ^{18}O as the source of atmospheric oxygen indicated that more than 50% of the oxygen atoms in the CO_2 and CO molecules come from the atmosphere (1884).

19.1.2 Nitrogen Oxides

NO_x in tobacco smoke has been quantified by calorimetric analyses (189, 3441, 3720) such as the Saltzman method (19A07) and by the chemical emission method (2122) which has been shown to be a rapid method for quantification (1884). Most of the NO_x present in fresh MSS is NO; only a small amount of NO_2 is present (189, 816, 2803). The concentration of NO_2 in MSS increases (189, 2803, 3691) with the age of the smoke and can reach levels of 200 ppm after 60 s (189). NO_2 formation is believed to result from the autoxidation of NO. It has also been suggested that some of the NO_2

produced by oxidation is converted (2941, 4058) to methyl nitrite through a reaction with methanol in the smoke (1884). Predominate precursors of NO are nitrates (189) and other *N*-containing compounds in the tobacco. N_2O (2941) and HNO_3 (4058) have also been reported as components of MSS in addition to the earlier compounds (1884). The currently preferred method for the determination of NO_x is chemiluminescence (1930, 19A02).

19.1.3 Hydrogen Cyanide

HCN in smoke has been analyzed by colorimetry (110, 779, 780, 3088), by the ion-selective electrode method (3482), and by GC (513). An analysis of HCN in tobacco smoke by Vickroy and Gaunt (4053) illustrated that HCN can vary from 144 to 351 µg/cig depending on different brands of cigarettes. The concentration of HCN in MSS increases (110) with puff number similar to other MSS components. HCN is present in both the vapor phase and the particulate phase of MSS (110). Considerable amounts of HCN have also been found in cigarette butts (110, 779, 780). Today, the preferred method for the determination of HCN in the vapor and particulate phase of MSS is colorimetry. HCN is converted to cyanogen chloride, treated with pyridine, and complexed with diethyl acetone dicarboxylate (779, 780, 3145). Schmeltz and Hoffmann (3491) found that tobacco smoke contains $(CN)_2$ and that up to about 5% of the HCN analyzed was produced by conversion of HCN to $(CN)_2$ during analysis (1884).

19.1.4 Ammonia

The preferred method for the determination of NH_3 in MSS is currently ion-exchange chromatography (IEC) (2681a, 19A02). In this method, NH_3 is collected from Cambridge pads and sulfuric acid traps and then analyzed by IEC (19A02). Previous methods for the analysis of NH_3 in MSS such as titration and colorimetry suffered from interferences (2724, 2787, 19A01.), principally low-boiling amines. Quantification of NH_3 by means of selective electrodes (3693) has been attempted, but the results were affected (475) by methylamine. GC (129, 475, 2541) has also been employed with good results since the effects of the presence of other substances can be substantially reduced. Early methods for the determination of NH_3 involved trapping MSS in an aqueous acidic solution. The trapped MSS solution was then steam distilled under alkaline condition to obtain the sample for analysis. It was discovered that this early method produced extra NH_3 (30%–80%) during the steam distillation procedure (475, 1884). NH_3 collected from MSS should be analyzed directly to achieve accurate quantification (1884). Cigarette blends with higher levels of nitrogen such as blends high in burley tobacco tend to have higher yields of MSS NH_3. The yield of NH_3 in MSS is known to vary with the permeability of the cigarette wrappers, when cigarettes were tested with comparable blends (475). The amount of NH_3 produced was greater for wrappers with higher air permeability. The rate of formation of NH_3 depended strongly on temperature. The yield of NH_3 increased with decreasing temperature (1884). Therefore, it was thought that variations in the burning temperature resulting from differences in wrapper quality or its air permeability determined the amount of NH_3 produced (1884).

Table 19.5 is a catalog of the fixed and variable gases in tobacco, tobacco smoke, and tobacco substitute smoke. The catalog contains only 36 entries. This number of entries represents a very small fraction of the total number of identified compounds in tobacco and tobacco smoke, but amazingly, the weight contributed by fixed and variable gases represents about 90% of the whole smoke from a cigarette.

TABLE 19.5
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	7664-41-7	Ammonia NH_3	30, 31, 50, 126b, 129, 167, 172, 173a, 174a, 174b, 174c, 195, 197, 198, 213, 237, 239, 364, 365, 375, 376, 402, 407, 408, 424, 472, 473, 475, 480, 491, 688, 827, 916, 985–987, 989, 1051, 1063–1066, 1068–1075, 1091, 1099, 1100, 1128b,1137, 1140, 1222, 1245, 1263, 1277, 1293, 1335, 1348–1351, 1354, 1369, 1375a, 1386, 1388–1390, 1437, 1442, 1445, 1469, 1489, 1492, 1522, 1524, 1531, 1532, 1539, 1580, 1589, 1673, 1674, 1709, 1741, 1744, 1808, 1841, 1842, 1853b, 1884, 1902, 1911, 1966, 2079, 2083–2085, 2133, 2134a, 2142, 2161, 2170, 2217, 2224, 2263, 2267, 2270, 2326, 2330, 2338, 2342, 2342a, 2343, 2368, 2480, 2524, 2529, 2541, 2543, 2545, 2607, 2627, 2688, 2691–2695, 2724, 2761, 2762, 2775, 2777, 2781, 2782, 2804, 2858, 2919, 2927, 2928, 2934, 2936, 2937, 2939, 2973, 2986–2988, 3007, 3022, 3029, 3059, 3140, 3187, 3190, 3213, 3214, 3251, 3254, 3255, 3257, 3266, 3300, 3302, 3306, 3308, 3324, 3369, 3385, 3482, 3491, 3493, 3583, 3584, 3623, 3659, 3693, 3695, 3797, 3844, 3909, 3910, 3934, 3955, 3956, 3973, 3992, 4005–4007, 4009–4011, 4041, 4052, 4056, 4060–4062, 4064, 4065, 4136, 4226, 4245, 4249, 4301, 4319, 4332, 4406, 4636, 4686, 4743, 5042, 5049, 5082, 5079, 5099, 5100, 5129, 5189, 5263, 5359, 5382, 5389, 5512, 5548, 5811b, 5836, 5869a, 19A02	129, 174b, 212, 385, 555, 622, 677b, 826a, 856, 927, 989, 1053, 1063–1066, 1068–1074, 1128b, 1189, 1222, 1244, 1263, 1329, 1330, 1332, 1333, 1335, 1351, 1369, 1493, 1527, 1835b, 1941, 2079, 2313a, 2330, 2337, 2338, 2339b, 2356, 2381, 2394a, 2453, 2529, 2543, 2545, 2607, 2746, 2761, 2762, 2765, 2766, 2787, 2914, 2919, 2939, 2987, 3022, 3214, 3254, 3261, 3266, 3385, 3420, 3491, 3499, 3693, 3707, 3780, 3797, 3974a, 3974b, 4244, 4249, 4837a, 5018, 5079, 5126, 5165, 5186, 5189, 5194, 5298, 5382, 5389, 5396, 5669, 5712, 5803, 5811b, 5872, 5907, 17B40	50, 1354, 1375a, 4052, 4056, 4249
2.	7440-37-1	Argon Ar	172, 238, 239, 1140, 1284, 1375a, 1377, 1420, 1437, 1744, 1842, 2059, 2068, 2270, 2310, 2607, 2781, 2804, 2939, 3120, 3302, 3308, 3897, 4249, 4332, 5512		1375a, 1377, 4249
3.	7726-95-6	Bromine Br_2	15, 50, 2667, 2779, 4249, 5811b	2667, 2779, 2913a, 3973, 4249, 5811b	50, 4249
4.	124-38-9	Carbon dioxide CO_2	28, 30, 31, 90, 126a, 126b, 162–170, 172, 174, 217, 199, 220, 222–224, 238, 239, 337, 375, 403, 421, 445, 474, 480, 491, 499, 544–546, 568b, 621, 686, 722, 855, 857, 916, 918a, 920, 957, 966, 1048a, 1051, 1063–1074, 1099, 1119, 1140, 1202, 1205, 1208, 1243, 1263, 1284, 1329,	212, 256, 568b, 1053, 1206a, 2079, 3266, 4249, 4577, 4795, 4926, 5079, 5132, 5165, 5189, 5192, 5193, 5811b, 17B40	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 2506, 2507, 3192, 4052, 4056, 4249

TABLE 19.5 (continued)
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Carbon dioxide (cont.)	1330, 1332–1334, 1348–1350, 1352, 1354, 1373, 1375a, 1377, 1378, 1388–1390, 1413, 1419, 1420, 1437, 1442, 1445, 1464, 1466, 1468, 1477, 1478, 1492, 1541, 1589, 1600, 1664, 1668, 1673, 1674, 1693, 1709, 1744, 1760, 1803, 1837, 1842, 1924, 1935–1937, 1963, 1966, 1977, 2029, 2059, 2060, 2062, 2066, 2068, 2079, 2117, 2124, 2133, 2134a, 2142, 2170, 2183, 2196, 2198, 2252, 2263, 2265, 2270, 2293, 2310, 2326, 2342, 2343, 2348, 2457, 2506, 2507, 2524, 2537, 2543, 2545, 2548, 2549, 2555, 2571, 2582, 2624, 2634, 2659, 2662, 2683, 2761, 2762, 2777, 2780, 2782, 2798, 2799, 2799a, 2804, 2866, 2867, 2913, 2919, 2920–2922, 2928, 2939, 2942, 2973, 3059, 3088, 3102, 3116, 3120, 3121, 3132, 3190, 3224, 3254, 3255, 3257, 3266, 3302, 3308, 3317, 3324, 3336, 3378, 3412, 3482, 3493, 3511, 3516, 3522, 3548, 3564, 3640, 3795, 3870, 3876, 3880, 3882, 3883, 3897, 3909, 3910, 3929, 3930, 3939, 3973, 3987, 3992, 4052, 4055, 4056, 4064, 4067, 4078a, 4079, 4145, 4162, 4212, 4215, 4249, 4251, 4319, 4332, 4360, 4364, 4365, 4406, 4418, 5047, 5079, 5140, 5207, 5359, 5512, 5811b		
5.	51-90-1	Carbon-^{14}C dioxide	916a, 1051d, 2763, 4249		
6.	75-15-0	Carbon disulfide CS_2	237, 722, 1140, 1373, 1420, 1422, 1741,1831, 2310, 2313a, 2799a, 2939, 2940, 2945, 3255, 3257, 3265, 3300, 3302, 3729, 3797, 4249, 4319, 4332, 5039, 5811b, 5869a	5079, 5189, 21A05	
7.	630-08-0	Carbon monoxide CO	28, 30, 31, 82, 83, 90, 123a, 126, 126a, 126b, 130, 162–170, 172, 173, 173a, 174, 174a, 174b, 174c, 199, 217, 220, 221, 238, 239, 251, 288, 335, 337, 354, 357a, 375, 376, 383, 386, 401, 403, 421, 445, 447, 469a, 474, 480, 488, 489, 491, 492, 499, 534, 544–546, 603, 621, 636, 686, 688, 722, 781, 855, 886, 893, 916, 918a, 920, 929a, 957, 966, 988a, 1007, 1048a, 1051, 1063–1074, 1089, 1099, 1119, 1140, 1166, 1167, 1202, 1205, 1208, 1243, 1263, 1276, 1292, 1284, 1306, 1329, 1330, 1332–1334, 1331, 1343, 1344,	4249, 4795, 5811b	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 4052, 4056, 4249

(*continued*)

TABLE 19.5 (continued)
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Carbon monoxide (cont.)	1348–1350, 1354, 1361, 1373–1375, 1375a, 1377, 1378, 1352, 1386, 1388–1390, 1419, 1420, 1435, 1437, 1442, 1443, 1445, 1466–1468, 1476–1478, 1492, 1493a, 1503, 1504, 1506, 1541 1586, 1589, 1605, 1629, 1639, 1664, 1668, 1673, 1674, 1692, 1693, 1695, 1699, 1709, 1719, 1741, 1744, 1760, 1803, 1807a, 1830, 1842, 1847, 1855, 1920, 1921, 1924, 1931, 1932, 1935–1937, 1956, 1963, 1966, 1976, 1977, 1986a, 1989, 2012, 2029, 2030, 2055, 2059, 2060, 2062, 2066, 2068, 2079, 2117, 2123, 2124, 2133, 2134a, 2142, 2159, 2170, 2183, 2196, 2203, 2213, 2252, 2265, 2270, 2293, 2310, 2323, 2326, 2330, 2326, 2342a, 2343, 2344, 2347, 2348, 2358, 2359, 2400c, 2400d, 2419, 2445a, 2457, 2518, 2524, 2537, 2540, 2543, 2344, 2347, 2348, 2358, 2359, 2400c, 2400d, 2419, 2445a, 2457, 2518, 2524, 2537, 2540, 2543, 2545, 2548, 2549, 2555, 2570, 2571,2582, 2624, 2626, 2634, 2659, 2662, 2683, 2690, 2761, 2762, 2777, 2780, 2782, 2785, 2798, 2799a, 2800, 2804, 2866, 2867, 2878, 2878a, 2913, 2928, 2929, 2920–2922, 2927, 2928, 2939, 2942, 2965, 2970, 2973, 3007, 3059, 3087, 3088, 3102, 3110, 3112–3120, 3132, 3135–3137, 3139, 3140, 3142, 3143, 3148a, 3190, 3254, 3255, 3257, 3300, 3302, 3308, 3317, 3324, 3336, 3370, 3378, 3407, 3412, 3441a, 3482, 3493, 3516, 3522, 3548, 3557, 3564, 3640, 3722, 3729, 3795, 3844, 3845, 3860, 3870, 3876, 3880–3883, 3898, 3907, 3909, 3910, 3917a, 3929, 3939, 3952, 3973, 3987, 3992, 4009–4011, 4052, 4055, 4056, 4064, 4065, 4067, 4078a, 4079, 4105, 4120, 4121, 4137, 4143, 4145, 4162, 4212, 4215, 4249, 4251, 4285, 4319, 4330, 4332, 4342, 4364–4366, 4391, 4398, 4406, 4418, 4581, 4745, 4980, 5006, 5030, 5042, 5045, 5047, 5065, 5071, 5079, 5124, 5140, 5154, 5189, 5207, 5219,5263, 5313, 5359, 5411, 5483, 5484, 5512, 5532, 5546, 5558, 5575, 5643a, 5679, 5811b, 5835, 5836, 5869a, 19A02, 19A05		
8.	7665-54-5	Carbon-^{14}C monoxide	606b, 916a, 1935, 2763, 4249		

TABLE 19.5 (continued)
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
9.	463-58-1	Carbon oxide sulfide {carbonyl sulfide} COS	126b, 621, 722, 1140, 1445, 1674, 1828, 1832, 2025, 2079, 2142, 2170, 2270, 2293, 2310, 2634, 2799a, 2866, 2939, 2940, 2942, 3059, 3105, 3106, 3255, 3300, 3302, 3308, 3516, 3583, 3584, 3729, 3797, 3897, 3939, 4135, 4249, 4319, 4332, 4360, 4395, 5039, 5811b, 5835		
10.	75-44-5	Carbon oxychloride {phosgene} $COCl_2$	1375b (0), 3254 (0), 3901a (0), 4249, 5046, 5059	2483a, 4249	
11.	2944-05-0	Carbon sulfide CS	1140, 1429, 4249, 5811b		
12.	7782-50-5	Chlorine Cl_2	50, 1240, 2779, 3797, 4249, 5811b	1127b, 1240, 2779, 3973, 3974a, 3974b, 4108, 4249, 4512, 5654, 5688, 5811b	50, 4249
13.	460-19-5	Ethanedinitrile {cyanogen} NC-CN	513, 1741, 1971, 1991, 2079, 2634, 2724, 2939, 3300, 3302, 3308, 3491, 3932, 4249, 4332, 5070, 5811b		
14.	7782-41-4	Fluorine F_2	50, 3797, 4249, 5079, 5410, 5811b	3973, 3974a, 4249, 4692, 5811b	50, 4249
15.	302-01-2	Hydrazine $H_2N\text{-}NH_2$	126, 126a, 126b, 172, 237, 239, 427, 1148, 1217, 1373, 1437, 1445, 1507, 1557, 1571a, 1580, 1674, 1706, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1781, 1808, 1870, 1871, 2133, 2384, 2385, 2825, 3255, 3257, 3260, 3265, 3300, 3491, 3493, 3714, 3811a, 4010, 4011, 4249, 5512, 5811b, 5869a	1571a, 1580, 1581, 2385, 3481, 3491, 3493, 3811a, 3973, 3974b, 4249	
16.	74-90-8	Hydrocyanic acid {hydrogen cyanide} HCN	80–83, 110, 112, 126b, 167, 172, 174a, 174b, 174c, 174e, 213, 237–239, 267, 269, 270, 314, 337, 402, 429a, 480, 491, 513, 577, 603, 631, 688, 722, 747, 748, 765, 779, 780, 804, 861, 916, 918a, 920, 966, 1051, 1063–1074, 1077a, 1091, 1092, 1099, 1119, 1140, 1202, 1235, 1276, 1283, 1284, 1292, 1329, 1330, 1332–1336, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1331, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1442, 1445, 1466, 1467, 1469, 1492, 1497, 1498, 1589, 1668, 1673, 1674, 1693, 1695, 1719, 1741, 1744, 1746, 1751, 1760, 1781, 1803, 1807a, 1842, 1932, 1956, 1966, 1967, 2059, 2062, 2067, 2068, 2079, 2083–2086, 2133, 2134a, 2142, 2157, 2159, 2170, 2252, 2270, 2293, 2310, 2313a, 2313c, 2313d, 2326, 2342, 2342a, 2343, 2344, 2502, 2506, 2507, 2537, 2543, 2545, 2570, 2607, 2608, 2628, 2634, 2679, 2683, 2724, 2761, 2762, 2775, 2777, 2780, 2782, 2799a, 2801, 2804, 2805, 2866,	2607, 3290, 3633, 4064, 4271a, 5079, 5189, 5811b	1330 (0), 1332 (0) 1354, 1375a, 1377, 1378, 2506, 2507, 4052, 4056, 4249

(*continued*)

TABLE 19.5 (continued)
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Hydrocyanic acid {hydrogen cyanide} (cont.)	2939, 2942, 2956, 2971, 2973, 3007, 3029, 3059, 3087, 3088, 3101, 3116, 3120, 3121, 3121a, 3132, 3135–3137, 3139, 3140, 3145, 3148, 3149, 3190, 3251, 3254, 3255, 3257, 3290, 3300–3302, 3306, 3308, 3370, 3482, 3491, 3493, 3524, 3525, 3530, 3557, 3690, 3724, 3729, 3844, 3872, 3876, 3880–3882, 3897, 3909–3911, 3917a, 3939, 3952, 3973, 3976, 3984, 3992, 3996, 4005–4007, 4010, 4011, 4052, 4053, 4056, 4063, 4064, 4109, 4143, 4162, 4202, 4249, 4259, 4260, 4301, 4319, 4342, 4360, 4365, 4398, 4418, 4502, 4743, 4745, 4816, 5042, 5079, 5140, 5189, 5208, 5219, 5263, 5512, 5531, 5546, 5547, 5554, 5587, 5811b, 5835, 5836, 5869a		
17.	1333-74-0	Hydrogen H_2	168, 172, 237, 239, 480, 722, 1140, 1263, 1373, 1420, 1437, 1485, 1664, 1668, 1674, 1744, 1842, 2059, 2060, 2066, 2068, 2252, 2270, 2310, 2662, 2782, 2804, 2866, 2878, 2939, 3121, 3302, 3308, 3880, 3882, 3883, 4151, 4249, 4332, 5079, 5512, 5811b		3192
18.	7783-06-4	Hydrogen sulfide H_2S	199, 239, 782, 916, 957, 1067, 1128, 1140, 1202, 1240, 1276, 1283, 1419, 1437, 1445, 1466, 1469, 1495, 1526, 1741, 1744, 1828, 1832, 1842, 2067, 2079, 2170, 2252, 2270, 2293, 2310, 2313a, 2342, 2343, 2502, 2524, 2607, 2621, 2782, 2799a, 2804, 2939, 2940, 3121a, 3187, 3300, 3302, 3308, 3493, 3524, 3525, 3797, 3817a, 3880, 3882, 3897, 3933, 3973, 4052, 4056, 4063, 4187, 4202, 4215, 4249, 4319, 4332, 4360, 5034, 5039, 5042, 5079, 5140, 5189, 5512, 5811b, 5835, 5869a	2607, 4249, 4795, 5079, 5323	4052, 4056
19.	7553-56-2	Iodine I_2	50, 641, 4249, 5811b	3797, 3973, 3974a, 4249, 4273, 5079, 5281, 5283, 5284, 5373, 5811b	50, 641, 4249
20.	75-13-8	Isocyanic acid H-N═C═O	199, 239, 782, 916, 957, 1067, 1128, 1140, 1202, 1240, 1276, 1283, 1419, 1437, 1445, 1466, 1469, 1495, 1526, 1741, 1828, 1832, 1842, 2067, 2079, 2170, 2252, 2270, 2293, 2310, 2313a, 2342, 2343, 2502, 2524, 2607, 2621, 2782, 2799a, 2804, 2939, 2940, 3121a, 3187, 3300, 3302, 3308, 3493, 3524, 3525, 3797, 3817a, 3880, 3882, 3897, 3933, 3973, 4052, 4056, 4063, 4187, 4202, 4215, 4249, 4319, 4332, 4360, 5034, 5039, 5042, 5079, 5140, 5189	3973, 4249	

TABLE 19.5 (continued)
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
21.	7727-37-9	Nitrogen N_2	167, 172, 237, 239, 421, 621, 1140, 1284, 1373, 1375a, 1377, 1420, 1437, 1668, 1744, 1842, 1924, 1963a, 2059, 2060, 2066, 2068, 2079, 2133, 2142, 2270, 2310, 2607, 2634, 2724, 2780, 2781, 2782, 2804, 2939, 3120, 3121, 3132, 3302, 3308, 3491, 3564, 3973, 4249, 4332, 5079, 5512, 5811b	193, 260, 559, 1127b, 2665, 2688, 2724, 3974b, 3491, 4249, 5079, 5189, 5192, 5193, 5597, 5622, 5625, 5434, 5654, 5666, 5715, 5803, 5843	1375a, 1377, 3192
22.	11104-93-1	Nitrogen oxide	2122, 3302, 4249, 5811b		
23.	10024-97-2	Nitrogen oxide {nitrous oxide} N_2O	167, 480, 1140, 1420, 1659, 2142, 2270, 2293, 2310, 2724, 2939, 2940, 2941, 2946, 3059, 3302, 3491, 3564, 3882, 4249, 4319, 4332	1175a, 4249	
24.	10102-43-9	Nitrogen oxide {nitric oxide} NO	21, 28, 199, 172, 173a, 189, 239, 386, 387, 401, 480, 499, 574, 603, 688, 753, 815, 816, 845, 855, 887, 960b, 988a, 1051, 1063–1074, 1089, 1140, 1331, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1465, 1602, 1634, 1693, 1741, 1833, 1834, 1859, 1929, 1930, 1952, 1955, 1956, 1963, 2062, 2079, 2083–2085, 2122, 2133, 2134a, 2142, 2159, 2270, 2293, 2297, 2310, 2360, 2545, 2557a, 2634, 2690, 2724, 2738, 2782, 2800, 2801, 2803, 2804, 2806, 2878a, 2919, 2927, 2939, 3007, 3116, 3132, 3135–3137, 3139, 3149, 3255, 3300, 3302, 3308, 3370, 3441, 3491, 3557, 3587, 3655, 3671, 3691, 3694, 3720, 3818, 3862, 3907, 3952, 3973, 3993, 3997, 4005–4007, 4052, 4056, 4162, 4219, 4249, 4250, 4252, 4319, 4332, 4365, 5008, 5034, 5042, 5590, 5811b, 5836	1175a, 4249	642, 1375a, 1377, 1378, 3192, 4052, 4056, 4249
25.	10102-44-0	Nitrogen oxide {nitrogen dioxide} NO_2	172, 199, 213, 255, 386, 480, 486, 816, 960b, 1089, 1099, 1100, 1140, 1420, 1443, 1465, 1930, 1952, 1955, 1963, 2083–2085, 2134a, 2142, 2252, 2270, 2293, 2297, 2310, 2495, 2545, 2690, 2724, 2782, 2801, 2803, 2804, 2806, 2939, 3132, 3255, 3302, 3308, 3441, 3491, 3493, 3587, 3691, 3694, 3901, 3973, 4005–4007, 4249, 4319, 4332, 5008, 5042, 5811b, 5869a		
26.		Nitrogen oxides (N_2O + NO + NO_2) NO_x	82, 83, 126a, 126b, 174a, 174b, 237, 379, 386, 402, 499, 688, 804, 815, 816, 887, 960b, 1067, 1099, 1100, 1292, 1329, 1330, 1332–1334, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1388–1390, 1420, 1442, 1445, 1465, 1492, 1497, 1528, 1580, 1589, 1673, 1674, 1741, 1744, 1807a, 1842, 1955, 2036, 2051, 2293, 2313a, 2373, 2537,	2700, 4249, 5053	1330, 1332, 1354, 1375a, 1377, 4249

(*continued*)

TABLE 19.5 (continued)
Fixed and Variable Gases in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Nitrogen oxides (N_2O + NO + NO_2) (cont.)	2543, 2570, 2625, 2627, 2691–2695, 2733, 2736, 2761, 2762, 2775, 2777, 2782, 2803, 2804, 3190, 3251, 3254, 3255, 3308, 3388, 3441, 3587, 3694, 3844, 3848, 3880, 3939, 3952, 3992, 4010, 4011, 4232, 4249, 4301, 4319, 4332, 4342, 4581, 4980, 5512, 5569, 5590, 5836, 19A02, 19A07		
27.	7782-44-7	Oxygen O_2	168, 172, 237, 239, 411, 421, 480, 621, 1140, 1284, 1306, 1373, 1375a, 1377, 1420, 1437, 1664, 1668, 1744, 1842, 1924, 1969, 2059, 2060, 2066, 2068, 2079, 2133, 2252, 2310, 2607, 2634, 2736, 2780, 2781, 2782, 2804, 2939, 3120, 3121, 3132, 3302, 3308, 3516, 3880, 3882, 3883, 4249, 4332, 5042, 59079, 5512, 5811b	1206a, 2607, 5079, 5811b	1375a, 1377, 4249
28.	10028-15-6	Ozone		5811, 5811b	
29.	7803-51-2	Phosphine PH_3	575, 637, 3302, 4249, 5079	3633, 4271a, 5523, 5811b	641, 4249
30.	10043-92-2	Radon Rn		5079, 5167, 5811b, 20A11	
31.	14859-67-7	Radon, isotope of mass 222 ^{222}Rn	2466, 3302, 3308, 3989, 4005, 4249, 4319, 4332	5079, 20A11	
32.	7446-09-5	Sulfur dioxide SO_2	213, 270, 891a, 1140, 1445, 1828, 1832, 2083, 2084, 3255, 3257, 3300, 3302, 3306, 3729, 3880, 3882, 3973, 4005–4007, 4052, 4056, 4249, 4332, 5042	4908a, 5811b	4052, 4056, 4249
33.	7446-11-9	Sulfur trioxide (SO_3)	1240, 1941, 4249	1941,4249	
34.	463-56-9	Thiocyanic acid (HSCN)	1140, 1971, 2270, 2607, 2724, 2939, 2940, 3302, 3491, 3525, 3797, 4249, 4319, 4332, 5079, 5811b	2607, 3525, 5079	
35.	505-14-6 15941-77-2	Thiocyanogen $(SCN)_2$	1140, 1971, 2724, 2939, 2940, 3302, 3491, 3797, 3931, 4249, 5079, 5811b		
36.	7732-18-5	Water H_2O	50, 167, 172, 174, 194a, 211, 238, 239, 375, 403, 409, 427, 428, 445, 446, 480, 560, 568b, 603, 739b, 770, 825, 826, 846, 853, 916, 988a, 1063–1074, 1093, 1140, 1170, 1201, 1263, 1269, 1284, 1301, 1329, 1330, 1332–1334, 1346, 1354, 1375a, 1377, 1378, 1437, 1477, 1478, 1510, 1542, 1664, 1744, 1818, 1820, 1842, 1860, 1921, 1925, 1963, 1966, 2030, 2050, 2059, 2065, 2068, 2133, 2142, 2144, 2298, 2310, 2313b, 2274, 2398a, 2524, 2628, 2629, 2683, 2691–2695, 2721, 2741, 2744, 2843, 2854, 2855, 2920–2925, 2939, 3004, 3148a, 3187, 3190, 3224, 3228, 3258, 3266, 3302, 3308, 3370, 3531, 3548, 3569, 3572, 3575, 3583, 3584, 3696, 3876, 3900, 3917, 3976, 3992, 4060, 4078, 4120–4122, 4125, 4148, 4162, 4249, 4268, 5041, 5079, 5207, 5512, 5532, 5811b, 5836	69, 194a, 212, 480, 506, 541, 557, 568b, 918a, 954–956, 1053, 1115, 1164, 1206a, 1318, 1329, 1330, 1332, 1333, 1860, 1916a, 2151, 2153, 2603, 2739, 2740, 2744, 2765, 2766, 2914, 2939, 3029, 3266, 3370, 3569, 3575, 3576, 3797, 3819, 3941, 3962, 3973, 4043, 4249, 4272, 5018, 5031, 5053, 5079, 5165, 5419, 5585, 5609, 5612, 5656, 5723, 5774, 5803, 5811b, 5887	1330, 1332, 1354, 1375a, 1377, 1378, 3192, 4249

Note: The symbol (0) indicates the component was not identified in tobacco smoke studies or was not identified in the smoke from specific tobacco substitutes.

20 Metallic and Nonmetallic Elements, Isotopes, Ions, and Salts

20.1 ELEMENTS, ISOTOPES, AND IONS IN PLANTS

Plants require numerous nutrients and compounds to sustain life. There are at least 20 elements that are used by plants that are considered essential for growth and reproduction (20A06, 20A10). For higher plants (such as tobacco), a significantly higher number of other elements are needed.

Justus von Liebig (1803–1873) in the mid-nineteenth century stated that nutrients are essential for plant life:

> We have determined that a number of elements are absolutely essential to plant life. They are essential because a plant deprived of any one of these elements would cease to exist (20A58).

Von Liebig (20A58) taught of the absolute need to provide plants with essential minerals necessary for successful agricultural production. If the soil is not replenished with these essential elements and associated ions, plant yields decrease and numerous plant diseases occur. Healthy plants require and thus contain a great variety of elements, isotopes, and ions.

In general, significant efforts are normally exerted to maintain a plant's requirement for nitrogen (N), phosphorus (P), and potassium (K) through fertilization while taking for granted its basic need for carbon (C), hydrogen (H), and oxygen (O). Knowing the nutrients required to grow plants is only one aspect of successful crop production. Optimum plant yield also requires knowing the rate to apply, the method and time of application, the source of nutrients to use, and how the elements are influenced by soil and climatic conditions. The primary nutrients—N, P, and K—are commonly found in blended fertilizers, e.g., 10-10-10, or equivalent grades. Primary nutrients are utilized in the largest amounts by crops and, therefore, are applied at higher rates than secondary nutrients and micronutrients. The secondary nutrients—calcium (Ca), magnesium (Mg), and sulfur (S)—are required in smaller amounts than the primary nutrients. The major source for supplementing the soil with Ca and Mg is dolomitic lime, although these nutrients are also available from a variety of fertilizer sources. Sulfur is available in fertilizers in the form of potassium and magnesium sulfate, gypsum (calcium sulfate), and elemental sulfur. Micronutrients—iron (Fe), manganese (Mn), zinc (Zn), copper (Cu), boron (B), and molybdenum (Mo)—are required in even smaller amounts than secondary nutrients. They are available in manganese, zinc and copper sulfates, oxides, oxysulfates, and chelates, as well as in boric acid and ammonium molybdate.

Table 20.1 gives the elemental composition of a typical plant. It is interesting to note that about 96% of the makeup of a plant is C, H, and O. These elements come from carbon dioxide and water. The carbon dioxide in the atmosphere contributes the C and O found in plants. It is taken up by plants through small pores located in the leaves. Water, on the other hand, is taken up by the roots of plants and is responsible for contributing only H to the makeup of a plant. However, the H used to produce water also comes from the atmosphere. Table 20.1 also shows the classification of the elements in plants. The elements are classified as structural elements, primary and secondary nutrients, and micronutrients. Therefore, the atmosphere and sun provide about 96% of the necessary ingredients for plant growth, and minerals provide about 4% of the necessary ingredients for plant growth (20A10). The elemental composition in Table 20.1 of a typical plant is nearly identical with the elemental composition of tobacco, with the exception that tobacco generally has a slightly higher N level. Elemental analyses for C, H, and N in tobacco indicate that there is about 5% N in dry tobacco (2798, 20A06, 20A10). The percent C, H, and O (by difference) of dry tobacco leaf are about 43%, 6%, and 43%, respectively (2798, 20A06, 20A10), with the remainder being trace levels of metals and nonmetals (3973).

20.1.1 Elements, Isotopes, and Ions in Tobacco

As of 2007, the periodic table contains 117 elements whose discoveries have been confirmed. Ninety are found naturally on Earth, and the rest are synthetic elements that have been produced artificially in particle accelerators. Of these 90 naturally occurring elements, nearly 80 have been identified in tobacco. Additionally, 44 isotopes and 24 ions have been identified in tobacco. Tobacco is undoubtedly one of the most thoroughly evaluated plant materials evaluated for metal content. It should be noted that the omission of information about other microelements does not necessarily imply the absence of these elements in tobacco, but rather a lack of information (3973). The discovery of elements, isotopes, and ions in tobacco (and for that matter tobacco smoke) has only been limited by the discovery and advancement of new analytical techniques.

Over the years, numerous scientific articles, reviews, and books have been published that catalog the elements, ions, and isotopes found in tobacco. One of the earliest articles on the identification of metals in tobacco was published by Grandeau in 1862 (20A25) on the identification of rubidium

TABLE 20.1
Elemental Composition of a Typical Plant (1127b, 20A10)

Element	Symbol	Percent of Wet Weight	Percent of Dry Weight	Descriptor
Oxygen	O	81.0	45.0	Essential structural elements available from air and water
Carbon	C	6.8	44.5	
Hydrogen	H	11.5	6.0	
Nitrogen	N	0.2	1.5	
Phosphorus	P	0.03	0.2	Primary nutrients
Potassium	K	0.15	1.0	
Calcium	Ca	0.05	0.35	
Magnesium	Mg	0.03	0.20	Secondary nutrients
Sulfur	S	0.02	0.15	
Chlorine	Cl	0.015	0.10	
Iron	Fe	0.015	0.10	
Molybdenum	Mo	0.008	0.05	Micronutrients
Zinc	Zn	0.003	0.02	
Boron	B	0.003	0.02	
Copper	Cu	0.001	0.01	
Others		0.175	0.80	

(Rb) and cesium (Cs) in tobacco. Although it was well known in the 1860s that numerous metals and nonmetals existed in tobacco and higher plants (20A58), analytical techniques to isolate the small levels of metals were not established. A 1934 bibliography by Heffer and Sons (20A26) reviewed literature citations for 1921–1933 on antimony (Sb), bismuth (Bi), cadmium (Cd), chromium (Cr), cobalt (Co), Cu, lead (Pb), Mn, mercury (Hg), nickel (Ni), thallium (Tl), tin (Sn), and Zn. Johnstone and Plimmer (1971) published their review of chemical constituents of tobacco and tobacco smoke in 1959. In 1966, Tso (20A105) published an excellent historical review of elements identified in tobacco to that date. Stedman (3797), in his 1968 review, listed aluminum (Al), arsenic (As), Cu, Cr, Co, Fe, Pb, Mn, Mo, Ni, titanium (Ti), vanadium (V), and Zn as identified elements in tobacco and smoke. In 1974, Elliot (1127b) reviewed the nutritional requirements of tobacco including metals and metal ions, and Franzke et al. (1227) published their investigation of the heavy metals in tobacco. In 1977, Norman (2799a) reviewed the subject of metals in tobacco at the *Tobacco Chemists' Research Conference* (TCRC). The most recent review, in 1996, by Jones and Wilkinson (20A54), concerning historical agronomic achievements in tobacco science, provided current information on elements identified in tobacco. The most prolific writer on elements, isotopes, and ions in tobacco is Tso. From his 1966 review of the subject to his 1972 book on the physiology and biochemistry of tobacco plants (3972) and his 1990 book (3973) on the production, physiology, and biochemistry of the tobacco plant, Tso has continuously provided tobacco scientists with valuable information. His 1990 book (3973) devoted three chapters to metals, isotopes, and ions in tobacco. In Chapters 17 and 19 (3973), Tso discussed the presence, physiology, and biochemistry of the following elements in tobacco plants: Al, As, barium (Ba), beryllium (Be), Bi, B, bromine (Br), Cd, cerium (Ce), Cs, chlorine (Cl), Cr, Co, Cu, dysprosium (Dy), erbium (Er), fluorine (F), gadolinium (Gd), germanium (Ge), gold (Au), hafnium (Hf), holmium (Ho), indium (In), iodine (I), iridium (Ir), Fe, lanthanum (La), Pb, lithium (Li), Mg, Mn, Hg, Mo, neodymium (Nd), Ni, N, osmium (Os), palladium (Pd), P, platinum (Pt), polonium (Po), K, praseodymium (Pr), radium (Ra), rhenium (Re), rhodium (Rh), Rb, ruthenium (Ru), samarium (Sm), scandium (Sc), selenium (Se), silicon (Si), silver (Ag), sodium (Na), strontium (Sr), sulfur (S), tantalum (Ta), tellurium (Te), terbium (Tb), TI, thorium (Th), thulium (Tm), Sn, Ti, tungsten (W), uranium (U), V, ytterbium (Yb), Zn, and zirconium (Zr). As Tso stated (3973), "No attempt is made to include all publications about each element; in fact, some papers were eliminated intentionally to avoid duplication."

Tso (3973) estimated that tens of thousands of article have been written on the production, physiology, and biochemistry of the tobacco plant. In Chapter 18 (3973), Tso discussed radiochemical elements in tobacco and smoke, and in Chapter 19, he discussed the physiological disorders in tobacco plants associated with deficiencies in minerals and micronutrients.

Tobacco plants, like other higher plants, are autotrophs possessing the capacity to synthesize all of its complex organic materials, provided that carbon dioxide, water, minerals, and the proper physical environment are available. Their chemical composition is influenced by environmental factors such as light, temperature, moisture, soil type, and cultural practices, as well as inorganic nutrition.

The inorganic requirements of tobacco were considered in the 1962 book by Sutcliffe (20A101) and in reviews by Steinberg and Tso (20A98) and others, e.g., McMurtrey (20A66). The essential elements of tobacco may be grouped

into categories depending on their source and the relative amounts required. C, H, and O are considered structural elements and are grouped separately because they are derived from air or water. Obviously, C, H, and O are found in the vast number of the organic components identified in tobacco. Evans and Russell (20A20) described the requirements for these elements that were established when early investigators determined the basic chemical composition of tobacco matter and elucidated the essential nature of the respiratory and photosynthetic processes that occur in plants. Another group of elements referred to as primary nutrients include P, K, N, S, Ca, and Mg. These elements also make up a relatively large portion of the inorganic components of tobacco tissues and were established to be essential by plant physiologists such as Knop, Nobbe, and Sachs (20A101) prior to 1910. In this period, reagent chemicals were exceedingly crude and contained many of the essential trace elements that were being investigated. As a consequence, the proof of many trace elements in tobacco could not be established until chemists learned how to purify the analytical reagents for testing.

Another group of elements, including B, Cl, Co, Cu, Fe, Mn, Mo, and Zn, occur in exceedingly small concentrations in plant materials and are referred to as micronutrient elements. Fe was shown to be essential by Sachs (20A101) prior to 1910, but the other trace elements were demonstrated to be essential only after 1920 (20A20).

During the period 1923–1931, Sommer and Lipman (20A96) established that a variety of plants including tobacco required Zn and Cu. During the same period, Warrington (20A111) in England demonstrated that boron was a required in micronutrient in broad beans. Since then, it has become clear that these elements are needed for a variety of species, including tobacco. In 1939, Arnon and Stout (20A05) demonstrated that tomato plants required Mo and since then it has become apparent that all species need this element for metabolism (20A20).

The biochemical role of minerals in metabolic processes of various organisms has been covered in several reviews by Malstrom and Neilands (20A60), McElroy and Nason (20A65), Nason and McElroy (20A81), and Nicholas (20A84). The function of C, H, and O is obvious since they are constituents of fats, carbohydrates, and proteins. N and S are constituents of amino acids, proteins, coenzymes, and other compounds. Ca forms a complex with pectic acid and functions as a constituent of the middle lamella of cell walls. Dixon and Webb (20A13) showed that Ca also plays a role as a cofactor for certain adenosine triphosphate hydrolyzing enzymes, for phospholipases, and as a cofactor for the amylases from a variety of plants. Many elements, especially the cations, play essential roles as cofactors for the enzymes of various metabolic sequences.

Tso (3973) provided numerous examples in which mineral deficiency such as Fe or Mo resulted in metabolic lesions that have been satisfactorily interpreted on the basis of detailed knowledge of the biochemical role of metals in enzymes of important metabolic pathways. This biochemical approach to plant nutrition problems has proved exceedingly valuable to plant scientists and agricultural producers in terms of identifying diseases and finding solutions to improve crop yields. Today, an enormous amount of work is being undertaken to understand the total genome of tobacco (429b, 429c). Detailed analyses of the metabolic pathways, involved enzymes, and feedback control and gene repressor mechanisms, including the metal and nonmetal elements and ions, as essential catalysts in tobacco, are being thoroughly documented (429b, 429c).

Mineral ions participate in a wide variety of metabolic processes, electron transport mechanisms, and in nitrate reduction. By manipulation of the level of inorganic elements and ions in the nutrient medium, it is possible to influence the constituents in plants. For over 100 years, tobacco scientists have employed a fundamental research approach in attempts to understand the complex physiology and biochemistry of tobacco involved in the biosynthesis of compounds in tobacco (3973). Their efforts have greatly improved the economics of tobacco production and have led to advancements associated with health issues associated with tobacco and its various commercial uses (20A20).

Inorganic ions play a very important role in tobacco metabolism (20A20). There are various sites where inorganic ions, e.g., Ca^{+2}, Mn^{+2}, Mg^{+2}, PO_4^{-3}, Zn^{+2}, and K^{+1}, participate in glycolytic reactions. Phosphate participates in a majority of the reactions as a component of sugar-phosphate compounds. Phosphate also functions as an important component of coenzymes such as uridine diphosphate-glucose, di- and triphosphopyridine nucleotides, adenosine di- and triphosphate, etc. Practically every reaction in which phosphate is transferred requires Mg as a cofactor, but most of these enzymes are not highly specific for a divalent cation activator and will respond to other cations such as Mn (2489). Another interesting aspect of the glycolytic enzymes is that Zn is required for alcohol dehydrogenase, lactic acid dehydrogenase, aldolase, and triosephosphate dehydrogenase. The role of Zn as an important inorganic ion, as a bound component of dehydrogenases and other enzymes, has been discussed in detail by Vallee (20A110).

K ion is a cofactor for the aldolase reaction. Pyruvic kinase from all known sources also requires univalent cations, in addition to a divalent cation. This enzyme needs K, ammonium, or Rb ions as a cofactor. Mg ions serve an important function in photosynthetic processes in tobacco as it is an essential constituent of chlorophyll a and chlorophyll b. Some heavy metal and nonmetal ions are toxic to tobacco and can serve as metabolic inhibitors. The toxicity of fluoride, for example, is explained in part on the basis of the formation of a magnesium-fluorophosphate complex which inhibits the enolase reaction in glycolysis. Other enzymes are inhibited by substrate analogs, sulfhydryl complexing agents, and metal chelating agents.

Several cations function as essential cofactors for enzymes of the citric acid cycle. Magnesium is necessary for the pyruvic acid oxidase complex, and ferrous Fe is necessary for the activity of aconitase from certain sources (20A20). The isocitric dehydrogenase system which catalyzes a

dehydrogenation of isocitric acid and also the decarboxylation of oxalosuccinate to yield α-ketoglutarate requires Mn for the decarboxylation step (20A03). Mg is a necessary cofactor for the α-ketoglutarate dehydrogenase complex, and Fe is a cofactor for succinate dehydrogenase (20A19, 20A64, 20A65, 20A80, 20A84). There are numerous cofactors (Fe^{+2}, -SH compounds, Mn^{+2}, Mg^{+2}, PO_4^{-3}) and inhibitors (SCN^{-1}, Br^{-1}, I^{-1}, Cl^{-1}, Na^{+1}, Cu^{+2}, Hg^{+2}, CN^{-1}) of citric acid cycle enzymes in tobacco. It is apparent that the various enzymes not only require cations but are also inhibited by substrate analogs, substrate competitors, heavy metals, and sulfhydryl complexing agents (20A20).

Mineral ions play important roles in the electron transport portion of the terminal respiratory process in tobacco. In this process, nonheme Fe serves an important function in the electron transfer process. There is also convincing evidence that Cu ion is important in the process (20A20). Mineral ions also play an important role in the electron transport processes of the initial reactions of photosynthesis. In the photosynthetic processes of tobacco, Fe, Cu, Mn, and chloride ions are essential to the electron transfer processes (20A20).

Metal ions play an important role in nitrate reduction. The discovery and characterization of the pyridine nucleotide enzymes involved in nitrate reduction (20A18, 20A65, 20A81, 20A83) made it possible to understand the role of mineral ions in the nitrate reduction processes. Reduced pyridine nucleotides and flavin adenine dinucleotide function as cofactors in reduction of nitrate, nitrite, hyponitrate, and hydroxylamine. The first step of the reaction involves the reduction of nitrate to nitrite, and Mo is essential for this reaction. The reduction of nitrite to hyponitrite and hyponitrite to hydroxylamine requires Cu and Fe ions (20A20).

Many types of tobacco contain radioactive elements such as ^{226}Ra and ^{210}Po at concentrations ranging from 0.1 to 0.47 pCi/g (1742, 2815, 3982, 3983). Phosphate fertilizers are the major source of these radioelements (3982, 3983); minor contributions come from airborne particles carrying ^{210}Pb and ^{210}Po. These particles are trapped by the trichomes on the undersides of the tobacco leaves (2467) and were first reported by Nystrom and Bellin (2815) in 1964.

The 1999 Coresta monograph on tobacco (910a) pointed out that trace elements and metal ions can have a profound effect on tobacco quality. Fe, for example, has been implicated in the speckling effects which develop in "gray tobacco" deficiency of Virginia tobacco (2338). Aluminum is associated with development of the black color of cured tobacco or so-called black tobacco (20A57). Tso (3973) devoted an entire chapter in his 1990 book on the absolute need for trace elements in tobacco disease prevention (3973, 20A106). Although concentrations of most of these metals are not very high in tobacco (usually well below percent levels, typically in the low to middle ppm range), many of these elements are extremely important to the health of the plant. Trace levels of metals (Mn, Fe, etc.) in tobacco are important as quality factors as they can affect the combustibility and smolder rate of tobacco. Some of the metals in tobacco are desirable as quality factors while others are not (Cd, Pb, and Cr) as they have been associated with human health concerns (20A100). The type and amount of certain inorganic ions are also important factors in determining the burn and smolder properties of tobacco. Peterson and Tibbitts (20A86) found that the concentrations of K^{+1}, Cl^{-1}, SO_4^{+2}, S^{-2}, Mg^{+2}, and NO_3^{-1} in tobacco (descending order of importance) account for 80% of the variation in leaf combustibility and smolder (4332).

Tobacco is probably the most frequently examined plant in the study of microelements. Many microelements are important for normal tobacco growth and development (3973). However, the specific roles of some of these elements are still not well understood. Frequently, the presence of certain microelements is merely a result of the circumstances of site, season, or species and therefore may not bear any physiological or agronomic significance. Tobacco plants are widely distributed in various locations of the world under different climatic, soil, and culture conditions. Any report of a certain microelement regarding its level, distribution, and fertilizer and soil requirements may or may not be applicable to that particular element under different circumstances. In 1986, Isakander et al. (20A47) determined 28 elements were in American cigarette tobacco. Today, nearly 150 elements, ions, and isotopes have been identified in tobacco.

20.1.2 Elements, Isotopes, and Ions in Tobacco Smoke

In 1954, Kosak (2170) published a list of components reported to be present in tobacco smoke. His list included "inorganic components." The inorganic compounds included ammonia, carbon monoxide, carbon dioxide, hydrogen cyanide, hydrogen sulfide, thiocyanic acid (?), oxygen, arsenic (probably present as As_2O_3), "acetates" (?), "chlorides" (?), "cyanides" (?), and "nitrates" (?). The question marks in Kosak's publication indicated that he did not consider the evidence in the literature to be definitive proof of the identity of the component. Since then, a tremendous amount of research has been conducted and published on metals and ions in tobacco smoke. During the late 1950s, Cogbill and Hobbs (769) conducted pioneering work on elements found in tobacco smoke. Two reviews in 1959 by Johnstone and Plimmer (1971) and Bentley and Berry (282) documented elements found in tobacco smoke. During the late 1960s and throughout the 1970s, a tremendous amount of research was published by the Martin Brinkman Co. (2468), Celanese Fiber Marketing Co. (641), Nadkarni (2666, 20A70), Nadkarni et al. (2667, 20A71–20A79), Morie and Morrisett (2633), Jenkins (20A49), Franzke et al. (1227), John (2052), Allen and Vickroy (50), and Perinelli and Carugno (2929) on elements, isotopes, and ions in tobacco smoke. Concurrently, scientists within the tobacco industry were conducting research on metals in tobacco smoke. Much of this work was reviewed by Jenkins of Philip Morris in 1990 on the uses of nuclear radiation in tobacco and smoke research (1933).

At present, 80 metals and nonmetal elements, 24 isotopes, and 12 ions have been identified in tobacco smoke by

numerous classical and instrumental analytical techniques. It is an amazing achievement that nearly 90% of the naturally occurring elements have now been identified in tobacco and tobacco smoke. Although numerous ions in tobacco were known, research on their identity in tobacco smoke was not established until the advent of commercial application of ion chromatography (IC) in the late 1980s. Since then, many laboratories have gathered extensive experience in the application of IC for the analysis of inorganic and organic anions, in both tobacco and tobacco smoke (250, 1273, 2931, 3160, 20A59, 20A114, 20A16, 20A17, 20A85).

The presence of radioactivity, both α- and β-particles, in leaf and tobacco smoke has been reported in many publications. At earlier periods, the main concern was for β-activity found in cigars, cigarettes, and tobacco ash (113, 2657, 3367, 20A97). The α-emitting radioactive isotopes were suggested to be significant because of health concerns to smokers. The total α-activity in tobacco varies widely in green leaf, cured leaf tobacco, and tobacco smoke (2466, 3367, 3973). A very minor amount of ^{210}Po is transferred into the mainstream smoke (MSS). Twenty-three isotopes have been identified in tobacco smoke. The discovery of elements, isotopes, and ions in tobacco smoke has only been limited by the discovery and advancement of new analytical techniques.

20.2 METHODS FOR THE DETECTION AND IDENTIFICATION OF METALS, IONS, AND ISOTOPES IN TOBACCO AND TOBACCO SMOKE

Numerous analytical techniques with a variety of different methodologies have been employed for the analysis of metals, nonmetals, isotopes, and ions in tobacco and tobacco smoke and various other types of organic matter. The subject of the choice of analytical methodology best suited for the detection of elements, isotopes, and ions in different matter has been reviewed by Fassel (20A21), Bock (20A08), Jones and Case (20A53), Jenkins (1933), Ivanova et al. (20A48), Thompson et al. (20A103), Sigg et al. (20A94), and Jimoh (20A51). The analytical methods included classical microanalytical determination (wet methods), colorimetric determinations, various atomic absorption spectrophotometric techniques (such as classical atomic absorption spectroscopy [AAS]) (with single or multiple element capability), cold vapor atomic absorption (CVAA), argon-supported inductively coupled plasmas (ICP), ICP with atomization–excitation processing, graphite furnace (GF) atomic absorption spectroscopy (AAS) (with/without Zeeman background correction), GF-AAS with deuterium lamp, inductively coupled plasma atomic emission spectrometry (ICP-AES), and microwave digestion), x-ray emission, competitive ligand-exchange/stripping voltammetry (CLE-SV), diffusion gradients through thin films (DGT), instrumental neutron activation analysis (INAA), IC, and high-performance liquid chromatography (HPLC). Hyphenated techniques are also becoming popular such as inductively coupled plasma mass spectrometry (ICP-MS) and IC-ICP-MS (20A51). The selection of the appropriate method depends on several factors such as the kind of equipment available, the ease of digestion, the kind of sample, elements of interest, fume removal, contamination considerations, matrix effects, and necessary safety precautions (20A08, 0A53, 20A103).

The inorganic components of tobacco and tobacco smoke have been determined by microanalytical techniques, classical colorimetric determinations, and modern instrumental methods. For example, Cogbill and Hobbs (769) described several colorimetric methods for the determination of metals in tobacco smoke.

X-ray emission spectroscopy has been used to the determination of metals and metal isotopes in tobacco and tobacco smoke (20A62).

Atomic absorption spectroscopy is widely used and is one of the most established methods for the determination of metals in tobacco and tobacco smoke. Although quite reliable, AAS can require separate analyses and recalibrations at varying ranges for each element, with a separate lamp for each analyte (dependent on the type of AAS equipment). Concurrent determination of multiple metals is possible, while speciation is often lacking in this method. The determination of metals in tobacco smoke is often more complicated. One reason for this difficulty is the conversion of smoke samples to homogeneous solutions so that they can pass through the aspirator of the instrument. Another is that for the determination of the ultratrace quantities of metals in cigarette smoke, a preconcentration step is often required. Solvent extraction is the method of preconcentration preferred over most other methods. The choice of solvents that can provide a high degree of selectivity over a broad pH range is limited. Alternately, metal complexes that are relatively insensitive to pH changes have been used, e.g., ammonium pyrrolidinecarbodithioate, successfully for a wide variety of metals (2633) in tobacco and tobacco smoke. The work of Morie and Morrisett (2633) on the use of AAS in the determination of metals in tobacco smoke serves as an excellent example.

ICP-AES and ICP-MS techniques are modern, sophisticated, very sensitive, and generally quite expensive. These methods have been successfully used for the determination of metals in tobacco and tobacco smoke (20A90, 20A112). The success of these two methods can be affected by the metal-solvent matrix employed. In many cases, preseparation procedures and other special handling techniques are required. Each method for analysis of metals in tobacco and tobacco smoke has its own set of advantages and challenges.

INAA is an extremely sensitive method for the determination of metals and metal isotopes. INAA has been successfully used by Nadkarni et al. (20A73), Jenkins et al. (1934), and Kubota (2214) to determine numerous inorganic constituents (elements and several elemental isotopes) in both tobacco and tobacco smoke (1933). The use of INAA for tobacco and tobacco smoke analysis has been accepted worldwide (1933). Tobacco is ideally suited for INAA because of its large abundance and variety of inorganic components. Tobacco is a readily available, easy-to-handle solid, produces little gas during irradiation, and is rapidly

assayed by INAA. The literature on the use of INAA in tobacco is very large because tobacco is often used as a model in nontobacco-oriented reactor facilities system for INAA (1933). However, the applicability of neutron activation analyses (INAA) is limited by the availability and cost of the necessary equipment. INAA requires a neutron flux source and gamma-ray counting facilities. The most conventional laboratories are thus unlikely to pursue this approach. Further, some elements are normally not determinable by INAA (Pb and Ni), either because of low sensitivity or strong interferences from other metals [Perini (20A85)]. Jenkins (1933) noted that despite the widespread use INAA for tobacco and smoke analysis, meaningful intercomparison of the INAA results published in the literature is difficult as there is a lack of descriptive experimental information on the exact types of the tobaccos or tobacco smoke tested. Many laboratories studied only tobaccos and tobacco smoke native to their own country.

Many laboratories have gathered extensive experience in the application of IC for the analysis of inorganic and organic anions. Small carboxylate anions, groups IA and IIA cations, and heavy metal ions have been identified in tobacco and tobacco smoke by this method. Several of these applications have been presented as TSRC papers (250, 2931, 1273). At the 1999 TSRC, Perini (20A85) presented a method associated with IC called transition metal IC (TMIC). TMIC can be used for specific resolution and speciation of transition metal ions in tobacco and related matrices. Perini showed that TMIC could be used to detect and speciate at least 19 transition metal ions.

20.3 THE TRANSFERENCE OF ELEMENTS, ISOTOPES, AND IONS FROM TOBACCO TO TOBACCO SMOKE

Nearly all trace metals in tobacco transfer at some small level into tobacco smoke. The transfer of metals from tobacco into MSS and sidestream smoke (SSS) has been of interest for a number of years (2133, 3836–3838, 2530). Transfer of metals from filters containing metal catalysts has also been of interest as they were thought to be a source of metals entrained into the MSS (2633). For example, experimental filters with permanganate salts (20A104) and hopcalite (20A69) have been reported to remove nitrogen oxides from smoke. The percent transfer rate of metals in tobacco to tobacco smoke varies greatly but generally falls within a 0.002%–7.0% range (20A91), although percentages as high as 19% have been reported for Sb (2666).

Numerous researchers have addressed the question of metal transference employing a variety of different cigarette types, collection devices, and analytical techniques. Depending on the metal or metals of interest, the method used, and the cigarette type, the reported results cover a wide range of values. In some cases, the range covers several orders of magnitude. For one to draw any significant conclusions from this mass of data would be tenuous. Some of the inadequacies associated with diversity of transfer rate reported by Morgan and Akers (20A68) are as follows:

- Tobacco types or blends of tobaccos were often not identified, and in most cases, tobacco filler types were not processed in a standard fashion.
- Cigarette configurations were often varied, and in many cases, the cigarette configuration and materials used to construct the cigarette were not mentioned.
- Often only one or two metal species were studied for a particular tobacco.
- TPM collection procedures were not uniform among studies.
- Analytical methods varied widely and were often not calibrated against standard materials of known metal content.
- Large analytical errors were often tolerated to obtain a numerical value.

Stöber (20A99) in his review of the generation, size distribution, and composition of tobacco smoke aerosols made the observation that more than one mechanism for the transport of metals into MSS is operative. The predominant mechanism is entrainment of small particulate matter. For the more volatile elements, however, vaporization followed by condensation into the particulate phase appears dominant. The rate of metal transfer to the smoke is dependent on the volatility, the temperature profiles in the burning cigarette, and the filter type. In cigarette smoke, element concentrations vary among brands and even within the same brand. Numerous factors influence the metal concentration found in tobacco, including soil type and pH, the atmosphere, genotype, stalk position, application of metal-containing fertilizers, or agricultural chemicals, e.g., herbicides and pesticides (3973). These same factors affect the concentration of elements transferred to MSS and SSS. Table 20.2 lists the percent transfer of selected metallic and nonmetallic elements between tobacco and tobacco MSS.

20.3.1 Elements in Tobacco Smoke of Special Interest

Eighty elements, 23 isotopes, and 12 ions have been identified in tobacco smoke. Table 20.2 contains data on the percent transfer of selected elements into tobacco smoke. Based upon literature data, small portions, at most a few percent of the metals and nonmetals, transfer from the tobacco into the smoke. The predominant route of exposure of humans to metals in cigarette smoke is inhalation. The smoker will likely inhale both the mainstream vapor and particulate phase of the smoke plus some of the smoke that is generated while the cigarette is smoldering between puffs (20A50). Nonsmokers may also be exposed to metals in cigarette smoke, through passive inhalation of environmental tobacco smoke (ETS), but these concentrations are hundreds of times more dilute (3257).

TABLE 20.2
Percent Transfer of Selected Metallic and Nonmetallic Elements between Tobacco and Tobacco Smoke

CAS No.	Name (per CA Collective Index)	Transference to Smoke (%)	References
7429-90-5	Aluminum	0.009–0.0014	1934
7440-36-0	Antimony	0.003–19	769, 1934,2666, 20A21, 20A67, 20A68,
7440-38-2	Arsenic	[0.016][a]–7.0	769, 1934, 2666, 20A21, 20A68, 20A76
7440-41-7	Beryllium	0–[4.0]	3711, 20A68
7726-95-6	Bromine	0.02–2.41	769, 1933, 1934, 2666, 20A21, 20A67, 20A68
7440-43-9	Cadmium	7–22	2530, 20A68
7440-70-2	Calcium	ND–0.001	769, 1934
7440-45-1	Cerium	ND	1934
7440-46-2	Cesium	1.27	2666, 20A21
7782-50-5	Chlorine	1.2–2.2	1933, 1934
7440-47-3	Chromium	0.43–1.74	769, 2666, 1934, 20A21, 20A67, 20A68
7440-48-4	Cobalt	0.5–4.2	769, 1934, 2666, 20A21, 20A67, 20A68
7440-50-8	Copper	0.71–1.7	769, 20A68
7440-57-5	Gold	0.002	2666
7439-89-6	Iron	0.014–1.3	769, 1934, 2666, 20A21, 20A67, 20A68
7439-91-0	Lanthanum	ND–11	1934, 2666
7439-92-1	Lead	0.16–6.3	769, 2530, 20A21, 20A67, 20A68
7439-95-4	Magnesium	0.0025	20A67
7439-96-5	Manganese	0.004–0.006	769, 1934, 20A67
7440-02-0	Nickel	<0.1–2.4	1934, 2530, 2666, 20A68
7440-09-7	Potassium	0.2–0.51	769, 20A67
7440-17-7	Rubidium	0.18–0.78	1934
7440-19-9	Samarium	ND	1934
7440-20-2	Scandium	0.018–2.6	1934, 2666, 20A21
7782-49-2	Selenium	2.5–5.2	2666, 20A21, 20A68
7440-22-4	Silver	0.60–1.08	2666, 20A21
7440-23-5	Sodium	0.25–1.06	769, 1934
7440-66-6	Zinc	0.4–2.7	769, 2530, 2666, 20A21, 20A67, 20A68

[a] [] = limit of detection.
ND, not detected.

Among the metals that transfer into the smoke and are thus inhaled, the International Agency for Research on Cancer (IARC) (1870) considered As, Be, Cr, Ni, and Cd as human carcinogens (1742, 20A28, 20A29) in 1985. In 1989, the U.S. Department of Health and Human Services (4012) listed Cr and Pb as possible carcinogenic agents in humans. Additionally, Zn in tobacco smoke has also been a metal of concern (20A49, 20A50). Today, the list of metals classified as group 1 (human carcinogens) has grown to include As, Be, Cd, Cr^{+6}, Ni, ^{32}P, ^{239}Pu, ^{240}Pu, α- and β-particle-emitting radionuclides (in general), ^{222}Rn, ^{224}Ra, ^{226}Ra, ^{228}Ra, and ^{232}Th. Additionally, smokeless tobacco (classified as a group 1 mixture) and ETS and tobacco smoke and tobacco smoking (classified as group 1 exposure circumstances) have been classified by IARC as agents considered carcinogenic to humans (Table 20.3). IARC listed the following agents identified in tobacco smoke as group 2A (probably carcinogenic to humans) or group 2B (possibly carcinogenic to humans): Pb, Co, Ni, nitrates, and nitrites.

Nearly all of the metals and isotopes found in tobacco that transfer to tobacco smoke are a consequence of the use of metals found naturally in the soil (some radionuclides in the soil from nuclear reactions and reactors in the area), use of fertilizer containing metals, or agrochemicals applied to the tobacco. The radioactive compounds found in highest concentration in cigarette smoke are ^{210}Po and ^{40}K. Other radioactive compounds present include ^{226}Ra, ^{228}Ra, ^{232}Th, and ^{228}Th (1870). As and As compounds and chromium and some chromium compounds are causally associated with cancer in humans, while nickel and cadmium and their compounds are probably carcinogenic to humans. Arsenic levels in tobacco have been elevated in the past due to the use of arsenical pesticides. Cd levels may be related to the presence of Cd in phosphate fertilizers (1870). Today, the so-called Hoffmann

TABLE 20.3
IARC Classification and References to Agents, Groups of Agents, Mixtures, and Exposure Circumstances Evaluated by IARC That Are Metals, Metallic Compounds, Radioisotopes, or Tobacco or Tobacco Smoke-Related Materials

Name	CAS No.	IARC Reference
Group 1		
Agents and Groups of Agents[a]		
Arsenic	7440-38-2	20A42, 20A36
Beryllium and beryllium compounds	7440-41-7	20A27, 20A28
Cadmium and cadmium compounds	7440-43-9	20A27, 20A28
Chromium [VI]	1333-82-0	20A32
Gallium arsenide	1303-00-0	20A33
Nickel and nickel compounds	7440-02-0	20A32
Phosphorus-32, as phosphate	14596-37-3	20A41
Plutonium-239 and its decay products (may contain plutonium-240 and other isotopes), as aerosols	15117-48-3 and 14119-33-6	20A41
Radionuclides, α-particle-emitting, internally deposited	Numerous isotopes in tobacco smoke	20A41
Radionuclides, β-particle-emitting, internally deposited	Numerous isotopes in tobacco smoke	20A41
Radium-224 and its decay products	13233-32-4	20A41
Radium-226 and its decay products	13982-63-3	20A41
Radium-228 and its decay products	15262-20-1	20A41
Radon-222 and its decay products	10043-92-2 or 14859-67-7	20A37, 20A41
Silica, crystalline (inhaled in the form of quartz or cristobalite from occupational sources)	14808-60-7	20A39
Thorium-232 and its decay products	7440-29-1	20A41
Mixtures[a]		
Tobacco, smokeless		20A44, 20A36, 20A40
Exposure Circumstances[a]		
Involuntary smoking (exposure to secondhand or ETS)		20A45
Tobacco smoking and tobacco smoke		20A45
Group 2A		
Agents and Groups of Agents[a]		
Indium phosphide	22398-80-7	20A33
Lead compounds, inorganic	7439-92-1	20A35
Nitrate or nitrite (ingested) under conditions that result in endogenous nitrosation	14797-55-8 and 14797-65-0	20A34
Exposure Circumstances[a]		
Cobalt metal with tungsten carbide		20A33
Group 2B		
Agents and Groups of Agents[a]		
Antimony trioxide	1309-64-4	20A43
Carbon black	1333-86-4	20A38, 20A30
Cobalt and cobalt compounds	7440-48-4	20A31
Cobalt sulfate and other soluble cobalt(II) salts	10026-24-1	20A33
Lead	7439-92-1	20A42, 20A36
Nickel, metallic and alloys	7440-02-0	20A32
Titanium dioxide	13463-67-7	20A43, 20A30
Vanadium pentoxide	1314-62-1	20A33
Exposure Circumstances[a]		
Cobalt metal without tungsten carbide		20A33

[a] Agents, groups of agents, mixtures, and exposure circumstances (associated with metals and nonmetals, or tobacco) evaluated in IARC Monographs Volumes 1–95. This list contains all agents evaluated as of November–December 2006 that are considered carcinogenic to humans (group 1), probably carcinogenic to humans (group 2A), and possibly carcinogenic to humans (group 2B). For details of the evaluation, the relevant monograph should be consulted (see http://monographs.iarc.fr/ENG/Classification/crthgr01.php).

analytes include the following metals, isotopes, and ions: As, Be, Cd, Pb, Cr, Cr^{+6}, Co, Hg, Ni, ^{210}Po, and Se (3300).

Despite ample scientific evidence to the contrary, many in the scientific community continue to contend that many of the Hoffmann analyte represent a "clear and present danger" to smokers. The following excerpts provide information and comments to the contrary (3300).

20.3.1.1 Arsenic

Over time, substantial decreases have been reported for As residues on tobacco and dramatic reductions in tobacco smoke. As, usually considered as As_2O_3 in tobacco, was removed from tobacco agronomy in 1952. Between 1917 and 1951, the As level in tobacco rose from about 12 to 57 µg/g (1459). By 1968, the As level in tobacco had decreased from the 1951 value of more than 50 µg/g to a 1968 value of 0.5–1.0 µg/g, a value similar to that reported by Griffin et al. (1391). Some of these chronological data were summarized by the U.S. Surgeon General in 1979 (20A107) and IARC (1871). In 1957, Cogbill and Hobbs (769) reported the transfer of As from a cigarette containing 7.1 µg of As to MSS to be 3.5%. With the tobaccos analyzed for As by Griffin et al. (1391), the As content of the MSS would range from 0.018 to 0.035 µg/cig. In 1968, Guthrie (1457) reported the As transfer from cigarette tobacco to its MSS varied between 4% and 12%. In 1990, Tso (3973) noted that for most tobaccos at that time, the As level was around 0.1–0.5 µg/g (3300).

20.3.1.2 Beryllium

Studies on laboratory animals exposed to high Be dose and epidemiological data have indicated that Be may cause cancer, although Be has been classified as a group 1 substance by IARC. However, IARC noted a number of limitations in the epidemiological studies, namely, poor exposure characterization, relatively low excess cancer risk, and the lack of discussion of exposure to other lung carcinogens. The potential of Be to induce developmental effects has not been investigated adequately (20A02). No literature information was found on the toxicity of Be by ingestion (20A116). The level of Be reported in cigarette MSS ranges from 0 to 0.5 ng/cig (1742, 1744, 3711).

20.3.1.3 Chromium, Cadmium, and Lead

The possible roles of Cr, Cd, and Pb in tobacco carcinogenesis are difficult to evaluate given the present database. In 1990, Hoffmann and Hecht (1727) stated:

> Taken together, the evidence for a major role of these materials as etiologic factors in tobacco carcinogenesis is not compelling.

20.3.1.4 Chromium VI

Seventeen years have elapsed since the IARC originally evaluated the carcinogenicity of Cr and Cr compounds. In 2000, De Flora (20A12) reviewed the toxicology of Cr compounds. A wealth of results indicate that Cr metal, Cr (III), and Cr (VI) can induce a variety of genetic and related effects *in vitro* (20A12). But there is a lack of carcinogenicity of Cr metal and Cr (III) compounds in experimental animals, and only a minority of animal carcinogenicity data with Cr (VI) compounds were positive (30 out of 70, i.e., 42.9%). Moreover, most positive studies used administration routes which do not mimic any human exposure and bypass physiological defense mechanisms. Typically, positive results were only obtained at implantation sites and at the highest dose tested. Exposure to Cr (VI) has been known for more than a century to be associated with induction of cancer in humans (20A12).

De Flora stated:

> Carcinogenicity requires massive exposures, as is only encountered in well defined occupational settings, and is site specific, being specifically targeted to the lung and, in some cases, to the sinonasal cavity. Increased death rates for cancers at other sites, which were occasionally reported in some epidemiological studies, were almost invariably not statistically significant and inconsistent (being counterbalanced by other studies which apparently showed decreased rates for the same cancers) (20A12). Chromium (VI) can be reduced in body fluids and nontarget cells, which results in its detoxification, due to the poor ability of chromium (III) to cross cell membranes. In target cells, chromium (VI) tends to be metabolized by a network of mechanisms leading to generation of reduced chromium species and reactive oxygen species, which will result either in activation or in detoxification depending on the site of the intracellular reduction and its proximity to DNA. When introduced by the oral route, chromium (VI) is efficiently detoxified upon reduction by saliva and gastric juice, and sequestration by intestinal bacteria. If some chromium (VI) is absorbed by the intestine, it is massively reduced in the blood of the portal system and then in the liver. These mechanisms explain the lack of genotoxicity, carcinogenicity, and induction of other long-term health effects of chromium (VI) by the oral route. Within the respiratory tract, chromium (VI) is reduced in the epithelial-lining fluid, pulmonary alveolar macrophages, bronchial tree and peripheral lung parenchyma cells. Hence, lung cancer can only be induced when chromium (VI) doses overwhelm these defense mechanisms. The efficient uptake and reduction of chromium (VI) in red blood cells explains its lack of carcinogenicity at a distance from the portal of entry into the body. All experimental and epidemiological data, and the underlying mechanisms, point to the occurrence of thresholds in chromium (VI) carcinogenesis (20A12).

Although Cr (VI) has often been alleged to exist in MSS, it has never been unequivocally identified in tobacco smoke (20A95).

20.3.1.5 Nickel

The USPHS (20A109) made the following statement on the occurrence of Ni in tobacco smoke and stated that "It is not likely that nickel plays a significant role in the etiology of lung cancer in cigarette smokers."

During the 1960s, the Sundermans reported that they had found Ni in MSS (3837). They speculated that Ni could possible react with CO in MSS to form nickel carbonyl. The Sundermans did not successfully induce lung cancer in rats exposed to tobacco smoke, although much furor was raised as to their allegations (3837, 3838).

20.3.1.6 Cobalt

Co has been identified in both tobacco and tobacco smoke. Co and Co-containing compounds have been evaluated by IARC and are classified as group 2B (possibly carcinogenic agents) (20A31).

This category [2B] is used for agents for which there is *limited evidence of carcinogenicity* in humans and less than *sufficient evidence of carcinogenicity* in experimental animals. It may also be used when there is *inadequate evidence of carcinogenicity* in humans but there is *sufficient evidence of carcinogenicity* in experimental animals. In some instances, an agent for which there is *inadequate evidence of carcinogenicity* in humans and less than *sufficient evidence of carcinogenicity* in experimental animals together with supporting evidence from mechanistic and other relevant data may be placed in this group. An agent may be classified in this category solely on the basis of strong evidence from mechanistic and other relevant data (IARC Preamble, see http://monographs.iarc.fr/ENG/Preamble/CurrentPreamble.pdf).

20.3.1.7 Mercury

Hg has been identified in both tobacco and tobacco smoke. Hg and inorganic Hg compounds (20A27) are classified by IARC as group 3 agents (not classifiable as to carcinogenicity to humans).

This category [3] is used most commonly for agents for which the evidence of carcinogenicity is *inadequate* in humans and *inadequate* or *limited* in experimental animals. Exceptionally, agents for which the evidence of carcinogenicity is *inadequate* in humans but *sufficient* in experimental animals may be placed in this category when there is strong evidence that the mechanism of carcinogenicity in experimental animals does not operate in humans. Agents that do not fall into any other group are also placed in this category. An evaluation in group 3 is not a determination of noncarcinogenicity or overall safety. It often means that further research is needed, especially when exposures are widespread or the cancer data are consistent with differing interpretations (IARC Preamble, see http://monographs.iarc.fr/ENG/Preamble/CurrentPreamble.pdf).

20.3.1.8 Selenium

Se has been identified in both tobacco and tobacco smoke. The MSS yield of Se in the University of Kentucky reference cigarette 1R4F is 1.2 ng/cig (3300). Se and Se compounds (20A36) are classified by IARC as group 3 agents (not classifiable as to carcinogenicity to humans). Se is not an antioxidant nutrient unto itself but is a component of antioxidant enzymes. It possesses excellent antioxidant, antimutagenic, and anticarcinogenic properties (1177a, 3257, 3685, 20A92, 20A93, 20A113, 20A46, 20A102).

El-Bayoumy (20A15) described the protective role of Se on genetic damage and on cancer. Fiökin et al. (20A22) conducted research that demonstrated protective effect of vitamin E and Se against ETS exposure through reduction in the occurrence of lipid peroxidation. Clark et al. (20A09) reported that taking a Se supplement decreased the incidence of prostate cancer in men by more than 60% (20A09). The final analysis of the trial, published in 2002, by Duffield-Lillico et al. (20A14) showed a 52% reduction of prostate cancer in men taking Se daily.

Two large randomized were conducted on antioxidants, e.g., β-carotene and α-tocopherol, and Se to determine their effects on cancer risk (Chinese Cancer Prevention Study and the Selenium and Vitamin E Cancer Prevention Trial [SELECT]). The Chinese study showed that a combination of β-carotene, vitamin E, and Se significantly reduced total mortality (9%), cancer mortality (13%), gastric cancer mortality (20%), and mortality of the other cancers (19%) (20A07). The SELECT is currently taking place in the United States, Puerto Rico, and Canada to determine if taking Se and/or vitamin E supplements can prevent prostate cancer in men age 50 or older (20A82).

20.3.1.9 ^{210}Polonium

For the last quarter of a century, there has been a controversy over the presence and health effects of ^{210}Po in tobacco smoke. The quantities of ^{210}Po found in the lungs of smokers are generally about three times higher than those in nonsmokers. However, the significance of ^{210}Po in tobacco-induced lung cancer has been questioned upon comparison of these data with those obtained in miners (1509, 1727). In the case of ^{210}Po, a recent in-depth study raises doubts on the significance of ^{210}Po as a factor contributing to lung cancer in smokers (3300). ^{210}Po is present in tobacco and tobacco smoke (0.03–1.0 pCi/cig); however, it is unlikely that these traces represent a major risk for the smoker (20A109).

20.3.1.10 ^{235}Uranium and ^{238}Uranium

In addition to the 1985 Sharma et al. study (5559), Sharma had also coauthored another paper on the uraniums in tobacco products (5526). Lal and Sharma were obviously knowledgeable in uranium analyses because of their previously published numerous uranium studies on a variety of foodstuffs such as milk, coffee, and cereals (5526a) as well as the uranium contents of drinking water, river water, farm plants, and different soils.

In a 1992 book on smokeless tobacco issued in duplicate—a U.S. government department issue and a privately published issue—Brunnemann and Hoffmann (5485) and Hoffmann et al. (5513) listed the two uraniums ^{235}U and ^{238}U, as well as ^{210}Po as carcinogens in snuff.

In 1996, Rana et al. (5554a) published another study on uraniums in chewing tobacco. An abstract of their article follows:

> The sandwiched pellet technique using Makrofol-E plastic track detectors has been employed to determine trace quantities of uranium in nine brands of flavored chewing tobaccos consumed by the Indian population. In this technique the nuclear reaction, 235-U(n,f), is used for the quantitative estimation of uranium. The maximum value of uranium (1.88 ppm) has been found in raw tobacco leaves (Surti), while the minimum (0.13 ppm) in Tulsi (Double Zero brand). Other seven brands showed intermediate values of U-contents which are also reported in this paper. These values are compared with the U-contents reported in the literature for other forms of tobaccos.

More recently in 2010, British American Tobacco (BAT) described its procedures for analyzing a host of components in smokeless tobacco (5482a). The analysis for uraniums was described as follows:

> Uranium-235 & -238 are determined by alpha-spectrometry following addition of U-232 internal tracer, ashing, dissolution in acid, co-precipitation, ion-exchange chromatography, and electro-deposition onto stainless-steel discs.

Also in 2010, Schaller and Nair (5558a) listed ^{235}U, ^{238}U, ^{210}Po, TSNAs, VNAs, formaldehyde, B[*a*]P, and nicotine as health problems in snus.

In 2002, Rodgman and Green (3300) published a cancer risk assessment on toxicants in tobacco and tobacco smoke. Where there were sufficient data on carcinogenicity (animal and/or human), incremental lifetime cancer risks (ILCR) were calculated for those elements and isotopes. None of the elements (discussed previously) called "Hoffmann analytes" exhibited more than a low to very low ILCR (3300). For some of the elements, there was insufficient cancer risk information necessary to calculate an ILRC, e.g., Co, Hg, Se, and Cr. For these elements, either there were little health concerns anticipated by regulatory bodies (such as USEPA or WHO) or studies documenting cancer associated with these elements were not available. In view of these various uncertainties in published data and comments made by known authorities and regulatory bodies (as to either the level of these elements in smoke or their carcinogenic potency of the element), it is difficult at the present time to conclude that any of the metals and metal isotopes represents a significant hazard to the human smoker.

20.4 SUMMARY

To date, 85 elements (metals and nonmetals), 51 isotopes, and 24 ions have been identified in tobacco and tobacco smoke. As indicated in Table 20.4, 155 have been identified in tobacco, 122 have been identified in tobacco smoke, and 117 are found in both tobacco and tobacco smoke. Table 20.5 provides a tabulation of the metallic and nonmetallic elements, isotopes, and ions in tobacco, tobacco smoke, and tobacco substitute smoke.

There are numerous compounds in tobacco and tobacco smoke that contain metals and nonmetals. No review articles have been published on these types of compounds in tobacco and smoke. In most papers, when they are mentioned, they are collectively called *miscellaneous compounds*. The compounds listed in Table 20.6 consist mainly of acid salts of sodium, potassium, magnesium, and calcium, metal oxides, hydroxides, carbonates, and carbonyl-containing compounds, halide salts of organic compounds, a variety of organometallic compounds, e.g., triphenylarsine, aluminum and magnesium phosphide, triphenylstannium hydroxide, certain agrochemicals that contain metals, e.g., Alloxydim-sodium®, potassium salt of gibberellic acid, and Zineb®, and several metal-containing biomolecules, e.g., globulins, cytochrome c6, and chlorophyll a and b. For the sake of completeness, several ammonium compounds and the acid salts and various ions of nitric, sulfuric, and phosphoric acids are included in Table 20.6. Overall, Table 20.6 contains 195 chemical components.

TABLE 20.4
Distribution of Metallic and Nonmetallic Elements, Isotopes, and Ions between Tobacco and Tobacco Smoke

	Number of Identified Metallic and Nonmetallic Elements, Isotopes, and Ions between Tobacco and Tobacco Smoke			
Component	**Total**	**Smoke**	**Tobacco**	**Smoke and Tobacco**
Elements: 85				
Metals	73	73	72	72
Nonmetals	12	12	10	10
Isotopes: 51				
Metal isotopes	45	21	44	20
Nonmetal isotopes	6	4	5	3
Ions: 24	24	12	24	12
Totals	160	122	155	117

TABLE 20.5
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	7440-34-8	Actinium	641, 2466, 3308, 4249	2466, 4249, 5079, 5167, 20A23, 20A55	
2.	20379-10-6	Actinium, isotope of mass 226		20A23	
3.	14331-83-0	Actinium, isotope of mass 228		20A55	
4.	7429-90-5	Aluminum	50, 160, 769, 966, 1933, 1934, 2079, 2799a, 2939, 3302, 3308, 3927, 4005–4007, 4134, 4230, 4242, 4249, 5079, 5811b	769, 1933, 1934, 2079, 2338, 2913a, 3797, 3973, 3974a, 4249, 4357, 5079, 5170, 5189, 5285, 5291, 5811b, 5883, 5896, 20A57	50, 641, 4249
5.	7440-36-0	Antimony	50, 2667, 2799a, 3302, 3775, 4230, 4249, 5811b	2667, 3775, 4249, 4357, 4381, 5079, 5811b, 20A26	50, 641, 4249
6.	14683-10-4	Antimony, isotope of mass 124	20A73	20A73, 20A115	
7.	14331-88-5	Antimony, isotope of mass 129		3973, 4249, 4381	
8.	7440-37-1	Argon	172, 238, 239, 1140, 1284, 1375a, 1377, 1420, 1437, 1842, 2059, 2068, 2270, 2310, 2607, 2781, 2804, 2939, 3120, 3302, 3308, 3897, 4249, 4332, 5512		1375a, 1377, 4249
9.	7440-38-2	Arsenic	47, 50, 126a, 159, 174b, 174c, 273, 373, 516, 603, 688, 769, 889, 889a, 933, 1026, 1148, 1163, 1217, 889, 1273, 1373, 1386, 1395, 1430, 1439, 1445, 1557, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1815–1817, 1842, 1845,1870, 1871, 2060, 2079, 2170, 2172, 2313a, 2468, 2524, 2609, 2667, 2799a, 2825, 2911, 2918, 2939, 2980, 3007, 3059, 3104, 3234, 3238, 3252, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3377, 3378, 3417, 3711, 3775, 3830, 3899, 3927, 3934, 4005–4007, 4009–4011, 4229, 4230, 4242, 4249, 4319, 4331, 4354, 5061, 5079, 5124, 5160, 5201, 5264, 5512, 5541, 5811b, 5869a	46, 47, 159, 174c, 373, 516, 769, 889, 889a, 1163, 1391, 1395, 1445, 1459, 1460, 1534, 1535 1815–1817, 2079, 2172, 2338, 2468, 2609, 2667, 2939, 2978–2980, 3059, 3104, 3138, 3234, 3238, 3377, 3416, 3417, 3699, 3775, 3797, 3834, 3973, 3974a, 3974b, 4070, 4071, 4249, 4273, 4357, 4381, 5018, 5053, 5061, 5079, 5119, 5120, 5139, 5142, 5160, 5189, 5264, 5281, 5283, 5284, 5322, 5338, 5438, 5541, 5600, 5648, 5684, 5729, 5811b, 5849	50, 4249
10.	15575-20-9	Arsenic, isotope of mass 76	20A73	3973, 4249, 4357, 4381, 20A115	
11.	22541-54-4	Arsenic, arsenious state As^{+3}	5061	5061	
12.		Arsenic, arsenic state As^{+5}	5061	5061	
13.	7440-39-3	Barium	50, 273, 1445, 4229, 4230, 4249, 5811b, 5836	2079, 2338, 2939, 3797, 3973, 3974a, 4249, 5001, 5079, 5103, 5218, 5245, 5278, 5422, 5811b, 5883	50, 4249
14.	7440-41-7	Beryllium	50, 641, 1217, 1445, 1741, 1743, 1744, 3265, 3300, 3711, 4229, 4230, 4243, 4249, 5512, 5811b, 5869a	3059, 3797, 3973, 3974a, 4243, 4249, 5001, 5811b	50 641, 4249
15.	7440-69-9	Bismuth	50, 641, 2799a, 3775, 4005–4007, 4230, 4249, 5811b	3775, 3973, 5079, 5811b, 20A26	50, 641, 4249

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
16.	14331-79-4	Bismuth, isotope of mass 210	3973	20A11	
17.		Bismuth, isotope of mass 216		20A23	
18.	7440-42-8	Boron	160, 641, 4229, 4230, 4249, 5079, 5811b	193, 1127b, 2079, 2338, 2939, 3797, 3973, 3974a, 3974b, 3978, 4249, 5079, 5189, 5261, 5279, 5281, 5291, 5283–5285, 5402, 5413, 5417, 5429, 5450, 5654, 5742, 5811b, 5896	641, 4249
19.	24959-67-9	Bromide	486, 618, 641, 273, 1445, 1933, 1933b, 1934, 1939, 2524a, 3255, 4249, 5811b	15, 618, 1933, 1934, 1939, 3918, 4249, 4357, 4381, 5811b	
20.	7726-95-6	Bromine	15, 50, 2667, 2779, 4249, 5811b	2667, 2779, 2913a, 3973, 4249, 5811b	50, 4249
21.	14686-69-2	Bromine, isotope of mass 82	20A73	3973, 4249, 4381, 20A115	
22.	7440-43-9	Cadmium	50, 126, 126a, 126b, 134–136, 172, 174b, 174c, 174e, 237, 239, 344, 461, 603, 623, 641, 688, 988a, 1125, 1126, 1148, 1185, 1217, 1227, 1273, 1329, 1373, 1386, 1437, 1445, 1454, 1557, 1673, 1674, 1727, 1740, 1743, 1744, 1773, 1781, 1842, 1870, 1871, 1896, 2012, 2133, 2134a, 2142, 2214, 2357, 2530, 2792, 2799a, 2825, 2929, 2933, 2953, 3007, 3135, 3136, 3255, 3257, 3265, 3300, 3370, 3376, 3378, 3441a, 3519, 3711, 3846, 3927, 4005–4007, 4009–4011, 4220, 4229, 4230, 4249, 4384, 4410a, 5512, 5541, 5811b, 5869a	54, 134, 174c, 250, 764, 1185, 1219, 1219a, 1219b, 1219c, 1227, 1329, 1330, 1445, 1454, 1896, 2313a, 2530, 2680, 2792, 2929, 2933, 3519, 3846, 3973, 3974b, 4074, 4220, 4249, 4357, 4384, 4721, 4816, 5018, 5051, 5053, 5079, 5094, 5514, 5531, 5541, 5811b, 20A26	50, 641, 4249
23.	7440-70-2	Calcium	50, 160, 273, 769, 1099, 1100, 1445, 1933, 1934, 2079, 2270, 2799a, 2939, 3302, 3308, 4005–4007, 4229, 4230, 4242, 4249, 5079, 5811b	176, 193, 260, 385, 555, 559, 677b, 769, 791, 864, 963, 1018, 1063–1066, 1068–1074, 1127b, 1212, 1329, 1330, 1332, 1333, 1933, 1934, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2529, 2543, 2545, 2627, 2665, 2688, 2761, 2762, 2765, 2766, 2939, 3797, 3973, 3974a, 3974b, 3976–3978, 4108, 4134, 4249, 4357, 4381, 5079, 5109, 5133, 5187, 5189, 5413, 5491, 5640, 5642, 5645, 5655, 5656, 5741, 5789, 5803, 5811b. 5815, 5868, 5896	50, 641, 4249

(*continued*)

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
24.	14127-61-8	Calcium, ion (Ca^{+2})		20A20	
25.	15124-81-9	Calcium, isotope of mass 49		3973, 4357, 20A115	
26.	7440-44-0	Carbon	2939, 5811b	2939, 5079, 5189, 5192, 5193, 5811b	
27.	14762-75-5	Carbon, isotope of mass 14	4249, 4541		
28.	7440-45-1	Cerium	17, 50, 1933, 1934, 4249, 5811b	17, 1933, 1934, 3973, 4249, 5079, 5479, 5811b	50, 4249
29.	14762-78-8	Cerium, isotope of mass 144		20A23	
30.	7440-46-2	Cesium	641, 2799a, 4249, 5811b	2338, 2939, 3797, 3973, 3974a, 4249, 5079, 5422, 5811b, 20A25	641, 4249
31.	13967-70-9	Cesium, isotope of mass 134	20A73	3973, 5811b, 20A73	
32.	10045-97-3	Cesium, isotope of mass 137	20A01	1190a, 4249, 4901, 5811b	
33.	16887-00-6	Chloride	641, 1628, 1933, 1933b, 1934, 1939, 2170, 2524a, 2931, 3255, 4249, 5079, 5811b	193, 256, 385, 486, 677b, 963, 1063–1066, 1068–1074, 1189, 1333, 1373, 1895, 1933, 1934, 1939, 2079, 2154, 2283, 2313a, 2338, 2356, 2529, 2543, 2545, 2627, 2761, 2762, 2765, 2766, 2847, 3160, 3797, 3976, 4249, 4261, 4262, 4357, 5053, 5079, 5113, 5126, 5189, 5195, 5252, 5277, 5293, 5302, 5337, 5448, 5642, 5811b	641, 4249
34.	7782-50-5	Chlorine	50, 1240, 2779, 3797, 4249, 5811b	1127b, 1240, 2779, 3973, 3974a, 3974b, 4108, 4512, 5654, 5688, 5811b	50, 4249
35.	14158-34-0	Chlorine, isotope of mass 38		3973, 4381, 20A115	
36.	7440-47-3	Chromium	50, 126a, 174b, 174c, 273, 603, 688, 746b, 769, 966, 1148, 1217, 1273, 1329, 1373, 1386, 1445, 1557, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 2214, 2270, 2667, 2799a, 2825, 2939, 3007, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3377, 3378, 3711, 3876, 4005–4007, 4230, 4242, 4249, 4331, 5512, 5541, 5811b, 5869a	174c, 769, 1219, 1219a, 1219b, 1329, 1330, 1445, 1951, 2079, 2270, 2313a, 2338, 2667, 2939, 3377, 3797, 3973, 3974a, 3974b, 4249, 4381, 4816, 5018, 5053, 5079, 5094, 5514, 5541, 5811b, 20A26	50, 641, 4249
37.	16055-83-1	Chromium ion (3+)	5811a		
38.	18540-29-9	Chromium ion (6+)	5811a		

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
39.	14392-02-0	Chromium, isotope of mass 51	20A73	3973, 4249, 4381, 20A115	
40.	7440-48-4	Cobalt	50, 273, 1445, 1673, 1741, 1743, 1744, 1870, 1871, 1933, 1934, 2667, 2792, 2799a, 3265, 3300, 3302, 3377, 3714, 3785, 3786, 4005–4007, 4229, 4230, 4249, 5512, 5541, 5811b, 5869a	1933, 1934, 2667, 2792, 3377, 3785, 3786, 3797, 3973, 3974a, 3974b, 4249, 4357, 4381, 5079, 5308, 5309, 5541, 5811b, 5883, 20A26	50, 4249
41.	10198-40-0	Cobalt, isotope of mass 60	20A73	4249, 4357, 4381, 20A115	
42.	7440-50-8	Copper	50, 160, 273, 769, 966, 1227, 1329, 1445, 2079, 2214, 2270, 2460, 2524a, 2630, 2633, 2792, 2799a, 2939, 3302, 3308, 3876, 4134, 4005–4007, 4229, 4230, 4242, 4249, 4319, 5079, 5811b, 5869a	193, 250, 769, 1127b, 1219, 1227, 1445, 2079, 2270, 2338, 2460, 2792, 2939, 3633, 3797, 3973, 3974a, 3974b, 4249, 4357, 5079, 5094, 5137, 5189, 5261, 5270, 5285, 5417, 5514, 5811b, 5896, 20A26	50, 641, 4249
43.		Copper, ion (Cu^{+2})		20A20	
44.	7429-91-6	Dysprosium	641, 4249	3973, 5811b	641, 4249
45.	7440-52-0	Erbium	641, 4249	3973	641, 4249
46.	7440-53-1	Europium	641, 4230, 4249, 5811b	2462, 2666, 4249, 5811b	641, 4249
47.	378750-46-0	Europium, isotope of mass 152	20A73	20A73	
48.	16984-48-8	Fluoride	641, 3302, 4249	4092, 4249, 4629, 4807, 4951, 5811b, 20A24	641, 4249
49.	7782-41-4	Fluorine	50, 3797, 4249, 5079, 5410, 5811b	3973, 3974a, 4249, 4692, 5811b	50. 4249
50.	7440-54-2	Gadolinium	50, 641, 4249, 5811b	412, 3973, 4249, 5811b	641, 4249
51.	7440-55-3	Gallium	50, 641, 4249, 5811b	412, 3973, 4249, 5811b	50, 641, 4249
52.	7440-56-4	Germanium	50, 641, 4249, 5811b	3973, 4249, 4871, 5811b	50, 641, 4249
53.	7440-57-5	Gold	641, 2667, 2799a, 4005–4007, 4249, 5811b	2462, 2667, 3973, 4249, 5811b	641, 4249
54.	7440-58-6	Hafnium	641, 4249, 5811b	16, 17, 1452, 3973, 4249, 5811b	641, 4249
55.	7440-60-0	Holmium	641, 4249	3973, 5811b	641, 4249
56.	1333-74-0	Hydrogen	168, 172, 237, 239, 480, 722, 1140, 1263, 1373, 1420, 1437, 1485, 1664, 1668, 1674, 1842, 2059, 2060, 2066, 2068, 2252, 2270, 2310, 2662, 2782, 2804, 2866, 2878, 2939, 3121, 3302, 3308, 3880, 3882, 3883, 4151, 4249, 4332, 5079, 5512, 5811b		641, 3192, 4249

(*continued*)

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
57.	7440-74-6	Indium	641, 4249	3973, 4249, 4893, 5811b	641, 4249
58.	20461-54-5	Iodide		486	
59.	7553-56-2	Iodine	50, 641, 4249, 5811b	3797, 3973, 3974a, 4249, 4273, 5079, 5281, 5283, 5284, 5373, 5811b	50, 641, 4249
60.	7439-88-5	Iridium	641, 4249, 5811b	3973, 5811b	641, 4249
61.	7439-89-6	Iron	50, 160, 273, 769, 968, 1445, 1933, 1934, 2079, 2270, 2633, 2667, 2799a, 3302, 3377, 3785, 3786, 3876, 4005–4007, 4229, 4230, 4242, 4249, 4319, 5079, 5552, 5811b	193, 250, 769, 1127b, 1445, 1933, 1934, 2079, 2270, 2283, 2338, 2529, 2667, 2939, 3377, 3785, 3786, 3797, 3973, 3974a, 3974b, 4249, 4381, 5079, 5132, 5137, 5153, 5176, 5189, 5262, 5282, 5285, 5412, 5666, 5811b, 5883, 5896	50, 641, 4249
62.	15438-31-0	Iron, ferrous ion (Fe^{+2})	5076	20A20	
63.		Iron, ferric ion (Fe^{+3})	5076		
64.	14596-12-4	Iron, isotope of mass 59	20A73	3973, 4249, 4381	
65.	7439-91-0	Lanthanum	641, 1933, 1934, 2667, 2799a, 4005–4007, 4249, 5811b	1933, 1934, 2667, 3973, 4249, 4381, 5811b	641, 4249
66.	13981-28-7	Lanthanum, isotope of mass 140	20A73	3973, 4249, 4381, 20A115	
67.	7439-92-1	Lead	50, 160, 174b, 174c, 174e, 273, 603, 623, 688, 769, 1217, 1227, 1273, 1329, 1386, 1445, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 1896, 2079, 2214, 2270, 2354, 2460, 2466, 2792, 2799a, 2825, 2901, 2929, 2939, 3007, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3376, 3442, 3714, 3846, 4005–4007, 4134, 4220, 4229, 4230, 4242, 4249, 4319, 4410a, 5079, 5512, 5541, 5811b, 5869a	174c, 250, 769, 1219, 1227, 1445, 1896, 2079, 2270, 2313a, 2338, 2460, 2792, 2929, 3138, 3442, 3797, 3846, 3973, 3974a, 3974b, 4046, 4220, 4249, 4357, 4816, 5018, 5053, 5079, 5094, 5514, 5541, 5811b, 5883	50, 641, 4249
68.	14255-04-0	Lead, isotope of mass 210	1823, 1842, 4249, 5811b	1180, 3969, 3983, 5811b, 20A11, 20A115	
69.	15092-94-1	Lead, isotope of mass 212		20A55	
70.	15067-28-4	Lead, isotope of mass 214		20A23	
71.		Lead, isotope of mass 218		20A23	
72.	7439-93-2	Lithium	50, 2079, 4229, 4230, 4249, 5811b	2079, 2338, 2939, 3797, 3973, 3974a, 4249, 5079, 5189, 5218, 5281, 5283, 5284, 5347, 5422, 5479, 5811b, 5883	50, 4249

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
73.	17341-24-1	Lithium, ion (Li^{+1})		20A20	
74.	7439-94-3	Lutecium	641, 4249, 5811b	3973, 5811b	641, 4249
75.	7439-95-4	Magnesium	50, 160, 769, 966, 1092, 1445, 1933, 1934, 2079, 2627, 2799a, 2939, 3302, 3377, 3548, 3876, 4005–4007, 4229, 4230, 4249, 5079, 5811b	193, 260, 385, 559, 769, 1063–1066, 1068–1074, 1127b, 1329, 1330, 1332, 1333, 1445, 1933, 1934, 2079, 2154, 2283, 2338, 2356, 2529, 2543, 2545, 2665, 2761, 2762, 2765, 2766, 2939, 3797, 3973, 3974a, 3974b, 3976, 3977, 4108, 4249, 4357, 5079, 5097, 5098, 5113, 5133, 5189, 5195, 5196, 5413, 5448, 5578, 5640, 5645, 5654–5656, 5811b, 5815, 5896	50, 641, 4249
76.	22537-22-0	Magnesium, ion (Mg^{+2})		20A20	
77.	7439-96-5	Manganese	50, 160, 273, 344, 769, 966, 1445, 1933, 1933b, 1934, 2079, 2270, 2393, 2524a, 2633, 2799a, 2939, 3302, 3308, 4005–4007, 4134, 4229, 4230, 4242, 4249, 4319, 5079, 5811b, 5869a	193, 250, 769, 1127b, 1333, 1933, 1934, 2079, 2270, 2283, 2338, 2489, 2529, 2939, 3797, 3973, 3974a, 3974b, 4249, 4357, 5079, 5137, 5189, 5268, 5285, 5448, 5514, 5654, 5666, 5811b, 5896, 20A02, 20A26	50, 641, 4249
78.	14681-52-8	Manganese, isotope of mass 56		3973, 4249, 4381, 20A115	
79.	16397-91-4	Manganese, ion (Mn^{+2})		20A20	
80.	7439-97-6	Mercury	50, 174b, 174c, 344, 623, 641, 672, 688, 1329, 1386, 1741, 2214, 2517b, 2799a, 3005, 3006, 3007, 3300, 4005–4007, 4249, 5054, 5811b, 5869a	174c, 1219, 2667, 3797, 3973, 3974a, 3974b, 4249, 4357, 4381, 5018, 5079, 5094, 5241, 5811b, 20A26	50, 641, 4249
81.	13982-78-0	Mercury, isotope of mass 203		3973, 4249, 4381, 20A115	
82.	7439-98-7	Molybdenum	50, 641, 4230, 4249, 5811b	193, 1127b, 3797, 3973, 3974a, 3974b, 4249, 4357, 5079, 5102, 5137, 5251, 5514, 5811b	50, 641, 4249
83.	16065-87-5	Molybdenum, ion (Mo^{+6})		20A20	
84.	7440-00-8	Neodymium	641, 4249	3797, 3973, 4249, 5811b	641, 4249

(*continued*)

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
85.	7440-02-0	Nickel	50, 126, 126a, 126b, 160, 172, 174b, 174c, 237, 239, 273, 344, 603, 623, 641, 688, 769, 918, 966, 1125, 1217, 1262, 1273, 1329, 1386, 1437, 1445, 1454, 1515, 1557, 1673, 1674, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 2133, 2134a, 2142, 2214, 2270, 2460, 2468, 2530, 2792, 2799a, 2825, 2886, 2929, 2939, 3007, 3255, 3257, 3265, 3300, 3308, 3370, 3378, 3711, 3714, 3775, 3785, 3786, 3837, 3838, 3846, 4005–4007, 4009–4011, 4220, 4229, 4230, 4246, 4249, 4319, 5079, 5512, 5541, 5629, 5811b, 5869a	174c, 250, 769, 918, 1125, 1219, 1445, 2270, 2313a, 2338, 2460, 2468, 2530, 2792, 2929, 2939, 3775, 3785, 3786, 3797, 3846, 3973, 3974a, 3974b, 4220, 4249, 5018, 5053, 5079, 5094, 5232, 5308, 5379, 5514, 5541, 5811b, 5883, 20A26	50, 641, 4249
86.	14833-49-9	Nickel, isotope with mass 65		5811b	
87.	7440-03-1	Niobium	50, 641, 4249, 5811b	412, 4249, 5811b	50, 641, 4249
88.	14797-55-8	Nitrate	1628, 2170, 2524, 2681a, 2931, 3257, 4249, 5079, 5811b	28, 29, 174b, 274, 379, 385, 468, 480, 486, 499, 504, 548–550, 553, 557, 670, 783, 826a, 933, 1003, 1007, 1010, 1014, 1051, 1063–1066, 1068–1074, 1122, 1123, 1175b, 1189, 1191, 1193, 1196–1200, 1222, 1329, 1330, 1332, 1333, 1385, 1388–1390, 1500, 1501, 1514, 1525, 1545, 1552, 1575, 1577, 1579, 1712, 1797, 1915, 1952, 1964, 2016, 2051, 2090a, 2118, 2283, 2313a, 2330, 2337, 2338, 2356, 2394a, 2395, 2484a, 2543, 2545, 2557a, 2635, 2646, 2738, 2761, 2762, 2765, 2766, 2801, 2914, 2917b, 2919, 2931, 2932, 3081, 3082, 3085, 3125, 3160, 3254, 3399, 3482, 3493, 3499, 3589, 3594, 3671, 3672, 3697, 3707, 3774, 3816, 3952, 3973, 3976, 3984, 3993, 4128, 4129, 4236, 4249, 4261, 4262, 5001, 5018, 5053, 5079, 5126, 5189, 5625, 5669, 5803, 5811b, 5824	

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
89.	14797-65-0	Nitrite	1628, 2681a, 2931, 4249, 5811b	379, 385, 486, 548–550, 553, 556, 557, 670, 933, 1005, 1007, 1014, 1051, 1175b, 1385, 1578, 1579, 1580, 1712, 2050, 2154a, 2313a, 2917b, 2931, 2932, 3125, 3774, 3973, 4128, 4129, 4236, 4249, 5001, 5053, 5811b	
90.	7727-37-9	Nitrogen	167, 172, 237, 239, 421, 621, 1140, 1284, 1373, 1375a, 1377, 1420, 1437, 1668, 1842, 1924, 1963a, 2059, 2060, 2066, 2068, 2079, 2133, 2142, 2270, 2310, 2607, 2634, 2724, 2780, 2781, 2782, 2804, 2939, 3120, 3121, 3132, 3302, 3308, 3491, 3564, 3973, 4249, 4332, 5079, 5512, 5811b	193, 260, 559, 1127b, 2665, 2688, 2724, 3974b, 3491, 4249, 5079, 5189, 5192, 5193, 5597, 5622, 5625, 5434, 5654, 5666, 5715, 5803, 5843	1375a, 1377, 1378, 3192, 4249
91.	7440-04-2	Osmium	641, 4249, 5811b	3973, 5811b	641, 4249
92.	7782-44-7	Oxygen	168, 172, 237, 239, 411, 421, 480, 621, 1140, 1284, 1306, 1373, 1375a, 1377, 1420, 1437, 1664, 1668, 1842, 1924, 1969, 2059, 2060, 2066, 2068, 2079, 2133, 2170, 2252, 2310, 2607, 2634, 2736, 2780, 2781, 2782, 2804, 2939, 3120, 3121, 3132, 3302, 3308, 3516, 3880, 3882, 3883, 4249, 4332, 5042, 5079, 5512, 5811b	1206a, 2607, 5079, 5811b	1375a, 1377, 4249
93.	7440-05-3	Palladium	641, 4249	3973	641, 4249
94.	14265-44-2	Phosphate	2627, 4249	1063–1066, 1068–1074, 1189, 1329, 1330, 1332, 1333, 2154, 2313a, 2338, 2395, 2543, 2545, 2761, 2762, 2765, 2766, 4249, 5053, 5079, 5126, 5640, 5811b	
95.	14066-20-7	Phosphate, dihydrogen		3973, 4249, 5811b	
96.		Phosphate, monohydrogen		3160, 4249	
97.	7723-14-0	Phosphorus	50, 412, 4229, 4230, 4249, 5811b	193, 260, 385, 559, 1127b, 2079, 2283, 2338, 2529, 2665, 2939, 3973, 3974b, 4249, 4957, 5079, 5113, 5133, 5189, 5413, 5448, 5666, 5738, 5811b, 5896	50, 4249
98.	14596-37-3	Phosphorus, isotope of mass 32		3973, 4249, 4957	

(*continued*)

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
99.	7440-06-4	Platinum	50, 4249, 5811b	2701, 3973, 5811b	
100.	13981-16-3	Plutonium, isotope of mass 238		2701, 3973, 4249	
101.	15117-48-3	Plutonium, isotope of mass 239	2663b	2663b, 2701, 3973, 4249	
102.	14119-33-6	Plutonium, isotope of mass 240	2663b, 4249	2663b, 3973, 4249	
103.	7440-08-6	Polonium	126, 237, 1148, 1217, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1870, 2468, 3071, 3265, 3300, 4005, 4249, 4332, 5512, 5811b	3973, 4249, 5811b	
104.	13981-52-7	Polonium, isotope of mass 210 ^{210}Po	126, 126a, 126b, 237, 264, 374, 1130, 1148, 1160, 1177, 1179, 1180, 1445, 1509, 1557, 1571a, 1674, 1722, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1823, 1842, 1864, 1870, 1871, 2069, 2158, 2396, 2468, 2536, 2663b, 2799a, 2813–2815, 2998, 3002, 3066–3070, 3255, 3257, 3265, 3300, 3302, 3308, 3408, 3442, 3680, 3981–3983, 4002, 4005, 4044, 4010, 4011, 4249, 4319, 4332, 4342, 5512, 5811b, 5869a	264, 265, 374, 1130, 1160, 1179, 1180, 1387, 1509, 2158, 2468, 2536, 2663b, 2815, 3002, 3005, 3066–3070, 3442, 3797, 3969, 3973, 3974a, 3974b, 3981–3983, 4044, 4249, 4383, 4810b, 5053, 5066, 5617, 5683, 5733, 5811b, 20A115	641, 4249
105.	7440-09-7	Potassium	50, 113, 160, 273, 294, 641, 769, 1445, 1628, 1933, 1934, 2079, 2270, 2543, 2627, 2657, 2679, 2761, 2762, 2799a, 2939, 3059, 3302, 3308, 3367, 3876, 4005–4007, 4134, 4229, 4230, 4242, 4249, 5079, 5811b	193, 256, 385, 555, 559, 677a, 769, 864, 963, 1017, 1063–1066, 1068–1074, 1127b, 1329, 1330, 1332, 1333, 1521, 1933, 1934, 2079, 2270, 2283, 2338, 2356, 2395, 2529, 2543, 2545, 2665, 2688, 2761, 2762, 2765, 2766, 2846, 2939, 3005, 3059, 3367, 3797, 3973, 3974a, 3974b, 3976, 3977, 4108, 4242, 4249, 4273, 4357, 4364, 4366, 5079, 5088, 5113, 5133, 5189, 5195, 5413, 5622, 5638, 5642, 5811b, 5896	50, 4249
106.	13966-00-2	Potassium, isotope of mass 40	113, 1842, 2657, 3302, 3367, 3442, 4002, 4005, 4249, 4319, 4332	2462, 3006, 3367, 3442, 4249, 5811b	
107.	14378-21-3	Potassium, isotope of mass 42		20A61	
108.	24203-36-9	Potassium, ion (K^+)	2681a, 5811b	20A63	
109.	7440-10-0	Praseodymium	50, 3973, 4249	3973, 5811b	
110.	7440-14-4 13982-63-3	Radium, isotope of mass 226	1842, 2083, 3302, 3989, 4005, 4249, 4319, 4332	682, 3005, 3797, 3974a, 3981, 3982, 4249, 5066, 5079, 5167, 5800, 5811b	641, 4249

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
111.	15262-20-1	Radium, isotope of mass 228		5079	
112.	10043-92-2	Radon		5079, 5167, 5811b, 20A11	
113.	14859-67-7	Radon, isotope of mass 222	2466, 3302, 3308, 3989, 4005, 4249, 4319, 4332	5079, 20A11	
114.	7440-15-5	Rhenium	641, 4249, 5811b	3973, 5811b	641, 4249
115.	7440-16-6	Rhodium	641, 4249, 5811b	3973, 5811b	641, 4249
116.	7440-17-7	Rubidium	17, 50, 1933, 1934, 4249, 5811b	1933, 1934, 2338, 2939, 3797, 3973, 3974a, 4249, 5079, 5479, 5811b, 20A25	50, 641, 4249
117.	22537-38-8	Rubidium, ion (Rb^+)		20A20	
118.	7440-18-8	Ruthenium	641, 4249, 5811b	2338, 3973, 5811b	641, 4249
119.	7440-19-9	Samarium	641, 1933, 1934, 4249, 5811b	1933, 1934, 2462, 3973, 4249, 5811b	641, 4249
120.	7440-20-2	Scandium	50, 641, 1933, 1934, 2667, 2799a, 4005–4007, 4249, 5811b	1933, 1934, 2667, 3973, 4249, 4381, 5811b	50, 641, 4249
121.	13967-63-0	Scandium, isotope of mass 46	20A73	3973, 4249, 4381	
122.	14391-97-0	Scandium, isotope of mass 49		20A115	
123.	7782-49-2	Selenium	50, 174b, 174c, 273, 641, 688,724, 1273, 1386, 1445, 1455, 1456, 1842, 2468, 2667, 2799a, 3007, 3257, 3265, 3300, 3685, 3775, 4005–4007, 4230, 4249, 5541, 5811b, 5869a	174c, 374, 721, 724, 1445, 1455, 1456, 2468, 2667, 3707, 3775, 3797, 3895, 3973, 3974a, 4249, 5018, 5053, 5079, 5094, 5274, 5541, 5811b	50, 641, 4249
124.	14265-71-5	Selenium, isotope of mass 75	20A73	20A73	
125.	7440-21-3	Silicon	50, 160, 641, 769, 966, 2079, 2270, 2799a, 2939, 3308, 3876, 4134, 4230, 4242, 4249, 5079, 5811b	385, 769, 2079, 2270, 2338, 2639, 2939, 3059, 3797, 3973, 3974a, 4249, 5079, 5113, 5269, 5811b	50, 641, 4249
126.	7440-22-4	Silver	50, 641, 2667, 2799a, 4005–4007, 4230, 4249, 5811b	951, 2667, 3797, 3973, 3974a, 4249, 5079, 5811b	50, 641, 4249
127.	14391-76-5	Silver, isotope of mass 110	20A73	20A73	
128.	7440-23-5	Sodium	50, 160, 641, 769, 966, 1628, 1933, 1933b, 1934, 2079, 2270, 2524a, 2799a, 2939, 3059, 3302, 3308, 3876, 4005–4007, 4134, 4229, 4230, 4242, 4249, 5079, 5811b	769, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1933, 1934, 2079, 2270, 2338, 2356, 2462, 3059, 3797, 3973, 3974a, 3974b, 4249, 4273, 4357, 5079, 5113, 5181, 5185, 5189, 5479, 5811b, 5896	50, 641, 4249
129.	17341-25-2	Sodium, ion (Na^{1+})	1556a, 2681a, 5811b	20A63	
130.	16759-28-7	Sodium, isotope of mass 24		20A61	

(*continued*)

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
131.	7440-24-6	Strontium	50, 160, 641, 769, 2079, 2799a, 2939, 3302, 4229, 4230, 4249, 5079, 5811b	769, 2079, 2338, 2939, 3005, 3797, 3973, 3974a, 4249, 5079, 5218, 5424, 5811b, 5883	50, 641, 4249
132.	14158-27-1	Strontium, isotope of mass 89		444, 3973, 4249	
133.	10098-97-2	Strontium, isotope of mass 90		444, 1190a, 3006, 4249	
134.	14808-79-8	Sulfate	1445, 2931, 4249, 5811b	385, 1545, 1895, 2154, 2338, 2356, 2543, 2545, 2627, 2761, 2762, 2765, 2766, 3160, 4249, 5053, 5079, 5189, 5195, 5670, 5715, 5811b	
135.	18496-25-8	Sulfide	2621, 2627, 4249, 5811b	4248, 20A89	
136.	14265-45-3	Sulfite	4249, 20A88	1243a, 4249	
137.	7704-34-9	Sulfur	50, 641, 1240, 1933b, 2270, 2524a, 3302, 4229, 4230, 4249, 5811b	116, 193, 1127b, 1240, 2079, 2270, 2283, 2338, 2393, 3476, 3633, 3797, 3973, 3974b, 4249, 5079, 5113, 5189, 5220, 5282, 5378, 5448, 5670, 5715, 5811b	50, 641, 4249
138.	7440-25-7	Tantalum	641, 4249, 5811b	3973, 5811b	641, 4249
139.	13494-80-9	Tellurium	50, 2799a, 3775, 4005–4007, 4230, 4249	3775, 3973, 4249	50, 4249
140.	7440-27-9	Terbium	17, 5811b	16, 3973, 4249, 5811b	
141.	7440-28-0	Thallium	50, 641, 2466, 3302, 3308, 4249, 5811b	1278, 3797, 3973, 3974a, 3974b, 4249, 5079, 5280, 5377, 5428, 5811b, 20A26	50, 641, 4249
142.	302-04-5	Thiocyanate	1445, 4249	20A56	
143.	14274-82-9	Thorium, isotope of mass 228	20A01, 20A87	16, 3873, 4249, 4836, 5066, 5811b, 20A55, 20A87	
144.	14269-63-7	Thorium, isotope of mass 230		5066	
145.	7440-29-1	Thorium, isotope of mass 232	50, 641, 2468, 4249, 5811b	16, 17, 2468, 3973, 4249, 5066, 5811b	50, 641, 4249
146.	7440-30-4	Thulium	641, 2799a, 4249	3973, 5811b	641, 4249
147.	7440-31-5 7740-31-5	Tin	50, 641, 4230, 4249, 5811b	3797, 3973, 3974a, 4249, 5079, 5448, 5811b, 20A26	50, 641, 4249
148.	7440-32-6	Titanium	50, 160, 273, 641, 769, 966, 1445, 2079, 2270, 2338, 2799a, 2939, 3302, 3876, 4230, 4242, 4249, 4319, 5079, 5811b	769, 2079, 2270, 2338, 2939, 3797, 3973, 3974a, 4249, 5079, 5218, 5422, 5448, 5811b, 5883	50, 641, 4249
149.	7440-33-7	Tungsten	641, 4249, 5811b	3973, 5811b	641, 4249
150.	13966-29-5	Uranium, isotope of mass 234		3973, 5066, 5811b	

TABLE 20.5 (continued)
Metallic and Nonmetallic Elements and Ions in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
151.	15117-96-1	Uranium, isotope of mass 235		5066, 5482a, 5485, 5513, 5526, 5554a, 5558a, 5559	
152.	7440-61-1	Uranium, isotope of mass 238	50, 641, 4249, 5811b	3797, 3973, 3974a, 4249, 5066, 5079, 5167, 5168, 5482a, 5485, 5513, 5526, 5554a, 5558a, 5559, 5811b	50, 641, 4249
153.	7440-62-2	Vanadium	50, 273, 641, 1445, 4230, 4249, 5541, 5811b	3797, 3973, 3974a, 4249, 5079, 5448, 5541, 5811b, 5883	50, 641, 4249
154.	7440-64-4	Ytterbium	641, 4230, 4249, 5811b	16, 3973, 4249, 4804, 5811b	641, 4249
155.	7440-65-5	Yttrium	50, 641, 4230, 4249	3005, 3973, 4249, 5811b	50, 641, 4249
156.	10098-91-6	Yttrium, isotope of mass 90		3006	
157.	7440-66-6	Zinc	50, 126b, 172, 237, 273, 623, 641, 769, 1329, 1445, 1674, 2079, 2133, 2134a, 2142, 2214, 2460, 2633, 2667, 2799a, 2929, 2939, 3255, 3302, 3376, 3377, 4005–4007, 4229, 4230, 4249, 4319, 5811b	193, 250, 769, 1127b, 1219, 1445, 2079, 2338, 2460, 2667, 2929, 2939, 3377, 3797, 3973, 3974a, 3974b, 4074, 4249, 4357, 4381, 5079, 5094, 5189, 5285, 5308, 5402, 5448, 5514, 5654, 5811b, 5883, 20A26	50, 641, 4249
158.	23713-49-7	Zinc, ion (Zn^{2+})		20A20	
159.	13982-39-3	Zinc, isotope of mass 65	20A73	20A73	
160.	7440-67-7	Zirconium	50, 641, 4230, 4249, 5811b	1735, 3973, 4249, 5811b	50, 641, 4249

TABLE 20.6
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

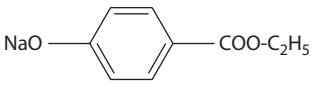
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	71-50-1	Acetate	1628, 2170, 2931, 3324, 5079, 5359, 5811	5811, 5811b	
2.	5743-26-0	Acetic acid, calcium salt, monohydrate		5811, 5811b	
3.	1932-50-9	Acetic acid, hydroxy-, potassium salt		5811b	
4.	142-72-3	Acetic acid, magnesium salt		5811, 5811b	
5.	373-02-4	Acetic acid, nickel salt		5811b	
6.	127-08-2	Acetic acid, potassium salt CH_3-COO-K		1271a, 4249, 4680, 5811b	
7.	127-09-3	Acetic acid, sodium salt CH_3-COO-Na	5811b	1053, 3266, 3464, 3498, 4249	
8.	1344-28-1	Aluminum oxide Al_2O_3		3973, 4249	
9.	1335-30-4	Aluminum silicate $Al_2(SiO_3)_3$	4249, 4508	2262, 4249	
10.	14798-03-9	Ammonium	1445, 1628, 5811b	1369, 3261, 5811b	
11.	12125-02-9	Ammonium chloride	5013		
12.	1336-21-6	Ammonium hydroxide		172a, 1053, 3266	
13.	12135-76-1	Ammonium sulfide		1053, 3266	
14.	7778-44-1	Arsenic acid, calcium salt		3633, 4249, 4271a, 4554	
15.	7645-25-2	Arsenic acid, lead salt $[Pb_3(AsO_4)_2]$		3633, 4241a, 4249, 4554	
16.	7784-40-9	Arsenic acid, lead salt $[PbH(AsO_4)]$		20A42	
17.	1327-53-3	Arsenic oxide (As_2O_3) {arsenious oxide}	46, 47, 373, 769, 889, 889a, 1163, 1395, 1430, 1816, 1817, 1845, 2170, 2172, 2524, 2609, 2646, 3104, 3417, 3899, 4242, 4249, 4319, 4354, 5079, 5124, 5160, 5201, 5811b	46, 47, 373, 769, 889, 889a, 1163, 1395, 2609, 2978, 3104, 3416, 3417, 3704, 3973, 4070, 4249, 5079, 5120, 5142, 5160, 5189, 5281, 5283, 5284, 5338, 5811b	
18.	7784-42-1	Arsine H_3As	1781		
19.	603-32-7	Arsine, triphenyl- $As(C_6H_5)_3$	3843		
20.	140-56-7	Benzenediazosulfonate, dimethylamino-, sodium salt {Fenaminosulf®}		3633	
21.	532-32-1	Benzoic acid, sodium salt		174b, 1053, 3266	
22.	35285-68-9	Benzoic acid, 4-hydroxy-, ethyl ester, sodium salt 		174b, 3266, 4249	
23.	5026-62-0	Benzoic acid, 4-hydroxy-, methyl ester, sodium salt		174b, 3266, 4249	
24.	35285-69-9	Benzoic acid, 4-hydroxy-, propyl ester, sodium salt		174b, 3266, 4249	
25.	7787-47-5	Beryllium chloride		5811	
26.		Butanedioate, hydroxy- {malate}	2931	3160	
27.	16426-50-9	Butanedioic acid, hydroxy-, calcium salt		5079, 5189, 5342	

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

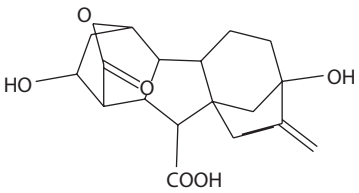
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
28.	585-09-1	Butanedioic acid, hydroxy-, dipotassium salt KOOC-CHOH-CH_2-COOK		4249, 4560, 5079, 5189, 5342	
29.	676-46-0	Butanedioic acid, hydroxy-, disodium salt NaOOC-CHOH-CH_2-COONa		5811b	
30.	869-06-7	Butanedioic acid, hydroxy-, magnesium salt		5079, 5189, 5342	
31.	921-53-9	Butanedioic acid, 2,3-dihydroxy-[R-(R*,R*)]-, dipotassium salt		2517a, 4249, 4560	
32.	4151-35-3	2-Butenedioic acid (*E*)-, dipotassium salt	5811, 5811a, 5811b		
33.	17013-01-3	2-Butenedioic acid (*E*)-, disodium salt	5811, 5811a, 5811b		
34.	10043-52-4	Calcium chloride		5811, 5811b	
35.	1305-62-0	Calcium hydroxide		5811b	
36.	1305-78-8	Calcium oxide CaO		1895, 3518, 4249, 5811b	
37.	137-42-8	Carbamic acid, *N*-methyldithio-, monosodium salt {Metham-sodium®}		3633, 3646a, 4271a	
38.	9006-42-2	Carbamodithioic acid, 1,2-ethylene(bis-, polymer with ammonia complex of zinc ethylenebisdithiocarbamate {Metiram®}		429b, 3633, 4249, 4271a, 5525	
39.	463-79-6	Carbonic acid		5079, 5382	
40.	10361-29-2	Carbonic acid, ammonium salt	3324, 3623, 4249, 5079, 5359	1053, 3266, 4249, 17B40	
41.	471-34-1	Carbonic acid, calcium salt		1053, 3266, 3476, 4249, 5811b	
42.	584-08-7	Carbonic acid, dipotassium salt {potash}		2154, 3973, 4249, 4560, 5079, 5126	
43.	497-19-8	Carbonic acid, disodium salt {sodium carbonate}		174b, 1053, 3266, 3476, 4249, 5529	
44.	13717-00-5	Carbonic acid, magnesium salt		3476, 4249, 5079, 5189, 5195, 5197	
45.	1066-33-7	Carbonic acid, monoammonium salt {ammonium hydrogen carbonate}	3266, 3623, 4249	1053, 3266, 4249, 17B40	
46.	298-14-6	Carbonic acid, monopotassium salt		3973, 4249, 4989	
47.	144-55-8	Carbonic acid, monosodium salt		1053, 3266	
48.	479-61-8 42617-16-3	Chlorophyll a {also listed under Magnesium} {Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]-}		120, 537, 543a, 677b, 830a, 832, 835, 838, 840, 1463, 1941, 2038, 2079, 2236, 2270, 2283, 2649, 2914, 2939, 3616, 3630, 3631, 3632, 3797, 3875, 3973, 3974a, 3974b, 4107, 4108, 4222, 4249, 5079, 5189, 5300, 5539, 5811b	
49.		Chlorophyll a, phytol		5539	

(*continued*)

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
50.	519-62-0	Chlorophyll b {also listed under Magnesium} {Magnesium, [3,7,11, 15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4, 8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*), 4β,21β]]]-}		120, 543a, 677b, 830a, 832, 835, 838, 840, 1941, 2236, 2270, 2914, 2939, 3630, 3631, 3632, 3797, 3875, 3973, 4222, 4249, 5079, 5189, 5300, 5811b	
51.	1406-65-1	Chlorophyll a and b		559, 830a, 832, 876, 877, 1927a, 1941, 2038, 2154, 2236, 2394a, 2914, 3448, 3491, 3630, 3631, 3632, 3797, 3973, 3974b, 4222, 4249, 4424, 5067, 5079, 5108, 5109, 5189, 5300, 5413, 5505, 5517, 5811b	
52.	11006-34-1	Chlorophyllin		830a, 3448, 4430, 4473, 4643, 4844, 4882, 4884, 4885	
53.	16055-83-1	Chromium ion (3+)	5811a		
54.	18540-29-9	Chromium ion (6+)	5811a		
55.	10210-68-1	Cobalt carbonyl	3785, 3786		
56.	1332-82-7	Cobalt chloride		5811	
57.	7447-39 4	Copper chloride (cupric chloride) $CuCl_2$		5811	
58.	1317-39-1	Copper oxide		3633, 4249	
59.	1332-40-7 1332-65-6	Copper oxychloride {RAME}		3633	
60.	8012-69-9	Copper oxychloride sulfate $Cu_2Cl(OH)_3 + Cu_4(OH)_6(SO_4)$		3633	
61.	1333-22-8	Copper oxysulfate $Cu_4(OH)_6(SO_4)$		5811	
62.	156-62-7	Cyanamide, calcium salt		3633, 4249	
63.	590-28-3	Cyanic acid, potassium salt		3633, 4249	
64.	55635-13-7	Cyclohexanecarboxylic acid, 2,2-dimethyl-2, 4-dioxo-3-(1-((2-propenyloxy)amino) butylidene)-, methyl ester, sodium salt {Alloxydim-sodium®}		3633, 4271a	
65.	9044-61-5	Cytochrome *b* 559		2079, 4249	
66.	9035-46-5	Cytochrome *c*6		429b, 4249, 4631	

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
67.		Ethanedioate {oxalate}		3160	
68.	14258-49-2	Ethanedioic acid, ammonium salt		4249, 4822	
69.	5794-28-5 17787-48-3	Ethanedioic acid, calcium salt (1:1): hydrate (2:5) = 17787-43-3, hydrate (1:1) = 5794-28-5		1814a, 4249, 4458, 4616	
70.	563-72-4 25454-23-3	Ethanedioic acid, calcium salt		1814a, 4249, 4458, 4616, 5079, 5126, 5189, 5342	
71.	583-52-8	Ethanedioic acid, dipotassium salt		3973, 4133, 4249, 4560	
72.	6018-94-6	Ethanedioic acid, nickel salt		3476, 4249	
73.	17480-26-1	Ethanedioic acid, tin salt {stannous oxalate}		3476, 4249	
74.	71-47-6	Formate	1628, 2931	5053, 5811b	
75.	125-67-7	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a, 7-trihydroxy-1-methyl-8-methylene-, 1, 4a-lactone, potassium salt {gibberellic acid, potassium salt} 		3633, 4249	
76.	9007-83-4	Globulins, γ-		120, 4249, 4615, 5079, 5432	
77.	14984-34-0	*D*-Glucuronic acid, monosodium salt		5811b	
78.	590-00-1 24634-61-5	2,4-Hexadienoic acid, potassium salt		174b, 1053, 3266, 3370, 4249	
79.	3615-82-5	myo-Inositol, hexakis(dihydrogen phosphate), calcium magnesium salt {phytin}		429b, 4249, 5079, 5384	
80.	71608-14-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]octadecyl hydrogen phosphate], disodium salt		429b, 1838, 4249	
81.	71608-17-8	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-1-[(2-hydroxy-1-oxopentacosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
82.	71608-15-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino] octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	

(*continued*)

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

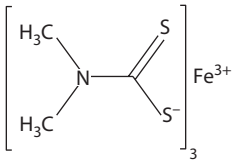
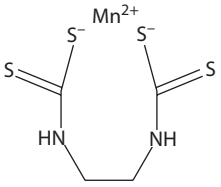
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
83.	71608-16-7	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]octadecyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
84.	71608-19-0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→ 4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl) amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
85.	71608-20-3	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→ 4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl) amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
86.	71608-21-4	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→ 4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
87.	71608-22-5	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxopentacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
88.	71608-23-6	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxohexacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		1838, 2056, 4249	
89.	14484-64-1	Iron, tris(dimethylcarbamodithioato-S,S′)-, (OC-6-11)- {Ferbam®} 		186, 3481, 3491, 3513, 3633, 4249, 4271a	
90.	15281-98-8	Iron carbonyl $Fe(CO)_4$	44, 3785, 3786, 4249		
91.	7705-08-0	Iron chloride (ferric chloride) $FeCl_3$		5811	

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
92.	1309-37-1 1332-37-2	Iron oxide (ferric oxide) Fe_2O_3		1895, 3476, 4249, 4679, 5811b	
93.	13463-40-6	Iron pentacarbonyl $Fe(CO)_5$	5811, 5811a, 5811b		
94.	1318-74-7	Kaolinite		5811, 5811b	
95.	12057-24-8	Lithium oxide (Li_2O)		5811b	
96.	14428-12-7	Magnesate(1-), [9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(3-)-N23, N24,N25,N26]-, hydrogen, [SP-4-2-[3S-(3α,4β,21β)]]- {chlorophyllide b}		4249, 4430, 4473, 4643, 4832a, 4844, 4882, 4884, 4885	
97.	14897-06-4	Magnesate(1-), [9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(3-)-N23,N24,N25,N26]-, hydrogen, [SP-4-2-[3S-(3α,4β,21β)]]- {chlorophyllide a}		4249, 4430, 4473, 4643, 4832a, 4844, 4882, 4884, 4885	
98.	15611-43-5 11006-34-1	Magnesate(3-), [18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12,17-tetramethyl-21*H*,23*H*-porphine-2-propanoato(5-)-N21,N22,N23,N24]-,trihydrogen,[SP-4-2-(2S-*trans*)]-{chlorophyllin}		830a, 3448, 4430, 4473, 4643, 4844, 4882, 4884, 4885	
99.	7791-18-6	Magnesium chloride		5811, 5811b	
100.	479-61-8 42617-16-3	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]- {chlorophyll a}		120, 537, 543a, 677b, 830a, 832, 835, 838, 840, 1463, 1941, 2038, 2079, 2236, 2270, 2283, 2649, 2914, 2939, 3616, 3630, 3631, 3632, 3797, 3875, 3973, 3974a, 3974b, 4107, 4108, 4222, 4249, 5079, 5189, 5300	
101.	519-62-0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-N23,N24,N25,N26]-, [SP-4-2-[3S-[3α(2E,7S*,11S*),4β,21β]]]- {chlorophyll b}		120, 543a, 677b, 830a, 832, 835, 838, 840, 1941, 2236, 2270, 2914, 2939, 3630, 3631, 3632, 3797, 3875, 3973, 4222, 4249, 5079, 5189, 5300	
102.	1309-48-4	Magnesium oxide (MgO)		1895, 3518, 4249	
103.	13446-35-0	Manganese chloride ($MnCl_4$)		2393, 4249	
104.	12427-38-2	Manganese, [[1,2-ethanediylbis[carbamodithioato]](2-)]- {Maneb®} 		3491, 3513, 3633, 3661a, 4249, 4271a, 5811b, 21A19	

(*continued*)

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

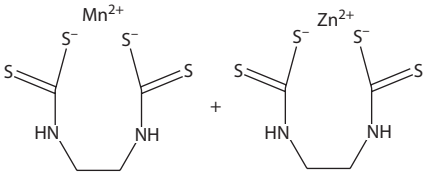
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
105.	8018-01-7	Manganese, [[1,2-ethanediylbis[carbamodithioato]](2-)] + zinc, [[1,2-ethanediylbis-[carbamodithioato]](2-)] {Mancozeb} 		2892a, 3633, 4271a, 5811b	
106.	1318-94-1	Muscovite $K_2O \cdot 3Al_2O_3 \cdot 6SiO_2 \cdot 2H_2O$		5811, 5811b	
107.	12612-55-4 13463-39-3	Nickel carbonyl $Ni(CO)_4$	44, 1781, 3300, 3302, 3308, 3785, 3786, 3836, 3837, 4005, 4249, 4319, 4332, 4342, 5811b		641, 4249
108.	125239-87-4	Nitrate, peroxy-	3000		
109.	7697-37-2	Nitric acid	1099, 1100, 1140, 3255, 3491, 4058, 4249, 5811b	857, 1140, 5079, 5126, 5298, 5811b	641, 4249
110.	6484-52-2	Nitric acid, ammonium salt		5811	
111.	10124-37-5	Nitric acid, calcium salt		5811, 5811b	
112.	3251-23-8	Nitric acid, copper salt		5811b	
113.	10099-74-8	Nitric acid, lead salt		5811	
114.	10377-60-3	Nitric acid, magnesium salt		5811, 5811b	
115.	7757-79-1	Nitric acid, potassium salt		3476, 5079, 5126, 5811b	
116.	7761-88-8	Nitric acid, silver salt		5811	
117.	7631-99-4	Nitric acid, sodium salt	5013	2913a, 5811b	
118.	10102-45-1	Nitric acid, thallium salt		5811	
119.	10102-06-4	Nitric acid, uranium salt		5811	
120.	7779-88-6	Nitric acid, zinc salt		5811	
121.	19059-14-4	Nitrite, peroxy-	2932, 3000		
122.	7782-77-6	Nitrous acid	1098, 1099, 1100, 3167, 3255, 5811b		
123.	430-75-1	Oxyacetate {glyoxylate} $O{=}CH\text{-}CO_2^-$		5811, 5811b	
124.		Pectic acid, calcium magnesium salt		1971, 5777	
125.	65028-58-2	Pectic acid, magnesium salt		1971, 2939, 4249	
126.	20859-73-8	Phosphide, aluminum $Al{\equiv}P$		2483a, 3633, 4249, 4271a	
127.	12057-74-8	Phosphide, magnesium Mg_3P_2		2483a, 3633, 4249, 4271a	
128.	7803-51-2	Phosphine PH_3	575, 637, 3302, 4249, 5079	3633, 4271a, 5523	641, 4249
129.	7664-38-2	Phosphoric acid		1053, 3266, 3476, 4249, 4518, 5811b	
130.	7757-93-9	Phosphoric acid, calcium salt (1:1)		3973, 4249, 4433, 5811b	
131.	7758-23-8	Phosphoric acid, calcium salt (2:1)		5811b	
132.	7783-28-0	Phosphoric acid, diammonium salt		1053, 2560, 3266, 3370, 3476, 4249, 4518	

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
133.	7558-79-4	Phosphoric acid, disodium salt		5811	
134.	14298-39-6	Phosphoric acid, holmium salt		5811	
135.	7757-86-0	Phosphoric acid, magnesium salt		5811b	4249, 4433
136.	13092-66-5	Phosphoric acid, magnesium salt $Mg(H_2PO_4)_2$		5811b	
137.	7722-76-1	Phosphoric acid, monoammonium salt $(NH_4)H_2PO_4$		5811	
138.	7778-77-0	Phosphoric acid, monopotassium salt	5811, 5811b	5811, 5811b	
139.	7558-80-7	Phosphoric acid, monosodium salt	5811, 5811a, 5811b	5811, 5811a, 5811b	
140.	7778-53-2	Phosphoric acid, tripotassium salt		3973	
141.	1314-56-3	Phosphorus oxide P_2O_5		1895, 3518, 4249, 5811b	
142.	7647-10-1	Platinum chloride		5811	
143.	7447-40-7	Potassium chloride KCl	4249, 4558	3973, 4249, 4560, 4654, 5811b	
144.	12136-45-7	Potassium oxide K_2O		1895, 3518, 4249	
145.	813-94-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, calcium salt		5079, 5189, 5342	
146.	3609-96-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, dipotassium salt		4249, 4560	
147.	3344-18-1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, magnesium salt		5079, 5189, 5342	
148.	18996-35-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monosodium salt		4249, 4760, 5548	
149.	866-84-2	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, potassium salt	5811b	174b, 1053, 3266, 4249, 5811b	
150.	68-04-2	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, sodium salt	5811b	174b, 1053, 3266, 4249, 5811b	
151.	6100-05-6	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripotassium salt, monohydrate		5079, 5189, 5342	
152.	927-20-8	1,2,3-Propanetriol, 1-(dihydrogen phosphate), magnesium salt (1:1)		429b, 4249, 4975	
153.	17603-42-8	1,2,3-Propanetriol, 1-(dihydrogen phosphate), sodium salt		4249, 4908a	
154.	1335-34-8	1,2,3-Propanetriol, mono(dihydrogen phosphate), potassium salt		4249, 4908a	
155.	65644-56-6	Propanoic acid, 2,3-dihydroxy-, calcium salt		5811b	
156.	72-17-3 16595-31-6	Propanoic acid, 2-hydroxy-, sodium salt H_3C-CHOH-COO-Na		3476, 4249, 5811, 5811b	
157.	16039-53-5	Propanoic acid, 2-hydroxy-, zinc salt		5811b	
158.	4151-33-1	Propanoic acid, 2-oxo-, potassium salt		5811b	
159.	51542-52-0	3,6-Pyridazinedione, 1,2-dihydro-, potassium salt		3636, 4249	
160.	65-30-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate (2:1)		3633, 3634, 3874c, 4249	
161.	6505-86-8	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate		3633, 3634, 3874c, 4249	
162.	2820-51-1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, hydrochloride, (S)-		4249, 4849	

(*continued*)

TABLE 20.6 (continued)
Various Ionic and Covalently Bonded Organic and Inorganic Compounds Containing Metals and Nonmetals, Miscellaneous Ions, and Organometallic Compounds Found in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
163.	58-56-0	3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride		429b, 4249, 4789	
164.	107-49-3	Pyrophosphoric acid, tetraethyl ester {TEPP} $[(H_3C\text{-}CH_2\text{-}O)_2\text{-}P{=}O]_2{=}O$		5079, 5439	
165.	10361-82-7	Samarium chloride		5811	
166.	7631-86-9	Silica	4249, 4508, 5501	1895, 2356, 2543, 2545, 2761, 2762, 2765, 2766, 4249, 5079, 5126, 5811b	
167.	60676-86-0	Silica, vitreous		5811b	
168.	19088-13-2	Silicic acid (H_2SiO_3), aluminum salt		2262	
169.	12141-45-6	Sillimanite $Al_2O(SiO_4)$	4508		
170.	7647-14-5	Sodium chloride		174b, 1053, 3266, 3476, 4249, 5811b	
171.	1310-73-2	Sodium hydroxide		1053, 3266	
172.	1313-59-3	Sodium oxide Na_2O		1895, 4249, 4679, 5811b	
173.		Sulfonium		2823, 5777	
174.	7664-93-9	Sulfuric acid		3476, 3633	
175.	7783-20-2	Sulfuric acid, ammonium salt		5811	
176.	7778-18-9	Sulfuric acid, calcium salt		5811, 5811b	
177.	7758-98-7	Sulfuric acid, copper salt		3633	
178.	10377-48-7	Sulfuric acid, dilithium salt		5811b	
179.	7778-80-5	Sulfuric acid, dipotassium salt		3973, 4249, 4560, 4722, 5811b	
180.	7757-82-6	Sulfuric acid, disodium salt		3973, 4249, 4894, 5811b	
181.	7487-88-9	Sulfuric acid, magnesium salt		5811, 5811b	
182.	7488-54-2	Sulfuric acid, rubidium salt		5811	
183.	7733-02-0	Sulfuric acid, zinc salt		5811	
184.	7757-83-7	Sulfurous acid, disodium salt		3973	
185.	7773-03-7	Sulfurous acid, monopotassium salt		3973	
186.	67-03-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride, monohydrochloride {thiamine hydrochloride}		1053, 3266, 4249	
187.	7772-98-7	Thiosulfuric acid, disodium salt		5811	
188.	1344-13-4	Tin chloride (stannic chloride) $SnCl_4$		5811	
189.	13463-67-7	Titanium oxide		5811b	
190.	76-87-9	Triphenylstannium hydroxide $(C_6H_5)_3{\equiv}Sn\text{-}OH$ {Fentin hydroxide®}		3633, 4271a	
191.	11105-12-7	Vanadium chloride		5811	
192.	1314-62-1	Vanadium pentoxide		3476	
193.	12122-67-7	Zinc, [[1,2-ethanediylbis[carbamodithioato]](2-)]- {Zineb®}		3481, 3491, 3513, 3633, 4249, 4271a, 4645, 4757, 5629, 5811b, 21A19	
194.	18920-65-5	Zinc, bis(thiocarbamato)-		3481, 3513, 4249	
195.	11126-30-0	Zirconium chloride		5811	

21 Pesticides and Growth Regulators

Since before 2500 BC, farmers have used pesticides to prevent damage to their crops. The first known pesticide was elemental sulfur, used to dust crops in Sumeria about 4500 years ago. By the fifteenth century, pesticides containing arsenic, mercury, and lead were being applied to crops. In the seventeenth century, nicotine was extracted from tobacco leaves as nicotine sulfate for use as an insecticide. In the nineteenth century, two more natural pesticides were introduced: pyrethrum (extracted from chrysanthemums) and rotenone (extracted from the roots and stems of several tropical and subtropical plant species of the genus *Lonchocarpus* or *Derris*) [Miller (21A46)].

From the 1860s until the advent in 1942 of DDT (1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene), there were numerous development and use of inorganic and naturally occurring compounds (inorganic and organic components extracted from plants and animals) for control of insects and plant diseases, particularly fungi. Little progress occurred in the discovery of natural or chemical means to control weeds. The chemistry of arsenicals was further exploited to control insects (Paris Green [copper(II) acetoarsenite]). Bordeaux mixture (copper sulfate and lime) was found to be extremely useful in the control of plant diseases, leading to its widespread usage. The invention of the pressure sprayer (both hand and power driven) made efficient large-scale application of pesticides feasible and economical. Aerial application was also invented (early 1920s), leading to expanded applications in agriculture. The availability of DDT, beginning in 1945 for civilian/agricultural usage, opened a new era of pest control, leading not only to its extensive usage but also to the development of numerous other synthetic organic insecticides, e.g., organophosphates (1946). About the same time (1944), selective synthetic organic herbicides were discovered, starting with 2,4-D (2,4-dichlorophenoxyacetic acid), which revolutionized weed control in agriculture and elsewhere. Also, synthetic organic fungicides (metal based) were developed as effective controls of plant diseases (and for other applications). During the 1950s and 1960s, granular pesticide formulations were developed, which led to large expansions of pesticide usage on major field crops [Aspelin (21A02)].

Prior to the advent of DDT (and other organic pesticides which rapidly followed), most pesticides used in agriculture were applied to protect high value/small acreage crops, principally fruits, vegetables, and cotton. This, however, changed dramatically in the 1950s, as major field crops, e.g., corn, sorghum, grains, tobacco, and soybeans, rapidly accounted for a majority of pesticide usage [Aspelin (21A02)].

By the 1960s, some very important new families of chemicals were discovered as herbicides, e.g., triazines, acetanilides, and dinitroanilines. In the 1970s, synthetic pyrethroids replaced much of the insecticide chemistry developed during the previous 20 years. During the 1980s, imidazolinone and sulfonylurea herbicides dramatically lowered application rates for weed control. During the 1990s and currently, agrochemical companies are employing new synthetic methods to produce safer pesticides (and growth regulators) for use on crops. The emphasis today in the development and use of pesticide and growth regulators is toward safer, more effective biological agents and pesticides applied at lower levels and enhanced stewardship in use of available pesticides [Aspelin (21A02)].

Tobacco is an agricultural product processed from the leaves of plants in genus *Nicotiana* of the nightshade family Solanaceae. *Nicotiana* is indigenous to North and South America, but numerous species of *Nicotiana* (over 60) are found throughout the world. The two main species cultivated and grown to produce tobacco and tobacco products worldwide are *Nicotiana tabacum* and *Nicotiana rustica*. *N. tabacum* is the most widely cultivated and used for production of tobacco leaf for cigarettes, cigars, chewing tobacco, snuff, snus, pipe tobacco, and other forms of tobacco products. *N. rustica* is the second most widely grown *N.* species. Its leaves are extracted for nicotine, pyridine products, and solanesol (3973).

Tobacco has evolved over the centuries to be resistant to many types of pests and infections. The plants produce numerous compounds that provide for its protection. For example, the plants contain high levels of nicotine. It constitutes 0.3%–5% in *N. tabacum* and up to 8%–10% in *N. rustica* based on the dry weight of the tobacco leaves. Its biosynthesis takes place in the roots, and it accumulates in the leaves. It is a potent neurotoxin for many pests with particular specificity to insects. Therefore, nicotine and salts of nicotine, e.g., Black Leaf 40 (nicotine sulfate), have been widely used as insecticides in the past (21A06, 21A07, 21A39–21A42), and currently, nicotine derivatives such as Imidacloprid [1-((6-chloro-3-pyridinyl)methyl)-*N*-nitroimidazolidinimine] continue to be widely used (3973).

Pesticides and plant growth regulators are important parts of modern agricultural and horticultural productivity. These pesticides can be naturally occurring in the plant or synthetically produced. Although naturally produced pesticides and growth regulators are effective, their concentrations in the plant are often lower than necessary to completely eradicate harmful pests and infections. Some naturally occurring pesticides are harvested from plants and sold commercially, e.g., *Bacillus thuringiensis*, *Derris* (rotenone), pyrethrum, Neem oil, and nicotine (nicotine salts) [EPA (21A21)]. Over the last 60–70 years, hundreds of synthetic pesticides and

growth regulators have been developed for application to tobacco at various stages in its development and during storage prior to use in commercial tobacco products to reduce or eradicate certain pests, e.g., insects, mice and other animals, unwanted plants (weeds), fungi, microorganisms such as bacteria and viruses, and infectious proteins. Some of the most effective pesticides and growth regulators are synthetic. Unfortunately, a number of highly effective synthetic pesticides are extremely harmful to both the environment and humans. One significant problem with synthetic insecticides is their longevity. This longevity is mostly due to the fact that many synthetic insecticides are not biodegradable.

Consequently, these pesticides remain in the ecosystem for long periods of time and can have disastrous consequences on organisms that subsequently absorb the insecticide. Arsenic salts (1459, 1460) and DDT (707–709) are good examples of synthetic pesticides that remained in the ecosystem for a long period of time and that have had considerable negative consequences. As a result of the possible harm to both humans and the environment, associated with synthetic pesticides, worldwide regulations are now in place. These regulations vary from country to country and apply to both synthetic agrochemicals and harvested natural pesticides [EPA (21A21)].

Based on a definition by the U.S. Environmental Protection Agency (EPA), a pesticide is any substance or mixture of substances intended for preventing, destroying, repelling, or mitigating any pest. The term pesticide also applies to herbicides, fungicides, and various other substances used to control pests. Under U.S. law, a pesticide is also any substance or mixture of substances intended for use as a plant regulator, defoliant, or desiccant. Pests are living organisms that are present where they are not wanted or that cause damage to crops or humans or other animals. In the United States, the EPA regulates both naturally occurring chemicals in harvested/extracted from plants as pesticides and growth regulators, as well as synthetic agrochemicals [EPA (21A21)].

There are five broad chemical classifications or categories of pesticides (four for synthetic pesticides and one for natural or plant-derived pesticides). Each of the following five chemical/biological categories of synthetic and harvested/extracted natural pesticides and growth regulators includes examples of commercial pesticides:

1. Organochloride pesticides: Aldrin, Chlordane, Dieldrin, DDT, Endosulfan, Endrin, Heptachlor, Lindane, Methoxychlor, Mirex, and TDE
2. Organophosphorus pesticides: Acephate, Azinphos-methyl, Chlorpyrifos, Chlorpyriphos-methyl, Diazinon, Dichlorvos (DDVP), Dicrotophos, Dimethoate, Disulfoton, Ethoprop, Fenamiphos, Fenitrothion, Fenthion, Fosthiazate, Malathion, Methamidophos, Methidathion, Methyl-parathion, Mevinphos, Naled, Oxydemeton methyl, Parathion, Phorate, Phosalone, Phosmet, Pirimiphos-methyl, Profenofos, Terbufos, Tetrachlorvinphos, and Trichlorfon
3. Carbamate pesticides: Aldicarb, Carbofuran, Carbaryl, and Methomyl
4. Pyrethroid pesticides: Allethrin, Bifenthrin, Deltamethrin, Permethrin, Resmethrin, Tetramethrin, and Tralomethrin
5. Plant-derived pesticides: Azadirachtin A and B (obtained from *Azadirachta indica*), *B. thuringiensis*, *Derris* (rotenone), Neem oil (obtained from *A. indica*), nicotine, Pyrethrum, Spinosad (a mixture of spinosyn A and spinosyn D) derived from soil bacterium *Saccharopolyspora spinosa*

Not every pesticide and growth regulator example listed earlier may be approved for use on tobacco.

This chapter provides information on pesticide and growth regulator residues (synthetic and natural occurring) identified on tobacco and identified in tobacco smoke. It also provides data of the transfer rates of these residues on tobacco to tobacco mainstream smoke (MSS) and certain examples of degradation/decomposition products from pesticide and growth regulator residues identified in MSS. Finally, a brief review of analytical methods for the analysis of pesticide and growth regulator residues on tobacco and in tobacco smoke is provided.

21.1 SYNTHETIC PESTICIDES AND PLANT GROWTH REGULATOR RESIDUES ON TOBACCO

Pesticide and growth regulator residues on tobacco and their transfer rates to MSS have been the subject of several reviews and multiple chapters in books. In the late 1960s, Guthrie and Bowery (21A25) and Guthrie (1457, 1458) reviewed the early literature dealing especially with residues of arsenic and the chlorinated hydrocarbon insecticides as well as those of carbamates and organophosphorus compounds used on tobacco. In another publication, Guthrie (21A24) summarized legislation on pesticide residues on tobacco and tobacco products in countries around the world as of 1973. In that paper, he also included an updated account of residues in U.S. tobacco and tobacco products. Ladisch in 1973 reviewed the known chlorinated pesticides in tobacco and tobacco smoke (21A31). Two reviews published in 1979 discuss the influence of growth regulators and herbicides [Steffens (3811a)] and insecticides and nematicides [Sheets and Leidy (3634)] on the chemistry of tobacco. These reviews contained updates on residues of pesticides. Ishiguro and Sugawara (1884) reviewed the known pesticides in tobacco and smoke and literature on decomposition products from pesticides in 1980. In 1986, Wittekindt (4271a) reviewed the pesticides recommended for use of tobacco in 22 countries, listed the maximum residues for 11 pesticides allowed on tobacco products in Germany, and presented a list of maximum amounts recommended by the German cigarette industry for 71 other pesticides. Davis et al. (21A17) and Meyer et al. (21A45) presented a detailed analysis of maleic

hydrazide (MH) residues in U.S. tobacco and discussed the toxicological implications of the residues. In 1989, the *43rd Tobacco Chemists' Research Conference* (TCRC) symposium was dedicated to the subject of regulation of insect and pathogen activity in tobacco and tobacco products. In that symposium, Benezet (21A05) reviewed chemical means to control pests in tobacco and tobacco products and their interaction. At that same symposium, Danehower (21A16) and Jackson et al. (21A29) reviewed the role of natural tobacco constituents that are effective pesticides (21A30). Cousins (21A14a) published a review on herbicides and suckering agents in 1989. In 1972 and again in 1990, Tso published books on the chemistry and biology of tobacco (3972, 3973). In both books, he devoted two chapters to pesticides and growth regulators (both compounds native to tobacco and applied agrochemicals). In 1991, Sheets (3633) presented a very thorough review of all known pesticides to that date. Davis and Nielsen edited a book in 1999 on tobacco production, chemistry, and technology (910a). Several chapters in that book reviewed various types of pesticides employed in the production of different types of tobacco (2483a, 2650b, 2892a, 3646a, 3661a). In 2002, Blanc et al. (21A06) reviewed the use of natural insecticides/pesticides for use on tobacco. Mueller (2650a) reviewed current approaches and tools for the management of pesticide residues on tobacco in 2005 at the *59th Tobacco Science Research Conference*. Most recently in 2005, Eberhardt (21A19) prepared an extensive review of pesticides used on tobacco, the transfer rates of pesticides to MSS and sidestream smoke (SSS), and decomposition products of pesticide residues identified in MSS.

The most commonly used commercial pesticides and growth regulators for tobacco, as of 1998, include the following:

Insecticides: Acephate, Aldicarb, *B. thuringiensis*, Carbaryl, Carbofuran, Chlorpyrifos, Diazinon, Disulfoton, Endosulfan, Ethoprop, Fenamiphos, Fonofos, Imidacloprid, Malathion, Methidathion, Methomyl, Spinosad, and Trichlorfon
Herbicides: Benefin, Clomazone, Diphenamid, Isopropalin, Napropamide, Pebulate, Pendimethalin, Sethoxydim, and Sulfentrazone
Fungicides: Dimethomorph, Mancozeb, Mefenoxam, and Metalaxyl
Plant growth regulator: Ethephon and Flumetralin
Plant growth regulators as herbicides: maleic hydrazide
Fumigants as insecticides: Chloropicrin
Fumigants as insecticides or herbicides: methyl bromide
Fungicides as insecticides or herbicides: 1,3-dichloropropene (1,3-D) (21A59)

Worldwide pesticide use has increased 50-fold since 1950, and 2.5 million tons of industrial pesticides is now used each year [Miller (21A46)]. More than 25 million pounds of pesticides is used in tobacco production in the United States, and tobacco ranks sixth among all agricultural commodities in the amount of pesticides applied per acre, according to the U.S. Government Accounting Office (GAO) (21A59).

Tobacco farmers use a considerable quantity of pesticides and growth regulators to increase leaf yield and quality and, hence, a greater profit for their crop. Even with the greatest caution used by farmers in applying the agrochemicals, a certain level of these pesticides and growth regulators remains on the leaf after harvesting and curing. Additional pesticides are often used on tobacco that is stored to control insect populations, and small but detectable levels of pesticides remain on tobacco prior to its use in manufacture of tobacco products. Therefore, certain residual pesticides are expected to be present on tobacco. Since about 1950, over 200 types of pesticides and growth regulators have been used on tobacco crops. Some are no longer used as many technological improvements have been made during that time and our knowledge of the effectiveness of different agrochemicals on pest has improved. All the newer pesticides are now regulated, and strenuous testing programs exist to assure that these agrochemicals meet safety (human and environmental [soil and air]) requirements (21A21). Additionally, agricultural breeding practices have generated new varieties of tobacco plants that are often more resistant to certain plant diseases and insects (21A21). Even with all the safety measures in place, residual levels of agrochemicals have been identified in both tobacco and tobacco smoke. Degradation products from the thermal degradation, pyrolysis, and combustion of these agrochemicals have also been identified on tobacco and in tobacco smoke. Generally, the level of residue tobacco pesticides and growth regulators is very small (ng/kg tobacco, ppm range). The transfer rate of these pesticides and growth regulators to MSS varies tremendously but is generally less than 30%, in many cases less than 10%, and in some cases less than 1% [Eberhardt (21A19)]. The existence of trace levels of pesticides and growth regulators in tobacco smoke was made possible by the advent of modern analytical methodologies, particularly gas capillary/gas chromatography (GC/GC), gas chromatography/mass spectrometry (GC/MS), and high-performance liquid chromatography (HPLC).

21.2 NATURALLY OCCURRING PLANT GROWTH REGULATORS AND PESTICIDES IN TOBACCO

Auxins are a class of plant growth substance (often called phytohormones or plant hormones). The most important member of the auxin family found in all plants is indole-3-acetic acid (IAA). It generates the majority of auxin effects in intact plants and is the most potent native auxin. Naturally occurring auxins include gibberellic acid, IAA, phenylacetic acid (PAA), and indole-3-butanoic acid (IBA) (3973). Gibberellic acid and several gibberellins are sold commercially as plant growth regulators. Auxins play an essential role in coordination of many growth and behavioral processes in the plant life cycle. When stimulated during normal plant growth or when applied to the plant at high concentrations, auxins produce ethylene.

Excess ethylene inhibits elongation growth, causes leaf abscission, and can even kill the plant (21A14). Synthetic auxins and commercially available auxins are effective herbicides by their effective promotion of ethylene in plants. Synthetic auxin analogs include 1-naphthaleneacetic acid (NAA), 2,4-D, IBA, and 2-methoxy-3,6-dichlorobenzoic acid [Hobbie and Estelle (21A27), Hobbie et al. (21A28), Lomax et al. (21A35)]. Additionally, compounds such as naturally occurring pyrethrins (21A15, 21A20, 21A23, 21A32–21A34), Neem oil (a mixture from *A. indica* of more than 135 compounds), Azadirachtin A and B from *A. indica* [Akol et al. (21A01), Biswas et al. (21A05a), Cousins (21A14a)], rotenone [Chamberlin and Madden (21A11)], and *B. thuringiensis* (B.t.) are effective naturally occurring pesticides (3973, 21A54). Of course, the most plentiful naturally occurring insecticide in tobacco is nicotine [Busbey and McIndoo (21A07, 21A08), McIndoo et al. (21A40–21A42), McIndoo (21A39), Steppuhn et al. (21A55)]. In 1989, Danehower (21A16) reviewed the field of naturally occurring tobacco growth regulators and pesticides at the 43rd TCRC. Numerous naturally occurring pesticides are found on the surface of tobacco leaves. Effective naturally occurring pesticides on the surface of tobacco leaves include *n*-, *iso*-, and *anteiso*-paraffinic hydrocarbons; aliphatic alcohols and acids; wax esters; α- and β-4,8,13-duvatrien-1-ols, the α- and β-duvatrienediols and monols; (12,*Z*)-labda-12,14-diene-8α-ol, *Z*-abienol; (13,*E*)-labda-12-ene-8α, 15-diol, labdenediol; numerous sucrose esters (C2–C8 acids); several labdane diterpenes (sclareol type); nicotine; nornicotine; formylnornicotine; acetylnornicotine; 3-hydroxy-acylnornicotines (C12–C16); acyl nornicotines (C12–C13) with *n*-, *iso*-, and *anteiso*-methyl branching; and numerous phenolic compounds derived from shikimic acid, e.g., caffeic acid, ferulic acid, gentisic acid, cichoriin, isoquercetin, rutin and their glucosides, and the mevalonic acid, e.g., capsidol, solavetivone, solanascone, occidol, and numerous other sequiterpenoids, biological pathways in tobacco.

21.3 TRANSFER RATES OF PESTICIDES AND PLANT GROWTH REGULATORS TO MSS

Tobacco, because it is subject to many types of pests, can be damaged both physically and chemically. Serious infections can result and have led to total crop failures. Efforts are continually being made to breed new varieties of tobacco resistant to disease and various pests (aphids, hornworms, various nematodes, etc.). Additionally, herbicides of various types are widely used to control unwanted vegetation in the fields. As a result, the use of pesticides and various plant growth regulators is widespread and at present is the primary means used by tobacco farmers to improve tobacco quality and yield. The level of pesticide (and plant growth regulator) residues on tobacco has always been a concern to tobacco growers, the tobacco industry, and governmental regulators in terms of the safety of the resulting tobacco products. Hundreds of tobacco pesticides and plant growth regulators have been developed and marketed in the past. Fewer than 25 are currently regulated and employed by farmers and the tobacco industry (3633). Regardless of the intended use of these pesticides and growth regulators, it seems inevitable that certain levels remain on the tobacco leaf. This is particularly true today, not necessarily because inordinate levels of pesticides are employed on tobacco but because tremendous advances in analytical chemistry have enabled scientists to detect extremely low levels (picogram to fentagram levels) of these residues (or their decomposition products). As certain agrochemicals used for pest control and growth regulation leave residues on cured tobacco leaves, some residual pesticides and growth regulators have been identified in tobacco smoke. An important question concerning consumer safety is whether the residual levels of pesticides (or growth regulators) represent a danger to the public.

At the completion in 1976 of the study of the second set of experimental cigarettes in the National Cancer Institute (NCI) decade-long study on the "less hazardous" cigarette, it was reported that the long-chained alcohols used as suckering agents on tobacco had no adverse chemical or biological effect on cigarette MSS. In the 1976 report, Gori (1330) summarized this aspect of the NCI second study as follows:

> The fatty alcohol, fatty alcohol x 100, and hand-suckered blends showed no significant difference among themselves or from the SEB II blend [see p. 2 in (1330)].
>
> No statistically significant differences were observed among Hand-suckered, Fatty Acid-Normal, and Fatty Acid x 100 Blends (variables 60, 61, and 62) [see p. 14 in (1330)]

In the fourth NCI study completed in 1980, the chemical and biological properties of the MSSs from cigarettes made from pesticide-treated tobacco and pesticide-free tobacco were compared. Gori wrote [see p. 7 in (1333)]:

> No significant differences were observed between cigarettes made from pesticide-treated tobacco leaves and pesticide-free tobacco leaves.

The pesticide-treated vs. pesticide-free tobaccos used in this phase of the NCI study were those grown in Prince Edward Island, Canada. The commercial pesticides used on the tobacco included Chlorpyriphos, Trichlorfon, diphenamide, Methomyl, DDT, Carbaryl, MH, and C10 alcohol. The pesticide-treated tobacco properties were described in 1980 by Tso et al. (3973, 3977):

> It appears that chemicals currently registered for use on tobacco, when applied as directed, are of no significance in increasing biological activity of cigarette smoke condensate [see p. 151 in (3973)].

In 2005, Eberhardt (21A19) reported on pesticide residues on tobacco, the transfer rates of selected pesticide residues, and pyrolysis products of some pesticide residues as part of the CORESTA subgroup study on pesticide residues. Information on 40 agrochemicals (used from the 1950s to the present) was obtained from 64 literature references. The agrochemicals evaluated were insecticides, fumigants, fungicides, herbicides, and growth regulators. These represented a diverse set of compounds including alcohols, acids, organophosphates, organohalides, carbamates, dithiocarbamates, pyrethrins, dinitro compounds, organonitrogen compounds, and heterocyclics. Prior to the work by Eberhardt (21A19), Rix (4857, 4858) evaluated the transfer of selected agrochemicals (Dicamba, Formothion, and Thiodan) from tobacco to smoke.

For the majority of the commercial pesticides (and plant growth regulators), reviewed by Eberhardt (21A19), only minimal information existed for their transfer into the smoke and for pyrolysis products. It must be noted that some of the agrochemicals listed, e.g., Leptophos and TDE, had only minor significance in tobacco cultivation and were added to tobacco for purely experimental reasons to study smoke transfer rates. Additionally, not all authors that provided information on transfer rates gave precise details on the pesticide concentrations in the original material used. There are only a few pesticides, such as DDT, MH, and several dithiocarbamates, where the transfer rates seemed to be adequately investigated, i.e., in sufficient number and by different research groups [Atallah et al. (1051d, 21A03, 21A04), Chopra et al. (707, 708, 712, 714, 716), Guthrie et al. (1457, 1458), Hoffmann and Rathkamp (1756), and Hoffmann et al. (1761, 1767)]. A number of publications by these authors used labeled agrochemicals (16 of the 64 studies), which provided information on the fate of the original substance in tobacco MSS and SSS as well as their presence in the vapor and particulate phases of the smoke streams. As most of the naturally occurring pesticides and plant growth regulators exist in tobacco, no information on the transfer rates to tobacco smoke is available. Table 21.3 lists the majority of known pesticides and plant growth regulators used on and identified in tobacco and tobacco smoke. Although Table 21.3 lists a great number of natural and synthetic pesticides and growth regulators found in tobacco and tobacco smoke, there are still other pesticides and plant growth regulators that could have been used on tobacco but where no information could be found in the literature. Additionally, individual pesticides and growth regulators often have multiple common names. Therefore, in reviewing Table 21.3, pesticides and growth regulators should be searched by Chemical Abstract number or chemical name. Table 21.3 contains only a selected number of naturally occurring pesticides and plant growth regulators found in tobacco and tobacco smoke. All of the compounds mentioned in this chapter as naturally occurring pesticides and plant growth regulators are covered in other chapters, e.g., the hydrocarbons are discussed in Section 1.1, the duvatrienediols are discussed in Chapter 2, and the nicotinoids are discussed in Section 17.2.

The evaluation by Eberhardt (21A19) of the available literature demonstrated that the transfer rate for all residues studied was much less than 100%. In most studies, the transfer rate of the pesticide to MSS is stated as being <30%. For a small number of agrochemicals, e.g., DDT, TDE, Lindane, and HCH-alpha, markedly higher transfer rates were found, although it should be kept in mind that very broad ranges in transfer rates exist for many of the pesticides examined. Only in a few studies were the transfer rates of residues in plain and filtered cigarettes presented and compared. The data suggested that the presence of a filter in cigarettes slightly reduces the transfer into MSS of some pesticides, e.g., DDT, Disulfoton, and TDE (1127). Several other factors also influenced the transfer rates, e.g., the type of tobacco tested, the form of the smoking article (e.g., cigarette, cigar, cigarillo, and pipe), the type of a filter employed, the method of adding the original substance and its amount, variation in smoking conditions (e.g., puff volume, and number of puffs), and the analytical methods employed to determine the agrochemical [Mussalo-Rauhamaa et al. (21A48), Mold and Walker (2596), Carugno (21A10), Schmid and Rastetter (21A52), Mestres et al. (21A43), Hengy and Thirion (1619), Hoffmann et al. (1761), Atallah and Dorough (21A03, 21A04), Thorstenson and Dorough (3915), Smith et al. (3724), Lorenz et al. (21A36–21A38), Guthrie (1457), Dickes et al. (21A18), Dorough and Atallah (1051d), Bowery et al. (415), Hawk et al. (1553), Ceschini and Chauchaix (644), Clark et al. (21A12), Moshy and Halter (21A47), Hengy and Thirion (1618), Meikle (2527), Sitaramaiah et al. (21A53), Thurm (21A57), Stone (21A56), Barkemeyer et al. (186), Chopra and Domanski (707), Chopra and Sherman (712), and Underwood (21A58)].

Table 21.1 shows the percentage transfer of selected pesticides applied to tobaccos that transfer to MSS. The percentage transfers were generally taken from the publication or were calculated based on data provided in the literature [Eberhardt (21A19)].

21.4 DECOMPOSITION PRODUCTS OF AGROCHEMICALS IN MSS

The decomposition products identified in MSS of various agrochemicals added to tobacco are shown in Table 21.2.

In some of the published studies reviewed by Eberhardt (21A19), the determination and quantification of the pyrolysis products were the primary objective of the study, e.g., Hoffmann et al. (1761), Mestres et al. (21A44), and Higman et al. (1645), and MSS transfer rates for the pesticide were not determined. In other studies, ^{14}C-labeled pesticides, e.g., Atallah and Dorough (21A03, 21A04), Frisch et al. (1243), and Clark et al. (21A12), were evaluated. In most

TABLE 21.1
Percent Transfer of Intact Agrochemicals to MSS (1884, 21A19)

Pesticide	Percent Transfer of Intact Compound
Anilazine	1
Azinphos-methyl	0.2–0.27
Benomyl	ND
Captan	ND–2.7
Carbaryl	1–11
Carbofuran	0.3–20
Chlorpyrifos	13.5–15
Cyhalothrin	5.2
Cypermethrin	1.51
DDT	1.2–83.3
Deltamethrin	2.64
Diamidofos	ND
Dieldrin	4–32
Diflubenzuron	6.9
Disulfoton	6–14.8
Dithiocarbamates	ND
Endosulfan	ND–15.3
Endosulfan sulfate	15.5–16.3
Endrin	18.18–31.58
Fenpropathrin	15.5
Fenvalerate	1.72
HCH-alpha	45
Heptachlor	4–5
3-Hydroxycarbofuran	0.1–3.26
Imidacloprid	5.3
Isobenzan	3.5–5.1
Leptophos	3–10
Lindane	3.1–40
Linuron	6.7
Malathion	ND–9.4
Maleic hydrazide	ND–23
Methoprene	38.2
Metobromuron	3.7–4
Mirex	9–23
Monolinuron	2.5–4.5
Naphthol	5.7–13.8
Parathion	ND–15.3
Phosphine	ND
TDE	0.007–63.75

ND, not determined.

cases, the agrochemicals tested were used as purchased, e.g., Comer et al. (21A13), Chopra et al. (716), and Chopra and Zuniga (717).

For the majority of the pesticides reviewed by Eberhardt (21A19), only minimal information existed for their transfer into smoke and for their pyrolysis products. There are only a few pesticides, such as DDT, MH, and several dithiocarbamates, where the transfer rates seem to be adequately investigated in a sufficient number of studies by different research groups [Atallah et al. (1051d, 21A03, 21A04), Chopra et al. (707, 708, 712, 714, 716), Guthrie et al. (1457, 1458), Hoffmann and Rathkamp (1756), and Hoffmann et al. (1761, 1767)].

21.5 METHODS FOR ANALYSES OF PESTICIDES AND PLANT GROWTH REGULATORS

Numerous analytical methods, e.g., GC/GC, GC/MS, and HPLC, have been published for the determination of various classes of pesticides [Haeberer and Chortyk (470, 21A26), Schmeltz et al. (3483), Sagredos and Eckert (3379–3381), Sagredos and Moser (3382), Nesemann and Seehofer (2699), Nesemann et al. (2697, 2698), Schmid and Rastetter (21A52), Schmid (3513), Dattilo et al. (904, 905), Guhlmann et al. (1451), Cai et al. (21A09), Carpenter and Frost (606), Nowell and Resek (21A50), Zaugg et al. (21A63), Werner et al. (21A60), Yamazaki and Tomara (21A62), and many others].

21.6 RESIDUES OF SYNTHETIC PESTICIDES AND PLANT GROWTH REGULATORS IDENTIFIED IN TOBACCO AND TOBACCO SMOKE

The number of pesticide, plant growth regulators, and their decomposition products identified in tobacco and tobacco smoke listed in Table 21.3 is 308. Of these, 114 have been identified in tobacco smoke, 302 in tobacco, and 108 in both tobacco and tobacco smoke. There are more natural pesticides and growth regulators known than are listed in Table 21.3 because only selected examples of these natural pesticides and growth regulators, described by Danehower (21A16), are given.

TABLE 21.2
Degradation Products of Pesticides in MSS (1884, 21A19)

Pesticide	Degradation Products of the Intact Compound	References
Anilazine	*o*-Chloroaniline	1457
Azinphos-methyl	Oxyguthion	419, 1457
Captan	CO_2	21A37
Carbaryl	Degradation products: 7 (not further characterized), CO_2	1051d, 21A03, 21A04
Carbofuran	Degradation products: 2 (not further characterized), CO_2	1051d, 1553, 21A03, 21A04
Chlorpyrifos	Decomposition into unknown fragments	717
DDT	1,1-Dichloro-2,2-bis(*p*-chlorophenyl)ethane (DDD = TDE), 1,1-dichloro-2,2-bis(*p*-chlorophenyl)ethylene (DDE), 1-chloro-2,2-bis(*p*-chlorophenyl)ethylene (DDM = TDEE), 4,4′-dichlorobenzophenone (DCBP), bis(*p*-chlorophenyl)methane (BCPM), CO_2, chloroform, methyl chloride, *trans*-4,4′-dichlorostilbene (DCS), DDD-olefins	644, 707, 712, 714, 708, 758, 1000, 1051d, 1457, 1756, 1767, 2697, 3915, 21A18, 21A37, 21A38, 21A43
Diamidafos	Phenol	2527
Dieldrin	Chlorinated and dechlorinated degradation products	21A57
Diflubenzuron	4-Chloroaniline, 4-chlorophenylurea	21A53
Dithiocarbamates	CO_2, carbon disulphide, COS, ethylene thiourea, hydrogen sulfide	124, 186, 21A10, 21A38, 21A44, 21A51
Endosulfan	Ether	1619
Imidacloprid	CO_2, CO (traces), urea compound	21A12
Leptophos	Degradation products: 4 (not further characterized), CO_2	1051d, 21A03, 21A04
Lindane	CO_2	21A36, 21A38
Linuron	3,4-Dichloroaniline	822
Malathion	CO_2	21A38
Maleic hydrazide	Acetonitrile, acrylonitrile, aminobutanoic acid, ammonia, aniline, butanoic acid, benzonitrile, CO_2, CO, cyanide, 1*H*-pyrrole-2,5-dione, hydrazine (traces), indole, succinimide	716, 1761, 2383–2385, 3724, 3725, 1553, 4274, 21A56
Methoprene	CO_2, CO	1243
Metobromuron	4-Bromoaniline	822
Mirex	Degradation products: 3 (not further characterized), CO_2	1051d, 21A03, 21A04
Monolinuron	CO_2, 4-chloroaniline	822, 21A37
Naphthol	Degradation products: 6 (not further characterized)	21A03, 21A04
TDE (DDD)	Dechlorinated TDE, 1,1-dichloro-2,2-bis(*p*-chlorophenyl)ethylene (DDE), 1-chloro-2,2-bis(*p*-chlorophenyl)ethylene (DDM = TDEE), 4,4′-dichlorobenzophenone (DCBP), bis(*p*-chlorophenyl)methane (BCPM), *trans*-4,4′-dichlorostilbene (DCS)	415, 416, 714, 758, 1457, 3915

TABLE 21.3
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

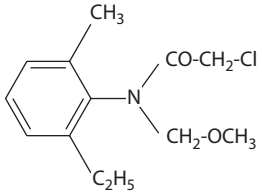
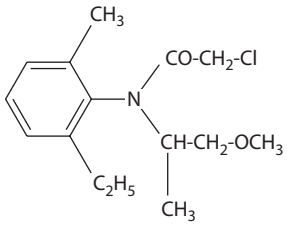
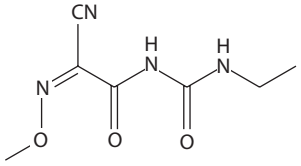
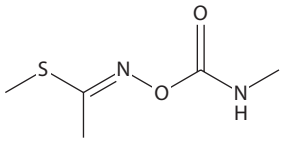
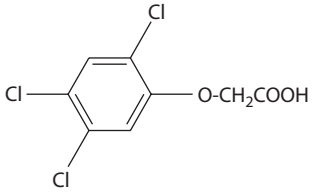
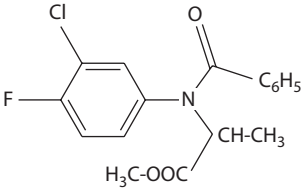
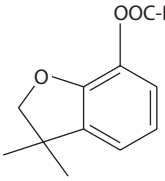
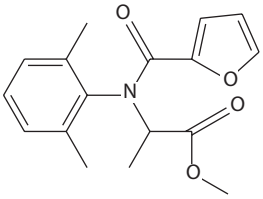
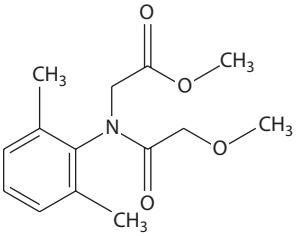
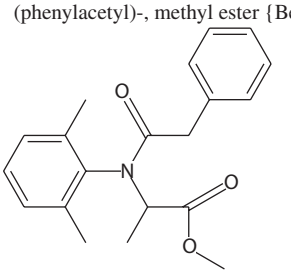
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	15972-60-8	Acetamide, 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)- {Alachlor®} 		2650a, 2913a, 3633, 4271a	
2.	51218-45-2	Acetamide, 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)- {Metolachlor®} 		2650b, 4271a	
3.	57966-95-7	Acetamide, 2-cyano-2-methoxyimino-*N*-(ethylcarbamoyl)- {Cymoxanil®} 		3633	
4.	16752-77-5	Acetamidic acid, thio-, *N*-[(methyl-carbamoyl)oxy]-, methyl ester {Methomyl®} 	1333	1219, 1219b, 1219c, 1333, 2650b, 3633, 3977, 4271a	
5.	94-75-7	Acetic acid, 2,4-dichlorophenoxy- {2,4-D}		3633, 5015, 5521, 5811b	
6.	93-76-5	Acetic acid, 2,4,5-trichlorophenoxy- {2,4,5-T®} 		3633, 5015	
7.	50-76-0	Actinomycin D		3108a	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
8.	52756-25-9	*DL*-Alanine, *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-, methyl ester {Flamprop-methyl®} 		4271a	
9.	82560-54-1	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy)carbonyl)methylamino)thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}  R = -NH-S-N[CH(CH$_3$)$_2$]-(CH$_2$)$_2$-COOC$_2$H$_5$		3633	
10.	57646-30-7	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(2-furanylcarbonyl)-, methyl ester {Furalaxyl®} 		3633	
11.	57837-19-1	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-, methyl ester {Ridomil®} 		2892a, 3633, 4271a	
12.	71626-11-4	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)-, methyl ester {Benalaxyl®} 		3633	
13.	53516-76-0	Ammonium chloride, alkyldimethylbenzyl- {Benzalkonium chloride®}		3633	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

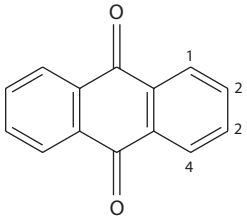
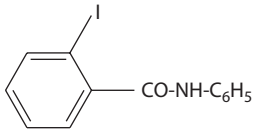
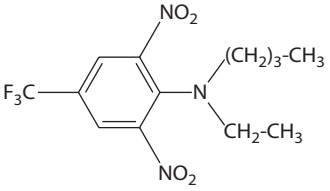
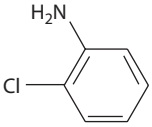
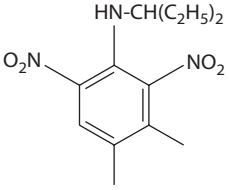
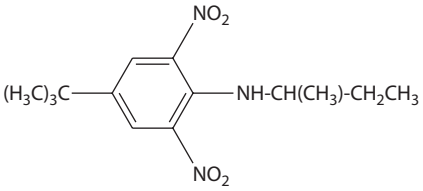
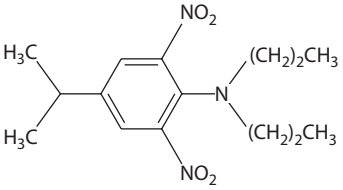
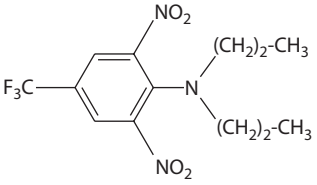
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
14.	84-65-1	9,10-Anthracenedione {9,10-anthraquinone} 	790b,1211, 1884, 2191, 2195, 2196, 2200, 2203, 2210, 2860, 3308, 3510, 3557, 3797, 4249, 5811b	2939, 3560, 3561, 3633, 3797, 3973, 3974a, 4249, 5811b	2210, 3402
15.	7440-38-2	Arsenic	47, 50, 126a, 159, 174b, 174c, 273, 373, 516, 603, 688, 769, 889, 889a, 933, 1026, 1148, 1163, 1217, 889, 1273, 1373, 1386, 1395, 1430, 1439, 1445, 1557, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1815–1817, 1842, 1845,1870, 1871, 2060, 2079, 2170, 2172, 2313a, 2468, 2524, 2609, 2667, 2799a, 2825, 2911, 2918, 2939, 2980, 3007, 3059, 3104, 3234, 3238, 3252, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3377, 3378, 3417, 3711, 3775, 3830, 3899, 3927, 3934, 4005–4007, 4009–4011, 4229, 4230, 4242, 4249, 4319, 4331, 4354, 5061, 5079, 5124, 5160, 5201, 5264, 5512, 5541, 5811b, 5869a	46, 47, 159, 174c, 373, 516, 769, 889, 889a, 1163, 1391, 1395, 1445, 1459, 1460, 1534, 1535 1815–1817, 2079, 2172, 2338, 2468, 2609, 2667, 2939, 2978–2980, 3059, 3104, 3138, 3234, 3238, 3377, 3416, 3417, 3699, 3775, 3797, 3834, 3973, 3974a, 3974b, 4070, 4071, 4249, 4273, 4357, 4381, 5018, 5053, 5061, 5079, 5119, 5120, 5139, 5142, 5160, 5189, 5264, 5281, 5283, 5284, 5322, 5338, 5438, 5541, 5600, 5648, 5684, 5729, 5811b, 5849	50, 4249
16.	22541-54-4	Arsenic, arsenious state As^{+3}	5061	5061	
17.		Arsenic, arsenic state As^{+5}	5061	5061	
18.	7778-44-1	Arsenic acid, calcium salt		3633, 4249, 4271a, 4554	
19.	7778-40-9	Arsenic acid, lead salt [$Pb_3(AsO_4)_2$]		3633, 4249, 4271a, 4554	
20.	7645-25-2	Arsenic acid, lead salt [$PbH(AsO_4)$]		20A42	
21.	68038-71-1	*B. thuringiensis* {Dipel®}		3633, 3634, 5237, 5238	
22.	15310-01-7	Benzamide, 2-iodo-*N*-phenyl- {Benodanil®} 		774a, 4249, 4271a, 4552	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
23.	1861-40-1	Benzenamine, *N*-butyl-2,6-dinitro-*N*-ethyl-4-(trifluoromethyl)- {Benefin®, Benfluralin®} 		2892a, 3633	
24.	95-51-2	Benzenamine, 2-chloro- {2-chloroaniline} 	3491, 4249, 5811b	3797, 4249, 5811b	
25.	99-30-9	Benzenamine, 2,6-dichloro-4-nitro- {Dicloran®}		3633	
26.	40487-42-1	Benzenamine, 3,4-dimethyl-2,6-dinitro-*N*-(1-ethylpropyl)- {Pendimethalin®} 		2650b, 2913a, 3633, 3811a, 4271a	
27.	33629-47-9	Benzenamine, 4-(1,1-dimethylethyl)-2,6-dinitro-*N*-(1-methylpropyl)- {Butralin®} 		2913a, 3585c, 3633, 3811a, 3973, 5568	
28.	33820-53-0	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(1-methylethyl)- {Isopropalin®} 		2892a, 3633, 4271a	
29.	1582-09-8	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)- {Trifluralin®} 		1219c, 2650a	
30.	108-90-7	Benzene, chloro- C_6H_5-Cl	707, 1884, 2570, 4249, 5811b		

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

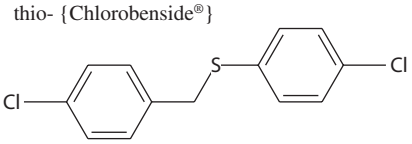
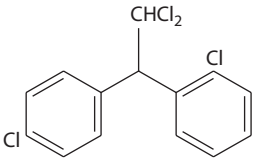
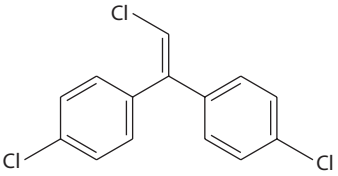
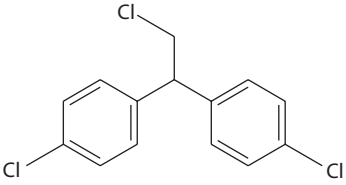
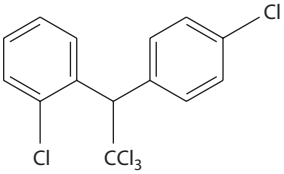
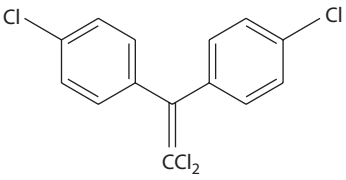
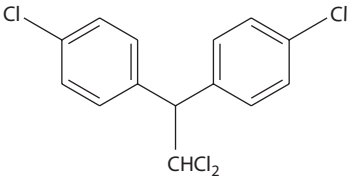
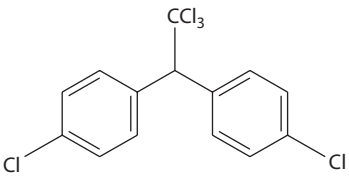
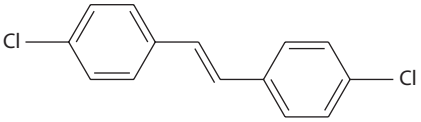
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	103-17-3	Benzene, 1-chloro-4-((4-chlorophenyl)methyl) thio- {Chlorobenside®} 		3633	
32.	53-19-0	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDD, *o,p′*-TDE} 	416, 518, 658, 758, 759, 1000, 1006, 1756, 1767, 1767a, 1781, 1884, 2550, 2596, 2697, 2767, 3493, 3634, 4249, 5811b, 21A19	518, 644, 713, 714, 758, 759, 1000, 1006, 1029, 1030, 1219, 1333, 1460, 1740, 1767, 2697, 3198, 3348–3350, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3977, 4249, 4271a, 5079, 5439, 5811b, 21A19	
33.	4329-12-8	Benzene, 1-chloro-3-[2,2-dichloro-1-(4-chlorophenyl) ethyl]- {*m,p′*-DDD}	1000, 1006, 1756, 1767, 1767a, 1781, 2767, 3493, 4249, 4342, 5811b, 21A19	1000, 1006, 1740, 3767a, 3770, 4249, 4271a, 5079, 5439, 21A19	
34.	1022-22-6	Benzene, 1,1′-(chloroethenylidene) bis[4-chloro- {DDM} 	707, 708, 713, 714, 758, 1000, 1006, 1767, 1781, 2767, 3557, 4005–4007, 4249, 5811b	708, 722, 758, 759, 1000, 1006, 1740, 1767, 2389, 2544, 4249, 5811b	
35.	2642-80-0	Benzene, 1,1′-(2-chloroethylidene) bis[4-chloro- {DDMS} 	707, 708, 713, 714, 758, 1000, 1006, 1767, 1781, 2767, 3557, 4005–4007, 4249	708, 722, 758, 759, 1000, 1006, 1740, 1767, 2389, 2544, 4249	
36.	789-02-6	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDT} 	517, 518, 758, 759, 1000, 1006, 1333, 1373, 1756, 1767, 1767a, 1781, 2697, 3257, 3493, 3685, 4005–4007, 4249, 4342, 5811b, 21A19	517, 518, 644, 722, 758, 759, 1000, 1006, 1029, 1030, 1219, 1219a, 1219b, 1333, 1460, 1740, 1767, 2697, 3138, 3633, 3637, 3767a, 3770, 3915, 3977, 3973, 3977, 3984, 4249, 4271a, 5079, 5439, 5811b, 21A19	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
37.	72-55-9	Benzene, 1,1′-(dichloroethenylidene) bis[4-chloro- {*p,p′*-DDE} 	518, 707, 708, 713, 714, 758, 759, 1000, 1006, 1375, 1375b, 1740, 1741, 1743, 1744, 1767, 1781, 2697, 2767, 3265, 3300, 3557, 4005–4007, 4249, 5512, 5811b	518, 644, 708, 722, 758, 759, 1000, 1006, 1029, 1030, 1219, 1219a, 1460, 1740, 2389, 2544, 2697, 3188a, 3633, 3637, 3770, 3915, 3974b, 4249, 4271a, 5811b	
38.	27013-25-8	Benzene, 1,1′-(2,2-dichloroethylidene)bis[chloro-	1000, 4249		
39.	72-54-8	Benzene, 1,1′-(2,2-dichloroethylidene)bis[4-chloro- {*p,p′*-DDD, *p,p′*-TDE} 	415, 419, 518, 658, 707, 708, 713, 714, 758, 759, 1000, 1006, 1375, 1375b, 1457, 1756, 1767, 1781, 1884, 2550, 2596, 2697, 2767, 2939, 3634, 4005–4007, 4249, 5811b	415, 419, 518, 644, 707, 708, 713, 714, 722, 758, 759, 1000, 1006, 1028–1030, 1219, 1219a, 1333, 1457, 1460, 1740, 1756, 1767, 2318, 2389, 2544, 2697, 2939, 3188a, 3348–3350, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3977, 3984, 4249, 4271a	
40.	50-29-3	Benzene, 1,1′-(2,2,2-trichloroethylidene)bis[4-chloro- {*p,p′*-DDT} 	517, 518, 707–709, 711, 712, 714, 758, 759, 1333, 1373, 1740, 1741, 1743, 1744, 1756, 1767, 1767a, 1781, 1884, 2697, 2825, 3257, 3265, 3300, 3493, 3634, 3685, 4249, 4342, 5512, 5811b, 5869a	517, 518, 644, 707–709, 711–714, 758, 759, 1028–1030, 1219, 1219a, 1333, 1460, 1756, 1767, 2318, 2697, 3138, 3188a, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3973, 3974b, 3977, 4249, 4271a, 5079, 5439, 5811b	
41.	5121-74-4	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro- {DCS = dichlorostilbene}	708, 1756, 1767, 1884, 3493, 4005–4007, 4010, 4011, 4249	722, 1460, 1756, 4249	
42.	1657-56-3	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-, (*E*)- {*trans*-DCS} 	707, 713, 714, 1756, 1781, 4249, 5811b	1756, 4249	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

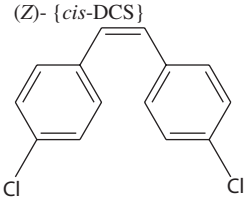
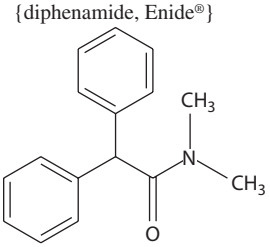
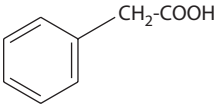
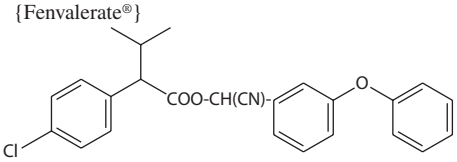
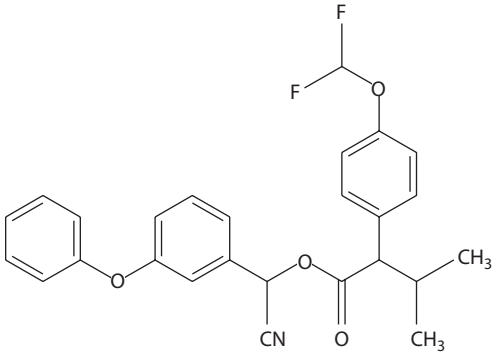
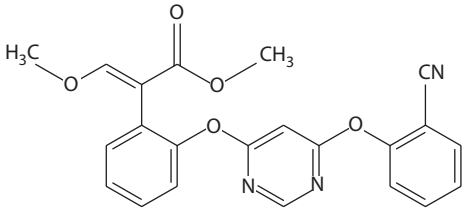
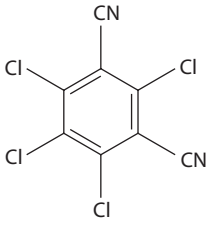
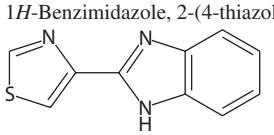
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
43.	2510-74-9	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-, (*Z*)- {*cis*-DCS} 	4249, 4342, 5811b		
44.	118-74-1	Benzene, hexachloro-		2389, 2544, 3152, 3188a, 3633, 3770, 4249, 4271a	
45.	15457-05-3	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)- {Fluorodifen®}		3633	
46.	82-68-8	Benzene, nitropentachloro- {Quintocen®}		3770	
47.	116-29-0	Benzene, 1,2,4-trichloro-5-((4-chlorophenyl) sulfonyl)- {Tetradifon®}		3633	
48.	957-51-7	Benzeneacetamide, *N,N*-dimethyl-α-phenyl- {diphenamide, Enide®} 	346, 1333, 4249	1219b, 1219c, 1333, 2650a, 3633, 3767a, 3973, 3977, 4249, 4271a, 5811b	
49.	103-82-2	Benzeneacetic acid {phenylacetic acid} 	172, 568b, 1132, 1063–1066, 1068–1074, 1099, 1165, 1359, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1587a, 1882, 1886, 2270, 2338, 2387, 2529, 2543, 2570, 2601a, 2641–2643, 2758, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3266, 3302, 3308, 3394, 3410, 3553, 3557, 4249, 5811b	120, 212, 404, 568b, 848, 908, 1053, 1165, 1587a, 1590a, 1620, 1999, 2014, 2270, 2283, 2338, 2386, 2389, 2529, 2544, 2758, 2862a, 2939, 3215, 3219, 3266, 3329, 3332, 3532, 3543, 3549, 3560, 3561, 3767a, 3973, 3974a, 3974b, 4249, 5708, 5811b	1360, 1375a, 2387
50.	51630-58-1	Benzeneacetic acid, 4-chloro-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®} 	21A19	3585e, 21A19	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
51.	70124-77-5	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl) methyl ester {Flucythrinate®} 		904	
52.	131860-33-8	Benzeneacetic acid, methyl (α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)- {Azoxystrobin®} 		5568	
53.	140-56-7	Benzenediazosulfonate, dimethylamino-, sodium salt {Fenaminosulf®}		3633	
54.	1897-45-6	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro {Chlorothalonil®} 		3585c, 3633	
55.	1861-32-1	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester {Chlorthal-dimethyl®, DCPA}		2913a, 3633	
56.	62924-70-3	Benzenemethanamine, 2-chloro-*N*-(2,6-dinitro-4-(trifluoromethyl)phenyl)-*N*-ethyl-6-fluoro- {Flumetralin®}		2913a, 3633, 5568, 5811b	
57.	19044-88-3	Benzenesulfonamide, 4-(dipropylamino)-3, 5-dinitro- {Oryzalin®}		4271a	
58.	148-79-8	1*H*-Benzimidazole, 2-(4-thiazolyl)- {Thiabendazole®} 	568b, 2207, 4249	568b, 2207, 3633, 4249	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

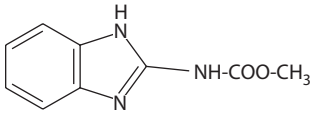
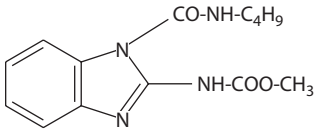
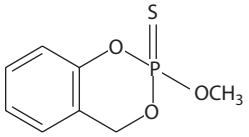
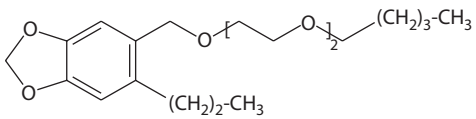
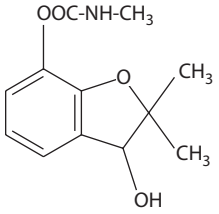
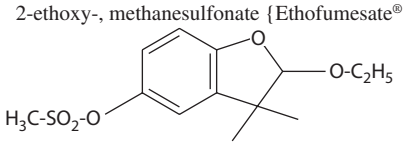
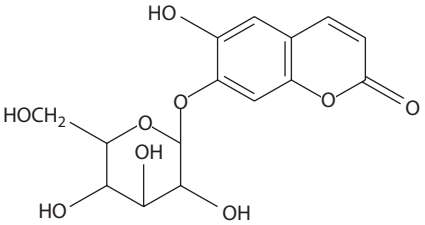
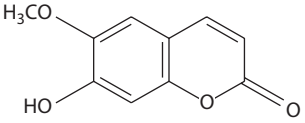
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
59.	10605-21-7	1*H*-Benzimidazole-2-carbamic acid, methyl ester {Carbendazim®} 		3585b	
60.	17804-35-2	1*H*-Benzimidazole-2-carbamic acid, 1-(butylcarbamoyl)-, methyl ester {Benomyl®} 		928a, 1219b, 1219c, 3585b, 3633, 3661a, 4271a, 21A19	
61.	3811-49-2	4*H*-1,3,2-Benzodioxaphosphorin-2-sulfide, 2-methoxy- {Salithion®} 		3381, 3633, 4271a	
62.	51-03-6	1,3-Benzodioxole, 5-[[2-(2-butoxyethoxy) ethoxy]methyl]-6-propyl- {piperonyl butoxide} 		3633, 4271a	
63.	16655-82-6	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate) {3-Hydroxycarbofuran®} 	1553, 21A19	1280, 1553, 1884, 3481, 5811b, 21A19	
64.	26225-79-6	7-Benzofuranol, 2,3-dihydro-3,3-dimethyl- 2-ethoxy-, methanesulfonate {Ethofumesate®} 		3633, 4271a	
65.	1918-00-9	Benzoic acid, 3,6-dichloro-2-methoxy- {Dicamba®}	4857	3633, 3973, 4249, 4857, 5015, 5521, 5811b	
66.	490-79-9	Benzoic acid, 2,5-dihydroxy- {gentisic acid}	3737, 3741, 3743, 4249, 5811b	3103, 3748, 3749, 3751, 4249, 4914	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
67.	121-34-6	Benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid}	568b, 1235, 1427, 1626, 1884, 1886, 2042–2044, 2046, 2939, 3219, 3302, 3308, 3553, 3712, 3737, 3741, 3743, 3797, 4163, 4249, 4377, 5811b	120, 568b, 908, 952, 1248, 1620, 2270, 2939, 2954 3103, 3219, 3329, 3532, 3560, 3561, 3748, 3749, 3751, 3797, 3973, 3974a, 4092, 4249, 4677, 5811b	
68.	531-58-8	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin} 		1309, 1626, 3797, 4249, 5811b, 5838	
69.	92-61-5	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin} 	419, 568b, 1284, 1373, 1626, 1842, 1884, 1898, 2377, 2524a, 2767, 2939, 3059, 3096, 3168, 3302, 3308, 3553, 3602, 3797, 3891, 3995, 4005–4007, 4119, 4121, 4123, 4124, 4164, 4249, 4319, 4373–4375, 5512, 5811b	72, 120, 254, 404, 568b, 677a, 830a, 831, 834, 835, 840, 890, 966, 1063–1066, 1068–1074, 1112, 1626, 1863, 2014, 2270, 2313a, 2338, 2361, 2389, 2531, 2544, 2557a, 2810–2812, 2914, 2939, 2954, 3059, 3103, 3109, 3161, 3194, 3219, 3329, 3631, 3641, 3646, 3705, 3738, 3794, 3797, 3973, 3974a, 3974b, 3984, 4249, 4269, 4373–4375, 5079, 5081, 5127, 5235, 5591, 5616, 5650, 5652, 5704, 5705, 5745, 5766, 5788, 5808, 5811b, 5830, 5831, 5842, 5876, 5888, 5889	
70.	21637-25-2	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		120, 1626, 1837a, 1971, 2023, 2270, 2939, 3059, 3194, 3555, 3667, 3794, 3797, 3973, 3974a, 4249, 5079, 5255, 5256, 5724, 5747, 5811b, 5888	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

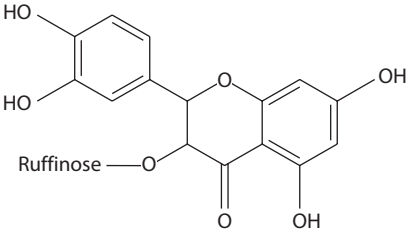
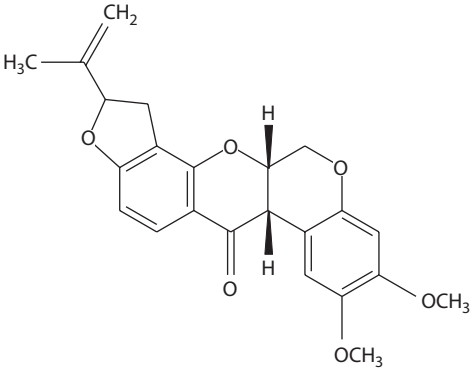
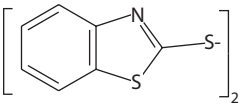
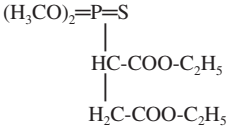
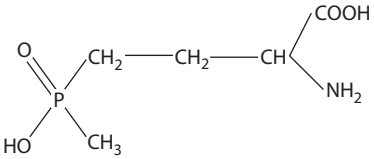
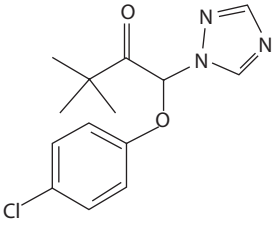
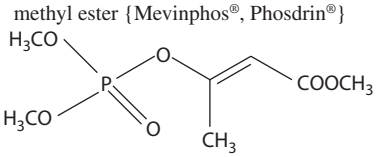
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
71.	153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} 		69, 72, 120, 248, 385, 598, 828b, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1063–1066, 1068–1074, 1309, 1329, 1333, 1485, 1626, 1971, 2014, 2079, 2153a, 2270, 2313a, 2338, 2361, 2379, 2395, 2514, 2529, 2531, 2557a, 2704a, 2810–2812, 2939, 3059, 3096, 3161, 3367a, 3400, 3462, 3551, 3555, 3628, 3629, 3631, 3641, 3646, 3700, 3705, 3738, 3767, 3794, 3974a, 3974b, 3984, 3999, 4005–4007, 4036, 4156, 4157, 4249, 4403, 4999, 5079, 5110, 5156, 5157, 5189, 5204, 5217, 5304, 5305, 5310, 5576, 5591, 5596, 5641, 5652, 5661, 5681, 5697, 5698, 5724, 5747, 5750, 5780, 5788, 5808, 5809, 5811b, 5831, 5834, 5888, 5889	
72.	83-79-4	Benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6a*H*)-one, 1,2,12,12a-tetrahydro-8, 9-dimethoxy-2-(1-methylethenyl)-, [2R-(2α,6aα,12aα)]- {Rotenone®} 		3633, 3634, 21A49, 21A14	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
73.	120-78-5	Benzothiazole, 2,2′-dithiobis- {Thiofide®} 		3476	
74.	8001-35-2	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated {Toxaphene®}		1028, 1029, 3633, 3770, 3973, 4249, 4271a, 5079, 5439	
75.	8001-50-1	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated + bicyclo[3.1.1]hept-2-ene, 2,6, 6-trimethyl-, polychlorinated {Strobane®, Dichloricide®}		3973	
76.	121-75-5	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester {Malathion®} 	1618, 1619, 1884, 3634, 4249, 5811b, 21A19	1219b, 1219c, 1618, 1884, 2058a, 2650b, 3633, 3634, 3767a, 3973, 4249, 4271a, 21A19	
77.	51276-47-2 53369-07-6	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®} 		5521	
78.	43121-43-3	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)- {Triadimefon®} 		3633	
79.	6923-22-4	2-Butenamide, 3-hydroxy-*N*-methyl-, dimethylphosphate, (*Z*)- {Monocrotophos®}		5811, 5811b	
80.	7786-34-7	2-Butenoic acid, 3[(dimethoxyphosphinyl)oxy]-, methyl ester {Mevinphos®, Phosdrin®} 		1219, 2058a, 3379, 3379a, 3380, 3633, 4271a	
81.	39300-45-3	2-Butenoic acid, 2-(1-methylheptyl)-4, 6-dinitrophenyl ester {Dinocap®}		3633, 3661a, 4271a	
82.	101-21-3	Carbamic acid, 3-chlorophenyl-, (1-methylethyl) ester {Chloropropham®}		4271a	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

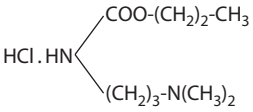
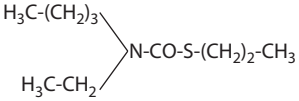
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
83.	23103-98-2	Carbamic acid, dimethyl-, 2-(dimethylamino)-5, 6-dimethyl-4-pyrimidinyl ester {Pirimicarb®}		3633, 4249, 4271a	
84.	25606-41-1	Carbamic acid, 3-(dimethylamino)propyl-, propyl ester, hydrochloride {Propamocarb hydrochloride®} 		3633	
85.	137-42-8	Carbamic acid, *N*-methyldithio-, monosodium salt {Metham-sodium®}		3633, 3646a, 4271a	
86.	9006-42-2	Carbamodithioic acid, 1,2-ethylene(bis-, polymer with ammonia complex of zinc ethylenebis-dithiocarbamate {Metiram®}		429b, 3633, 4249, 4271a, 5525	
87.	1114-71-2	Carbamothioic acid, butylethyl-, *S*-propyl ester {Pebulate®, Tillam®} 		1219b, 1219c, 2913a, 3633, 4271a	
88.	759-94-4	Carbamothioic acid, dipropyl-, *S*-ethyl ester {EPTC®}		3633	
89.	1929-77-7	Carbamothioic acid, dipropyl-, *S*-propyl ester {Vernolate®}		2650a	
90.	2303-17-5	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester {Triallate®}		2650a	
91.	124-38-9	Carbon dioxide	28, 30, 31, 90, 126a, 126b, 162–170, 172, 174, 217, 199, 220, 222–224, 238, 239, 337, 375, 403, 421, 445, 474, 480, 491, 499, 544–546, 568b, 621, 686, 722, 855, 857, 916, 918a, 920, 957, 966, 1048a, 1051, 1063–1074, 1099, 1119, 1140, 1202, 1205, 1208, 1243, 1263, 1284, 1329, 1330, 1332–1334, 1348–1350, 1352, 1354, 1373, 1375a, 1377, 1378, 1388–1390, 1413, 1419, 1420, 1437, 1442, 1445, 1464, 1466, 1468, 1477, 1478, 1492, 1541, 1589, 1600, 1664, 1668, 1673, 1674, 1693, 1709, 1760, 1803, 1837, 1842, 1924, 1935–1937, 1963, 1966, 1977, 2029, 2059, 2060, 2062,2066, 2068, 2079, 2117, 2124, 2133, 2134a, 2142, 2170, 2183, 2196, 2198, 2252, 2263, 2265, 2270, 2293, 2310, 2326, 2342, 2343, 2348, 2457, 2506, 2507, 2524, 2537, 2543, 2545, 2548, 2549, 2555, 2571, 2582, 2624,2634, 2659, 2662,	212, 256, 568b, 1053, 1206a, 2079, 3266, 4249, 4577, 4795, 4926, 5079, 5132, 5165, 5189, 5192, 5193, 5811b, 17B40	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 2506, 2507, 3192, 4052, 4056, 4249

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Carbon dioxide (cont.)	2683, 2761, 2762, 2777, 2780, 2782, 2798, 2799, 2799a, 2804, 2866, 2867, 2913, 2919, 2920–2922, 2928, 2939, 2942, 2973, 3059, 3088, 3102, 3116, 3120, 3121, 3132, 3190, 3224, 3254, 3255, 3257, 3266, 3302, 3308, 3317, 3324, 3336, 3378, 3412, 3482, 3493, 3511, 3516, 3522, 3548, 3564, 3640, 3795, 3870, 3876, 3880, 3882, 3883, 3897, 3909, 3910, 3929, 3930, 3939, 3973, 3987, 3992, 4052, 4055, 4056, 4064, 4067, 4078a, 4079, 4145, 4162, 4212, 4215, 4249, 4251, 4319, 4332, 4360, 4364, 4365, 4406, 4418, 5047, 5079, 5140, 5207, 5359, 5512, 5811b		
92.	75-15-0	Carbon disulfide	237, 722, 1140, 1373, 1420, 1422, 1741,1831, 2310, 2313a, 2799a, 2939, 2940, 2945, 3255, 3257, 3265, 3300, 3302, 3729, 3797, 4249, 4319, 4332, 5039, 5811b, 5869a	5079, 5189, 21A05	
93.	75-44-5	Carbon oxychloride {phosgene} $COCl_2$	1375b (0), 3254 (0), 3901a (0), 4249, 5046, 5059	2483a, 4249	
94.	56-23-5	Carbon tetrachloride	5811b	4249, 4271a	
95.	7440-50-8	Copper	50, 160, 273, 769, 966, 1227, 1329, 1445, 2079, 2214, 2270, 2460, 2524a, 2630, 2633, 2792, 2799a, 2939, 3302, 3308, 3876, 4134, 4005–4007, 4229, 4230, 4242, 4249, 4319, 5079, 5811b, 5859a	193, 250, 769, 1127b, 1219, 1227, 1445, 2079, 2270, 2338, 2460, 2792, 2939, 3633, 3797, 3973, 3974a, 3974b, 4249, 4357, 5079, 5094, 5137, 5189, 5261, 5270, 5285, 5417, 5514, 5811b, 20A26	50, 641, 4249
96.	1317-39-1	Copper oxide		3633, 4271a	
97.	1332-40-7 1332-65-6	Copper oxychloride {RAME}		3633	
98.	8012-69-9	Copper oxychloride sulfate $Cu_2Cl(OH)_3 + Cu_4(OH)_6(SO_4)$		3633	
99.	156-62-7	Cyanamide, calcium salt		3633, 4249	
100.	590-28-3	Cyanic acid, potassium salt		3633, 4249	
101.	608-73-1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {BHC, Lindane®}	644, 2160, 2697, 4249	644, 2544, 2650b, 2697, 3492, 3663, 3634, 3770, 3973, 4249, 4436, 5079, 5439	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

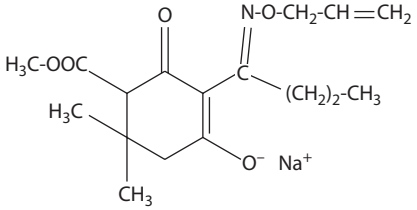
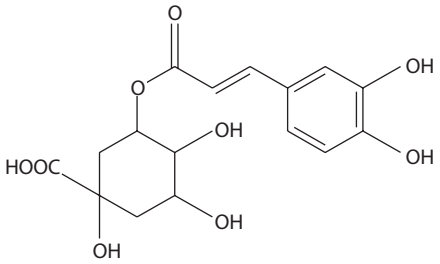
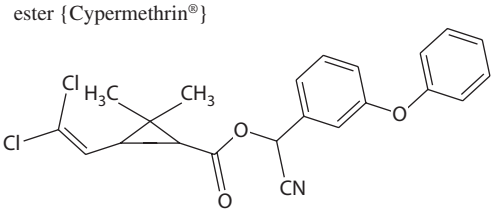
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
102.	319-84-6	Cyclohexane, 1,2,3,4,5,6-hexachloro- {alpha-HCH, HCH-Alpha, α-Lindane®}	518, 644, 1000, 1006, 4249, 21A19	518, 644, 1000, 1006, 1219, 1219b, 1219c, 1740, 2650b, 3633, 3634, 3770, 3973, 4249, 21A19	
103.	319-85-7	Cyclohexane, 1,2,3,4,5,6-hexachloro- {β-Lindane®}	518, 1000, 1006, 4249	518, 1000, 1006, 1740, 2650b, 3633, 3634, 3770, 3973	
104.	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1α,2α,3β,4α,5α,6β)- {gamma-HCH, HCH-Gamma, γ-Lindane®}	518, 644, 1000, 1006, 2697, 4249, 21A19	518, 644, 1000, 1006, 1740, 2389, 2544, 2650b, 2697, 3188a, 3633, 3634, 3770, 3973, 4249, 4271a, 5811b, 21A19	
105.	319-86-8	Cyclohexane, 1,2,3,4,5,6-hexachloro- {δ-Lindane®}	518, 1000, 1006, 4249	518, 1000, 1006, 1740, 2650b, 3633, 3770, 3973, 4249	
106.	55635-13-7	Cyclohexanecarboxylic acid, 2,2-dimethyl-2, 4-dioxo-3-(1-((2-propenyloxy)amino)butylidene)-, methyl ester, sodium salt {Alloxydim-sodium®} 		3633, 4271a	
107.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid} 	172, 602, 1884, 3257, 3302, 3792, 3797, 4249, 5811b	69, 72, 120, 254, 385, 486, 598, 602, 657, 665, 677b, 718, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1040, 1063–1066, 1068–1074, 1077b, 1309, 1329, 1333, 1352, 1485, 1625, 1626, 1923, 2014, 2056a, 2079, 2154, 2250a, 2270, 2283, 2313a, 2338, 2361, 2395, 2514, 2531, 2529, 2557a, 2810–2812, 2911c, 2911d, 2914, 2939, 2954, 3029, 3059, 3096, 3161, 3302,	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid} (cont.)		3366a, 3367a, 3400, 3459–3462, 3551, 3616, 3628, 3631, 3641, 3646, 3655b, 3700, 3705, 3738, 3748, 3749, 3751, 3754, 3792, 3794, 3797, 3806, 3973, 3974a, 3974b, 3984, 3999, 4005–4007, 4156, 4221, 4249, 4275, 4279, 4372, 4402, 4403, 4421, 4999, 5079, 5189, 5200, 5246, 5353, 5389, 5576, 5592–5594, 5596, 5604, 5652, 5665, 5672, 5673, 5681, 5697, 5698, 5700, 5705, 5713, 5722, 5737, 5761, 5782, 5784, 5788, 5808–5810, 5811b, 5812, 5827, 5831, 5834, 5839, 5850, 5856, 5889, 3890, 5896, 5900, 5908	
108.	74051-80-2	2-Cyclohexen-1-one, 2-[1-(ethoximino) butyl]-5-[2-(ethylthio)-propyl]-3-hydroxy- {Sethoxydim®}		3633	
109.	91465-08-6	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {λ-Cyhalothrin®}	21A19	2650b, 21A19	
110.	52315-07-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {Cypermethrin®} 	21A19	904, 1219b, 1219c, 3188a, 3585e, 3633, 4249, 4271a, 5568, 21A19	
111.	67375-30-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl) methyl ester {α-Cypermethrin®}	21A19	3633, 21A19	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

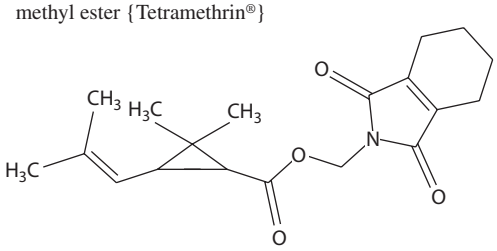
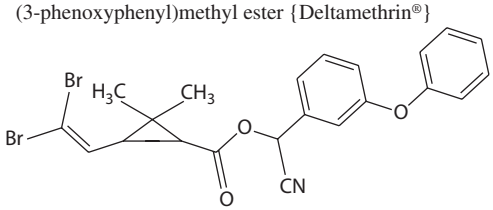
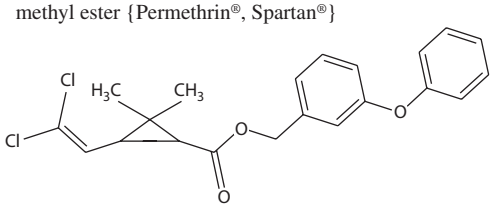
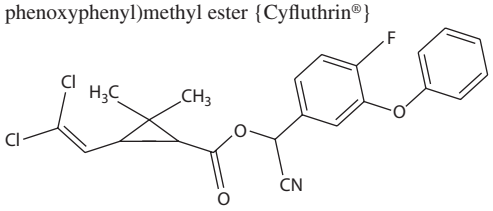
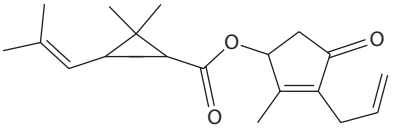
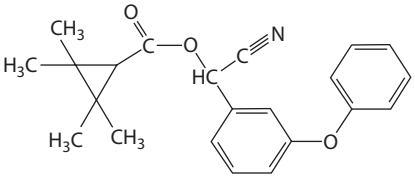
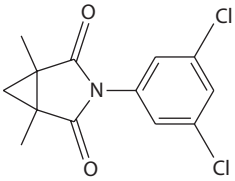
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
112.	121-29-9	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {Pyrethrin II}		3633, 3634	
113.	7696-12-0	Cyclopropanecarboxylic acid, 2, 2-dimethyl-3-(2-methyl-1-propenyl)-, (1-cyclohexene-1,2-dicarboximido) methyl ester {Tetramethrin®} 		904	
114.	121-21-1	Cyclopropanecarboxylic acid, 2, 2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {Pyrethrin I}		3633, 3634	
115.	10453-86-8	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, (5-phenylmethyl-3-furanyl)methyl ester {Resmethrin®}		21A05	
116.	52918-63-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano (3-phenoxyphenyl)methyl ester {Deltamethrin®} 	21A19	904, 1219b, 1219c, 3585e, 3633, 4271a, 21A19	
117.	52645-53-1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl) methyl ester {Permethrin®, Spartan®} 		904, 1219a, 1219b, 1219c, 2346, 2892a, 3188a, 3585e, 3633	
118.	68359-37-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester {Cyfluthrin®} 		904, 3633	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
119.	25402-06-6	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 3-(2-butenyl)-2-methyl-4-oxo-2-cyclopenten-1-yl ester {Cinerin I}		3633	
120.	4466-14-2	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester {Jasmolin 1}		3633	
121.	584-79-2	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl ester, (*E*)- {Allethrin®} 		3973, 4271a	
122.	66841-25-6	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-, cyano(3-phenoxyphenyl) methyl ester {Tralomethrin®}		21A05	
123.	39515-41-8	Cyclopropane carboxylic acid, 2,2,3,3-tetramethyl cyano(3-phenoxyphenyl)methyl ester {Fenpropathrin®, Danitol®} 	21A19	21A19	
124.	82657-04-3	Cyclopropanecarboxylic acid, 3-[(1*Z*)-2-chloro-3,3,3-trifluoro-1-propenyl]-2,2-dimethyl-, (2-methyl[1,1′-biphenyl]-3-yl)methyl ester, (1R,3R)-rel- {Bifenthrin®, Biphenthrin®}		21A05	
125.	32809-16-8	1,2-Cyclopropanedicarboximide, *N*(3,5-dichlorophenyl)-1,2-dimethyl- {Procymidone®} 		3585c	
126.	334-48-5	Decanoic acid {capric acid} H_3C-$(CH_2)_8$-COOH	60, 563, 565, 568b, 809, 1132, 1232, 1348, 1360, 1375, 1375a, 1375b, 1668, 1884, 2418, 2939, 3266, 3293, 3308, 3553, 3797, 4249, 4993, 5079, 5811b	60, 120, 172a, 174b, 404, 524, 568b, 848, 908, 565, 1053, 1893a, 1893b, 2270, 2356, 2283, 2389, 2544, 2592, 2611, 2917a, 3266, 3370, 3543, 3545, 3547, 3560, 3561, 3633, 3767a, 3974a, 4249, 4993, 5657, 5695, 5811b	1360, 1375a

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

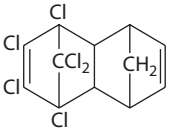
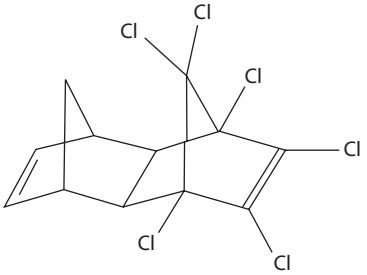
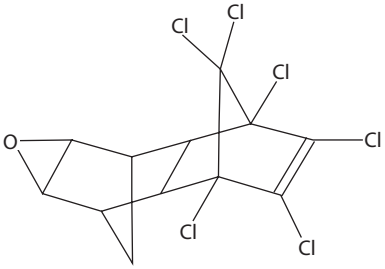
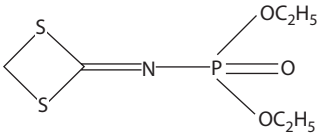
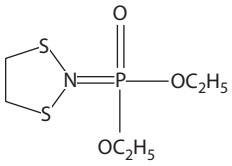
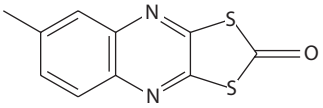
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
127.	112-30-1	1-Decanol {capric alcohol}	172, 568b, 1333, 1365, 3255, 3559, 4249, 5811b	568b, 1053, 1157, 1333, 2650a, 2650b, 3266, 3370, 3633, 3811a, 3973, 3977, 4098a, 4249, 5811b	
128.	309-00-2	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10, 10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5α,8α,8aβ)- [*endo, endo*] {Aldrin®} 	518, 644, 2697, 3633, 4249	518, 644, 1333, 1457, 2389, 2544, 2650a, 2650b, 2697, 3138, 3188a, 3633, 3770, 3973, 3977, 4249, 4271a, 5811b	
129.	465-73-6	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10, 10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5β,8β,8aβ)- [*endo, exo*] {Isodrin®} 		3770, 4249	
130.	60-57-1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9, 9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aα,3β,6β,6aα,7β,7aα)- {Dieldrin®} 	518, 644, 1000, 1006, 1884, 2697, 4249, 21A19	518, 644, 1029, 1000, 1006, 1219, 1219a, 1219b, 1333, 1740, 1884, 2650a, 2650b, 2697, 3188a, 3633, 3767a, 3770, 3797, 3915, 3973, 3977, 4249, 4271a, 5811b, 21A19	
131.	72-20-8	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4, 5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aβ,3α,6α,6aβ,7β,7aα)- {Endrin®}	415, 419, 518, 644, 1000, 1006, 1457, 1884, 2697, 3634, 4249, 21A19	415, 419, 518, 644, 1000, 1006, 1028, 1029, 1219, 1219a, 1333, 1457, 1740, 1884, 2318, 2389, 2544, 2650b, 2697, 2939, 3188a, 3633, 3634, 3637, 3767a, 3770, 3915, 3973, 3977, 4249, 4271a, 5811b, 21A19	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
132.	21548-32-3	1,3-Dithietan-2-ylidenephosphoramidic acid, diethyl ester {Fosthietan®} 		3633	
133.	947-02-4	Dithiolan-2-ylidenephosphoramidic acid, diethyl ester {Cyolane®, Phosfolan®} 		3380	
134.	2439-01-2	1,3-Dithiolo[4,5-b]quinoxalin-2-one, 6-methyl- {Quinomethionate®} 		3633	
135.	40596-69-8	2,4-Dodecadienoic acid, 11-methoxy-3, 7,11-trimethyl-, 1-methylethyl ester, (*E,E*)- {Kabat, Minex, Methoprene®, Altosid®} $(H_3C)_2{=}C(OCH_3)\text{-}(CH_2)_3\text{-}CH(CH_3)\text{-}CH_2\text{-}CH{=}CH\text{-}C(CH_3){=}CH\text{-}COO\text{-}CH(CH_3)_2$	1242, 1243, 21A19	1053, 1242, 1243, 1588, 2483a, 3266, 3633, 21A19	
136.	143-07-7	Dodecanoic acid {lauric acid} $H_3C\text{-}(CH_2)_{10}\text{-}COOH$	60, 172, 257, 258, 568b, 765, 809, 1132, 1232, 1375, 1586, 1785, 1906, 2418, 2529, 2570, 2767, 2939, 3266, 3293, 3302, 3308, 3557, 4030, 4249, 4319, 4993, 5079, 5811b	60, 101, 120, 172a, 174b, 404, 568b, 908, 1053, 1785, 1893a, 1893b, 2092, 2093, 2270, 2283, 2339a, 2356, 2529, 2862, 2917a, 3194, 3266, 3370, 3547, 3633, 3973, 3974a, 4249, 4280, 4993, 5695	
137.	112-53-8	1-Dodecanol {lauryl alcohol} $H_3C\text{-}(CH_2)_{10}\text{-}CH_2OH$	172, 568b, 2601a, 3559, 4249	58, 568b, 2356, 3633, 4098a, 4249	
138.	4602-84-0 3790-71-4	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- {farnesol}	1586, 2601a, 2767, 3224, 3251, 3266, 3284, 3285, 3302, 3557, 4249, 4570a, 5811b	172a, 174b, 404, 909, 1053, 2386, 2917a, 3266, 4249	
139.	106-93-4	Ethane, 1,2-dibromo- {ethylene dibromide, EDB®, Bromofume®} $Br\text{-}CH_2\text{-}CH_2\text{-}Br$		3188a, 3633, 3646a, 3973, 4249, 4271a, 5811b	
140.	25323-89-1	Ethane, 1,2,2-trichloro-		4249, 4271a	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

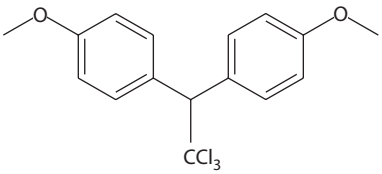
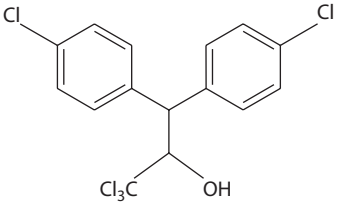
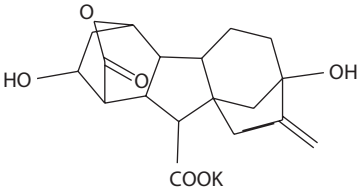
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
141.	72-43-5	Ethane, 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)- {Methoxychlor®} 		3188a, 3663, 3770, 4249, 4271a	
142.	23135-22-0	Ethanimidothioic acid, 2-(dimethylamino)-*N*-[[(methylamino)carbonyl]oxy]-2-oxo-, methyl ester {Oxamyl®} $(H_3C)_2$═N-CO-C(S-CH_3)═N-OOC-NH-CH_3		1280, 3633, 3634, 3646a, 3973, 4249, 4271a, 4891	
143.	59669-26-0	Ethanimidothioic acid, *N′,N′*-(thiobis ((methylimino)carbonyloxy))bis-, dimethyl ester {Thiodicarb®} S═[NH-COO-N═C(CH_3)-SCH_3]$_2$		3633	
144.	115-32-2	Ethanol, 2,2,2-trichloro-1,1-bis(4-chlorophenyl)- {Dicofol®} 		3633	
145.	74-85-1	Ethene {ethylene} H_2C═CH_2	85, 141, 143, 147, 151, 173a, 216, 239, 298, 544–546, 604, 605, 710, 722, 966, 1099, 1140, 1243, 1365, 1375a, 1377, 1437, 1445, 1472, 1664, 1821, 1842, 2060, 2079, 2252, 2270, 2293, 2310, 2583, 2634, 2782, 2799a, 2804, 2857, 2866, 2909, 2939, 2942, 2946, 3059, 3105, 3255, 3302, 3308, 3493, 3729, 3797, 3880, 3882, 3883, 3888, 3901, 3939, 4052, 4056, 4057, 4135, 4162, 4249, 4319, 4393, 5811b, 5835	2913a, 3633, 3973, 5811b	1228, 1375a, 1377, 3901, 4052, 4056
146.	125-67-7	Gibb-3-ene-1,10-dicarboxylicacid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, potassium salt {gibberellic acid, potassium salt} 		3633, 4249	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
147.	142-62-1	Hexanoic acid {caproic acid} $H_3C\text{-}(CH_2)_4\text{-}COOH$	172, 526, 563, 565, 568b, 960, 1132, 1140, 1232, 1360, 1364, 1365, 1371, 1375a, 1586, 1587a, 1668, 1903, 2079, 2088, 2271, 2338, 2543, 2545, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3263, 3266, 3308, 3410, 3555, 3557, 3797, 3799, 3800, 3809, 4064, 4249, 4319, 4993, 5079, 5811, 5811b	120, 172a, 174b, 404, 563, 568b, 848, 908, 1053, 1085, 1587a, 1590a, 1982, 1999, 2014, 2079, 2271, 2283, 2338, 2356, 2386, 2389, 2544, 2570, 2611, 2722, 2862a, 2917a, 2939, 3219, 3266, 3329, 3370, 3507, 3545, 3547, 3549, 3555, 3560, 3561, 3633, 3767a, 3797, 3973, 3974b, 4131, 4249, 4993, 5695, 5708, 5811, 5811b, 5846	1360, 1375a, 3393
148.	111-27-3	1-Hexanol {caproyl alcohol} $H_3C\text{-}(CH_2)_4\text{-}CH_2OH$	172, 568b, 1419, 3555, 4249, 5811b	172a, 174b, 568b, 937, 1053, 2339a, 2917a, 3266, 3547, 3555, 4249, 5811b	
149.	74-90-8	Hydrocyanic acid {hydrogen cyanide} HCN	80–83, 110, 112, 126b, 167, 172, 174a, 174b, 174c, 174e, 213, 237–239, 267, 269, 270, 314, 337, 402, 429a, 480, 491, 513, 577, 603, 631, 688, 722, 747, 748, 765, 779, 780, 804, 861, 916, 918a, 920, 966, 1051, 1063–1074, 1077a, 1091, 1092, 1099, 1119, 1140, 1202, 1235, 1276, 1283, 1284, 1292, 1329, 1330, 1332–1336, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1331, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1442, 1445, 1466, 1467, 1469, 1492, 1497, 1498, 1589, 1668, 1673, 1674, 1693, 1695, 1719, 1741, 1746, 1751, 1760, 1781, 1803, 1807a, 1842, 1932, 1956, 1966, 1967, 2059, 2062, 2067, 2068, 2079, 2083–2086, 2133, 2134a, 2142, 2157, 2159, 2170, 2252, 2270, 2293, 2310, 2313a, 2313c, 2313d, 2326, 2342, 2342a, 2343, 2344, 2502, 2506, 2507, 2537, 2543, 2545, 2570, 2607, 2608, 2628, 2634, 2679, 2683, 2724, 2761, 2762, 2775, 2777, 2780, 2782,	2607, 3290, 3633, 4064, 4271a, 5079, 5189, 5811b	1330 (0), 1332 (0), 1354, 1375a, 1377, 1378, 2506, 2507, 4052, 4056, 4249

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

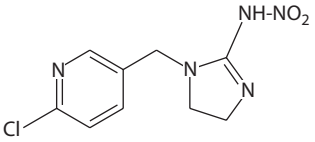
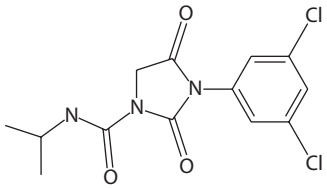
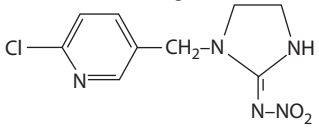
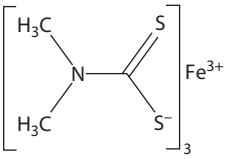
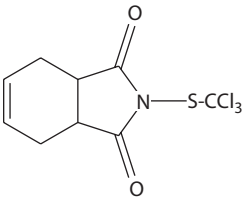
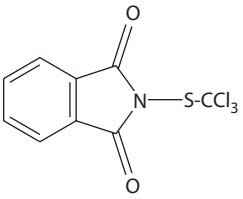
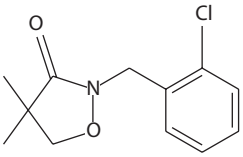
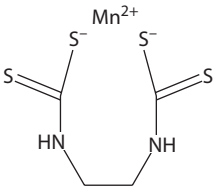
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Hydrocyanic acid {hydrogen cyanide} (cont.)	2799a, 2801, 2804, 2805, 2866, 2939, 2942, 2956, 2971, 2973, 3007, 3029, 3059, 3087, 3088, 3101, 3116, 3120, 3121, 3121a, 3132, 3135–3137, 3139, 3140, 3145, 3148, 3149, 3190, 3251, 3254, 3255, 3257, 3290, 3300–3302, 3306, 3308, 3370, 3482, 3491, 3493, 3524, 3525, 3530, 3557, 3690, 3724, 3729, 3844, 3872, 3876, 3880–3882, 3897, 3909–3911, 3917a, 3939, 3952, 3973, 3976, 3984, 3992, 3996, 4005–4007, 4010, 4011, 4052, 4053, 4056, 4063, 4064, 4109, 4143, 4162, 4202, 4249, 4259, 4260, 4301, 4319, 4342, 4360, 4365, 4398, 4418, 4502, 4743, 4745, 4816, 5042, 5079, 5140, 5189, 5208, 5219, 5263, 5531, 5546, 5547, 5554, 5587, 5811b, 5835, 5836, 5869a		
150.	105827-78-9	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl) methyl)-4,5-dihydro-*N*-nitro- {Admire®} 		2892a, 4249	
151.	36734-19-7	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2, 4-dioxo- {Iprodione®} 		3585c, 3633, 3661a	
152.	138261-41-3	Imidazolidinimine, 1-((6-chloro-3-pyridinyl)methyl)-*N*-nitro- {Imidacloprid®} 	568b, 4249, 21A19	568b, 4249, 5064, 5568, 21A19	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
153.	87-51-4	1*H*-Indole-3-acetic acid	5811b	2058b, 3973, 4249, 5743, 5811b, 5854	
154.	133-32-4	1*H*-Indole-3-butanoic acid		3580a, 4249, 4487	
155.	14484-64-1	Iron, tris(dimethylcarbamodithioato-S,S′)-, (OC-6-11)- {Ferbam®} 		186, 3481, 3491, 3513, 3633, 4249, 4271a	
156.	133-06-2	1*H*-Isoindole-1,3(2*H*)-dione, 3a,4,7, 7a-tetrahydro-2- [(trichloromethyl)thio]- {Captan®} 	1884, 3302, 4249, 21A19	1219c, 1884, 3633, 21A19	
157.	133-07-3	1*H*-Isoindole-1,3(2*H*)-dione, 2-[(trichloromethyl) thio]- {Folpan®} 		3633	
158.	556-61-6	Isothiocyanic acid, methyl- {Trapex®} $H_3C\text{-}N{=}S$	4570A	3633, 3646a, 3973, 4271a	
159.	81777-89-1	3-Isoxazolidinone 2-[(2-chlorophenyl)methyl]-4, 4-dimethyl- {Clomazone®} 		2913a, 3633	
160.	12427-38-2	Manganese, [[1,2-ethanediylbis[carbamodithioato]] (2-)]- {Maneb®} 		3491, 3513, 3633, 3661a, 4249, 4271a, 5811b, 21A19	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

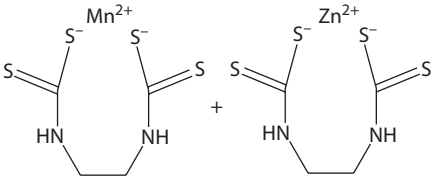
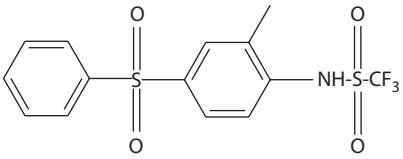
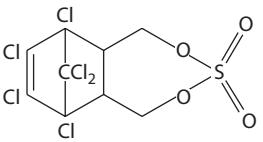
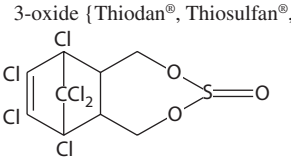
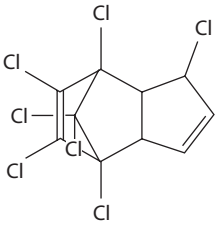
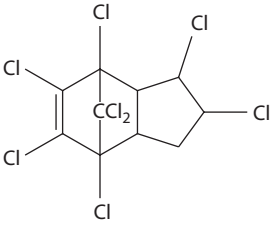
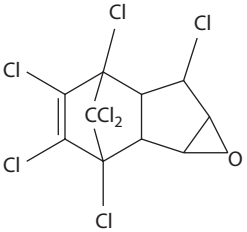
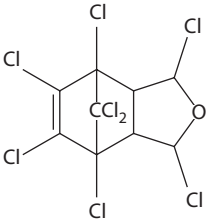
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
161.	8018-01-7	Manganese, [[1,2-ethanediylbis[carbamodithioato]] (2-)] + zinc, [[1,2-ethanediylbis-[carbamodithioato]] (2-)] {Mancozeb} 		2892a, 3633, 4271a, 5811b	
162.	9002-91-9	Metaldehyde {acetaldehyde tetramer}		3633, 3973	
163.	74-83-9	Methane, bromo- {Brom-o-Gas®, Meth-o-Gas®, ProFum®, Terr-o-Gas®, Zytox®}	1884, 3255	3633, 3634, 3646a, 3722b, 3973, 5811b	
164.	74-87-3	Methane, chloro- H_3C-Cl	112, 126b, 199, 172, 239, 298, 348, 604, 605, 621, 712, 1140, 1153, 1154, 1375a, 1377, 1437, 1440, 1939, 1962, 1966, 2060, 2079, 2142, 2270, 2634, 2782, 2939, 2940, 3059, 3106, 3255, 3302, 3308, 3493, 3583, 3584, 3692, 3882, 3901, 3939, 4005–4007, 4052, 4056, 4162, 4249, 4395, 5811b, 5869a	722, 1595, 4249	1375a, 1377, 3901, 4052, 4056, 4249
165.	75-09-2	Methane, dichloro- $H_2C{=}Cl_2$	222–224, 568b, 712, 1140, 4249, 5811b	568b, 984, 1595, 4249	
166.	76-06-2	Methane, nitrotrichloro- {Chloropicrin®}		3633, 3646a, 3973	
167.	67-66-3	Methane, trichloro- {chloroform} H-CCl_3	39, 568b, 703, 712, 1939, 3300, 4249, 4570a, 5811b, 5869a	568b, 722, 4249	641, 4249
168.	37924-13-3	Methanesulfonamide, trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl)- {Perfluidone®} 		4271a	
169.	1031-07-8	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10, 10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3, 3-dioxide {Thiodan® sulfate, Endosulfan® sulfate} 	644, 1619, 3634, 4249, 21A19	644, 1028, 1219, 1219a, 1458, 1619, 1884, 2650a, 3188a, 3633, 3634, 3770, 3797, 3915, 4249, 21A19	
170.	115-29-7	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8, 9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide {Thiodan®, Thiosulfan®, Endosulfan®} 	419, 644, 1457, 1619, 1884, 3302, 3634, 4249, 4858	419, 644, 1028, 1219, 1219a, 1219b, 1219c, 1457, 1458, 1619, 1884, 2650a, 2650b, 3188a, 3633, 3634, 3770, 3797, 3973, 4249, 4271a, 4858, 5811b	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
171.	33213-65-9	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10, 10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aα,6β,9β,9aα)- {β-Endosulfan®}	644, 3634, 4249	644, 2650a, 3188a, 3633, 3634, 3770, 4249, 5811b	
172.	959-98-8	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10, 10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aβ,6α,9α,9aβ)- {α-Endosulfan®}	3634, 4249	2650a, 3633, 3634, 3770, 4249, 5811b	
173.	76-44-8	4,7-Methano-1*H*-indene, 1,4,5,6,7,8,8-heptachloro-3a, 4,7,7a-tetrahydro- {Heptachlor®} 	606, 2697, 4249, 21A19	2697, 3138, 3188a, 3633, 3770, 3973, 4249, 4271a, 21A19	
174.	5103-71-9	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8, 8-octachloro-2, 3,3a,4,7,7a-hexahydro- {α-Chlordane®} 		1219, 1219a, 1219b, 3138, 3633, 3634, 3770, 3973, 4249, 4271a	
175.	57-74-9 12789-03-6	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8, 8-octachloro-2, 3,3a,4,7,7a-hexahydro- {γ-Chlordane®}		2650b, 3138, 3188a, 3633, 3634, 3770, 4249, 5811	
176.	1024-57-3	2,5-Methano-2*H*-indeno[1,2-*b*]oxirene, 2,3,4,5,6,7, 7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)- {Heptachlor epoxide®} 	606, 4249	1219, 1219a, 1219b, 3188a, 3633, 3770, 4249	
177.	297-78-9	4,7-Methanoisobenzofuran, 1,3,4,5,6,7,8, 8-octachloro-1,3,3a,4,7,7a-hexahydro- {Isobenzan®, Telodrin®} 	1457, 1458, 1884, 4249, 21A191	1457, 1884, 3797, 4249, 21A19	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

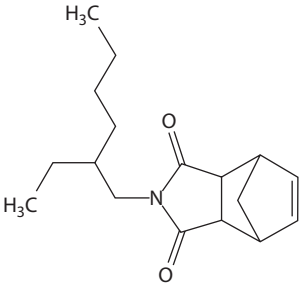
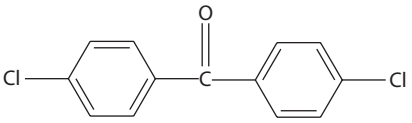
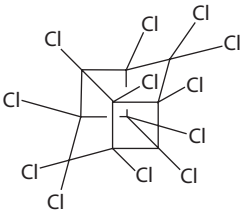
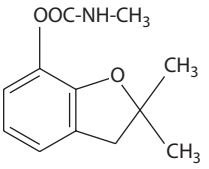
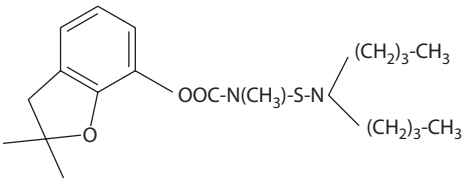
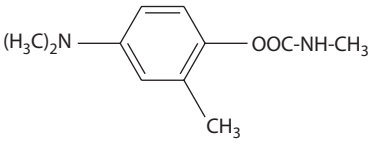
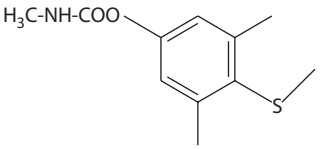
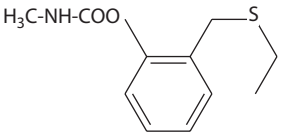
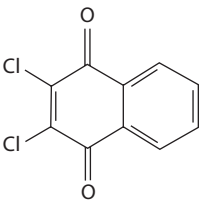
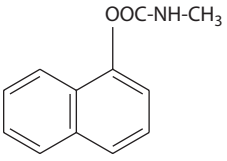
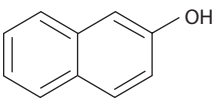
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
178.	113-48-4	4,7-Methano-1*H*-isoindole-1,3(2*H*)-dione, 2-(2-ethylhexyl)-3a,4,7,7a-tetrahydro-		3633	
					
179.	5293-97-0	Methanone, bis(2-chlorophenyl)-	2570, 4249	2389, 2544, 4249	
180.	90-98-2	Methanone, bis(4-chlorophenyl)-	707, 708, 713, 714, 2570, 4249	4249, 5811b	
					
181.	2385-85-5	1,3,4-Metheno-1*H*-cyclobuta[*cd*]) pentalene, 1,1a,2,2,3,3a,4,5,5,5a,5b, 6-dodecachlorooctahydro- {Mirex®}	21A19	21A19	
					
182.	1563-66-2	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester Sometimes listed as 7-benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate {Furadan®, Carbofuran®}	1553, 21A19	1280, 1553, 2650b, 3481, 3633, 3973, 4249, 4271a, 5811b, 21A19	
					
183.	55285-14-8	Methylcarbamic acid, 2,3-dihydro-2, 2-dimethyl-7-benzofuranyl [(di-*N*-butylamino)thio] ester {Carbosulfan®}		3633	
					

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
184.	2032-59-9	Methylcarbamic acid, 4-(dimethylamino)-3-methylphenyl {Aminocarb®} 		2650a, 3633, 4271a	
185.	2032-65-7	Methylcarbamic acid, 3,5-dimethyl-4-(methylthio) phenyl- {Methiocarb®} 		3633, 4271a	
186.	29973-13-5	Methylcarbamic acid, 2-((ethylthio)methyl) phenyl- {Ethiofencarb®} 		3633, 4271a	
187.	110488-70-5	Morpholine, 3-(3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl)- {Dimethomorph®, Acrobat®}		2892a, 3633, 4249	
188.	86-87-3	1-Naphthaleneacetic acid		3973	
189.	117-80-6	Naphthalene-1,4-dione, 2,3-dichloro- {Diclone®} 	3797	2095, 3797, 4249, 4666a	
190.	63-25-2	1-Naphthalenol, methylcarbamate {Sevin®, Carbaryl®} 	418, 419, 1333, 1457, 1884, 3224, 3302, 3634, 21A19	418, 419, 1219a, 1219c, 1280, 1333, 1457, 1884, 2650b, 2698, 3481, 3633, 3634, 3637, 3727, 3797, 3973, 3977, 4249, 4271a, 5811b, 21A19	
191.	135-19-3	2-Naphthalenol {2-naphthol = β-naphthol} 	414, 568b, 765, 786–789, 789a, 869, 1025, 1365, 1378, 1626, 1649, 1879, 1884, 2079, 2195, 2939, 3059, 3263, 3302, 3474, 3616, 3746, 3747, 3753, 3797, 3999, 4005–4007, 4249, 4319, 5811b, 21A19	568b, 4249, 21A19	1378, 3395, 4249

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

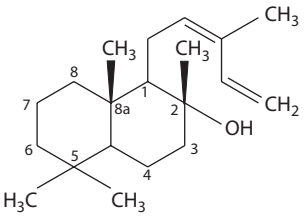
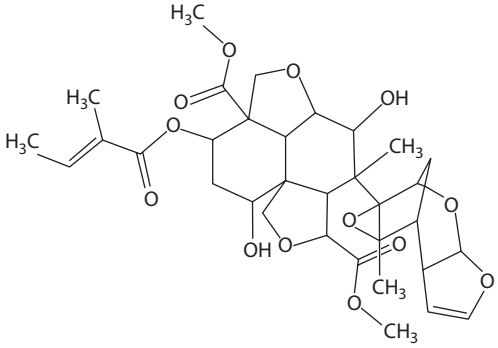
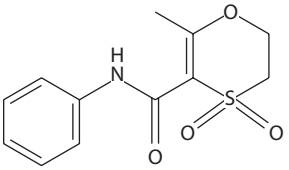
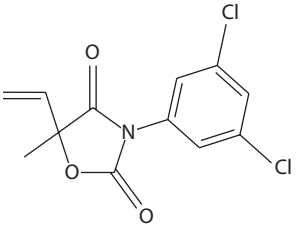
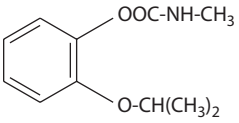
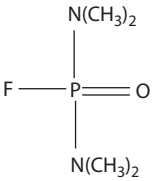
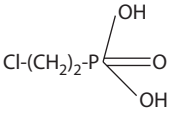
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
192.	1616-86-0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-(1α,2β,4aβ,8aα)]-{*Z*-abienol} 		897, 898, 2338, 2341a, 2786, 2914, 3099, 3607, 3613a, 3621, 3703, 3704, 3706, 4073b, 4090, 4094, 4249	
193.	11141-17-6	1*H*,7*H*-Naphtho[1,8*a*,8-*bc*:4,4*a*-*c*′]difuran-3, 7a-dicarboxylic acid, (3*S*,3a*R*,4*S*, 5*S*,5a*R*, 5a[1]*R*, 7a*S*,8*R*,10*S*,10a*S*)-8-acetoxy-3,3a,4,5a,5a[1],7a,8,9, 10-decahydro-3,5-dihydroxy-4-{(1*S*,3*S*,7*S*,8*R*,9*S*,11*R*)-7-hydroxy-9-methyl-2,4,10-trioxatetracyclo [6.3.1.0[3,7].0[9,11]]dodeca-5-en-11-yl}-4-methyl-10 [(*E*)-2-methylbut-2-enoyloxy]-, dimethyl ester {Azadirachtin® A and B, Neem} 		21A01, 21A05a, 21A14a	
194.	8002-65-1	Neem oil		21A01, 21A05a, 21A14a	
195.	124-07-2	Octanoic acid {caprylic acid} $H_3C\text{-}(CH_2)_6\text{-}COOH$	172, 563, 565, 568b, 722, 809, 1132, 1232, 1348, 1364, 1371, 1587a, 1668, 1917, 1971, 2079, 2338, 2543, 2545, 2765, 2773, 2775, 2939, 3266, 3293, 3302, 3308, 3410, 3555, 3797, 4064, 4065, 4249, 4319, 4993, 5079, 5811b	120, 172a, 174b, 404, 568b, 848, 908, 1053, 1085, 1221, 1587a, 1590a, 1893a, 1893b, 1982, 1999, 2014, 2079, 2270, 2283, 2338, 2356, 2389, 2544, 2570, 2611, 2649, 2722, 2917a, 3219, 3266, 3370, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3633, 3767a, 3797, 3973, 3974a, 3974b, 4131, 4249, 4993, 5079, 5180, 5363, 5695, 5811b, 5846	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
196.	111-87-5	1-Octanol {caprylic alcohol}	172, 568b, 4249, 5811b	172a, 174b, 404, 568b, 1053, 2389, 2544, 2913a, 3266, 3547, 3811a, 3973, 4098a, 4249, 5811b	
197.	5259-88-1	1,4-Oxathiin-3-carboxamide 4,4-dioxide, 5, 6-dihydro-2-methyl-*N*-phenyl- {Oxycarboxin®} 		2650b	
198.	50471-44-8	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- {Vinclozolin®} 		2650a	
199.	114-26-1	Phenol, 2-(1-methylethoxy)-, methylcarbamate {Undene®, Propoxur®} 		1280, 2698, 3633, 4249, 4271a	
200.	118-79-6	Phenol, 2,4,6-tribromo-		2650a, 4249	
201.	300-76-5	Phosphate, 1,2-dibromo-2,2-dichloroethyl dimethyl {Naled®}		3633, 4271a	
202.	20859-73-8	Phosphide, aluminum $Al{\equiv}P$		2483a, 3633, 3634, 4249, 4271a	
203.	12057-74-8	Phosphide, magnesium Mg_3P_2		2483a, 3633, 4249, 4271a	
204.	7803-51-2	Phosphine {Detia, Gas Ex-B} PH_3	575, 637, 3302, 4249, 5079	3633, 4271a, 5523, 5811b	641, 4249
205.	115-26-4	Phosphine oxide, bis(dimethylamino)fluoro- {Dimefox®} 		2650b, 3633, 4271a	
206.	16672-87-0	Phosphonic acid, 2-chloroethyl- {Ethephon®, Ethrel®} 		2913a, 3633, 3811a, 3973, 5811b	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

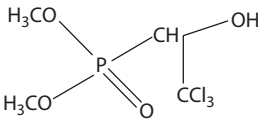
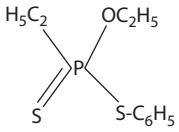
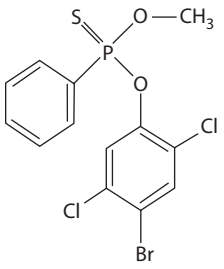
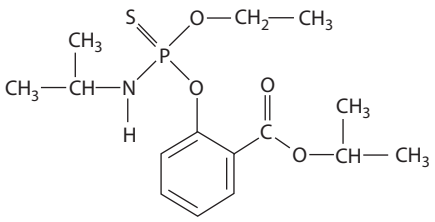
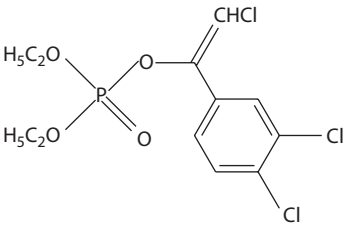
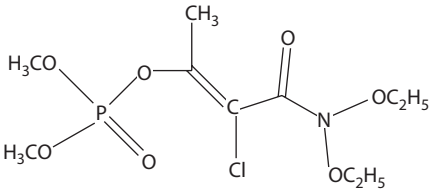
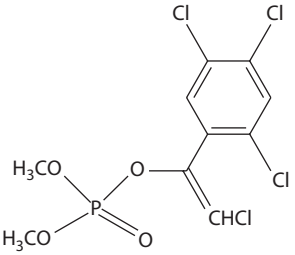
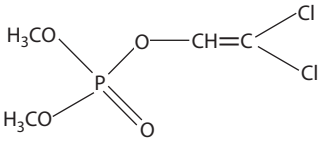
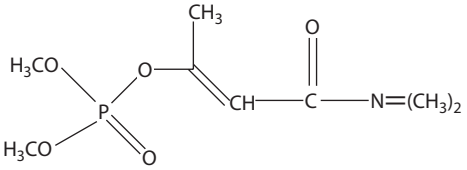
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
207.	52-68-6	Phosphonic acid, 2,2,2-trichloromethyl-1-hydroxyethyl-, dimethyl ester {Trichlorphon®, Dylox®, Dipterex®} 	1333	1333, 2650a, 3380, 3633, 3973, 3977, 4271a	
208.	98886-44-3	Phosphonodithioic acid, *O*-ethyl *S*-(1-methylpropyl) (2-oxo-3-thiazolidinyl)- {Fosthiazate®}		3633	
209.	944-22-9	Phosphonodithioic acid, ethyl-, *O*-ethyl S-phenyl ester {Fonofos®} 		3633, 4271a	
210.	21609-90-5	Phosphonothioic acid, phenyl-, *O*-4-bromo-2, 5-dichlorophenyl *O*-methyl ester {Leptophos®, Phosvel®} 	21A19	3381, 3634, 21A19	
211.	22224-92-6	Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylthio)phenyl ester {Fenamiphos®, Nemacur®}		2856a, 3381, 3633, 3646a, 3973, 4249, 4271a, 5811b	
212.	30560-19-1	Phosphoramidothioic acid, *N*-acetyl-, *O, S*-dimethyl ester {Orthene®, Acephate®}		1219a, 1219b, 1219c, 2058a, 2650b, 3633, 3634, 3973, 4271a	
213.	10265-92-6	Phosphoramidothioic acid, *O,S*-dimethyl ester {Methamidophos®}		2058a, 3633, 4271a, 5811b	
214.	25311-71-1	Phosphoramidothioic acid, *O*-ethyl *O-2* (1-methylethyl)carbonylphenyl-, (1-methylethyl) ester {Isofenphos®} 		3633, 21A61	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
215.	470-90-6	Phosphoric acid, 2-chloro-1-(2-dichlorophenyl) ethenyl-, diethyl ester {Chlorfenvinphos®, Birlane®}		3381, 3633, 4271a	
					
216.	13171-21-6	Phosphoric acid, 2-chloro-3-(diethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Phosphamidon®}		3380, 3633, 4271a	
					
217.	22248-79-9	Phosphoric acid, 2-chloro-1-(2,4,5-trichlrophenyl) ethenyl-, dimethyl ester {Tetrachlorvinphos®}		3381, 3633, 4271a	
					
218.	62-73-7	Phosphoric acid, 2,2,-dichloroethenyl-, dimethyl ester {DDVP, Dichlorvos®}		2058a, 3380, 3633, 4271a	
					
219.	141-66-2	Phosphoric acid, 3-(dimethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Dicrotophos®}		3380	
					

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

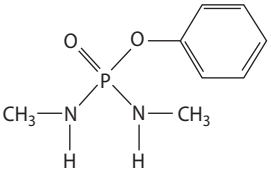
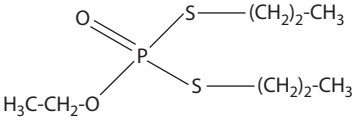
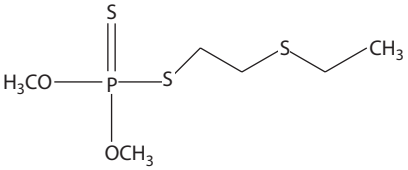
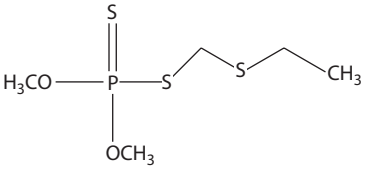
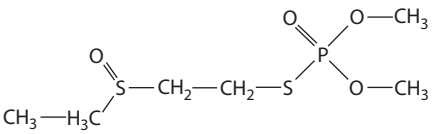
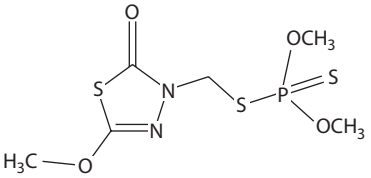
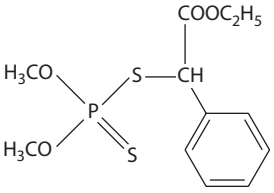
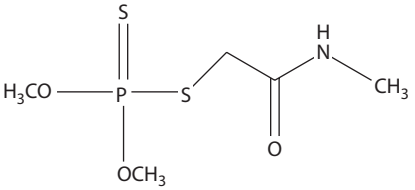
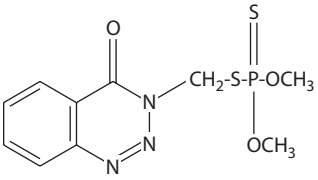
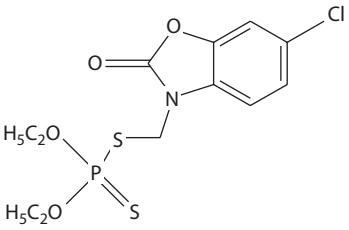
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
220.	1754-58-1	Phosphorodiamidic acid, *N,N′*-dimethyl-, phenyl ester {Diamidafos®} 	2527	1884, 2527, 21A19	
221.	13194-48-4	Phosphorodithioic acid, *O*-ethyl-*S,S*, dipropyl ester {Mocap®, Ethoprop®, Prophos®, Rovokil®, Ethoprophos®} 		2345, 3381, 3633, 3634, 3646a, 3767a, 3973, 4271a	
222.	13071-79-9	Phosphorodithioic acid, O,O-diethyl *S*-[(1,1-dimethylethyl) thio]methyl ester {Terbuphos®}		2650b, 3633	
223.	2497-06-5	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylsulfonyl)ethyl] ester {Thiodemeton sulfone®}		4249	
224.	298-04-4	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester {Di-syston®, Disulfoton®} 	1127, 21A19	1127, 2058a, 2345, 3633, 3634, 3973, 4249, 4271a, 5811b, 21A19	
225.	298-02-2	Phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio) methyl] ester {Phorate®} 		2058a, 3381, 3633, 4271a	
226.	301-12-2	Phosphorodithioic acid, *O*,*O*-dimethyl *S*-[2-(ethylsulfinyl)ethyl] ester {Oxydemeton methyl®} 		3633, 21A22	
227.	640-15-3	Phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Thiometon®}		4271a	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
228.	950-37-8	Phosphorodithioic acid, *O,O*-dimethyl-*S*-2, 3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl ester {Supracide®, Methidathion®} 		2058a, 3633, 3973, 4271a	
229.	2597-03-7	Phosphorodithioic acid, *O,O*-dimethyl-*S*-(α-ethoxycarbonylbenzyl) ester {Fenthoate®, Phenthoate®} 		3381	
230.	60-51-5	Phosphorodithioic acid, *O,O*-dimethyl-*S*-[2-(methylamino)-2-oxoethyl] ester {Dimethoate®} 	5553b, 5811b	3380, 3633, 3797, 3973, 4271a, 5811b	
231.	2642-71-9	Phosphorodithioic acid, *O,O*-diethyl *S*-[(4-oxo-1,2, 3-benzotriazin-3(4*H*)-yl)methyl] ester {Azinphos-ethyl®}		3633, 4271a,	
232.	86-50-0	Phosphorodithioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2, 3-benzotriazin-3(4*H*)-yl)methyl] ester {Guthion®, Azinphos-methyl®} 	417, 419, 1457, 1884, 3302, 4249, 21A19	419, 1219a, 1219c, 1457, 1884, 2650b, 3381, 3973, 4249, 4271a, 21A19	
233.	2310-17-0	Phosphorodithioic acid, *S*-[(6-chloro-2-oxo-3 (2*H*)-benzoxazolyl)methyl] *O,O*-diethyl ester {Phosalone®} 		3381, 4271a	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

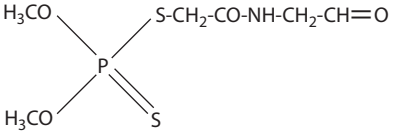
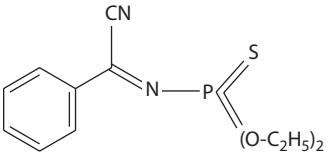
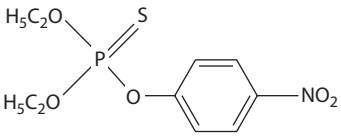
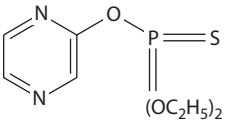
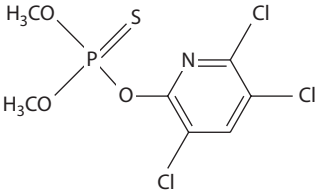
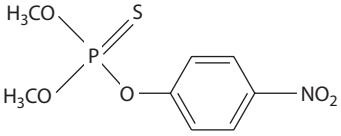
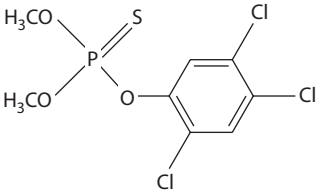
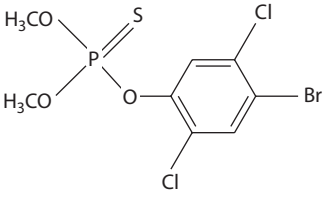
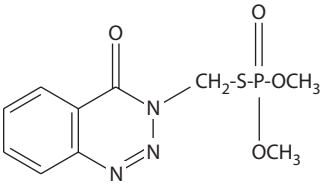
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
234.	2540-82-1	Phosphorodithioic acid, *S*-[2-(formylmethylamino)-2-oxoethyl] *O,O*-dimethyl ester {Formothion®} 	4858	2058a, 2650b, 3380, 3633, 4271a, 4858	
235.	41198-08-7	Phosphorothioic acid, *O*-(4-bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl ester {Profenophos®}		2058a	
236.	38527-91-2	Phosphorothioic acid, 2-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester {Ethaphos®}	5811, 5811a, 5811b		
237.	14816-18-3	Phosphorothioic acid, *O,O*-diethyl *O*-(α-cyanobenzylideneamino)- {Phoxim®} 		1492a, 4271a	
238.	333-41-5	Phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester {Diazinon®}	5811b	1219b, 1219c, 2058a, 2650b, 3633, 3973, 4249, 4271a	
239.	115-90-2	Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylsulfinyl)phenyl] ester {Fensulfothion®}		2650b, 3381, 3633, 3634, 3973, 4249, 4271a	
240.	56-38-2	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®} 	21A19	2058a, 3381, 3633, 3634, 3973, 4249, 4271a, 5079, 5439, 5811b, 21A19	
241.	24017-47-8	Phosphorothioic acid, *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) ester {Triazophos®}		2650a	
242.	297-97-2	Phosphorothioic acid, *O,O*-diethyl *O*-pyrazinyl ester {Thionazine®, Zinophos} 		3633, 4249, 4271a	
243.	2921-88-2	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyrifos®, Dursban®} 	717, 1333, 5811b, 21A19	717, 1219a, 1219b, 1219c, 1333, 2058a, 3381, 3633, 3919, 3977, 4249, 5811b, 21A19	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
244.	298-00-0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-nitrophenyl) ester {Parathion-methyl®} 	5811b	2058a, 3381, 3633, 3973, 4271a	
245.	299-84-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester {Fenchlorphos®, Phenchlorphos®} 		3381, 3633	
246.	2104-96-3	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-bromo-2,5-dichlorophenyl) ester {Bromophos®} 		3381, 3633, 4271a	
247.	919-86-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Demeton-S-methyl®}		2058a, 3633, 4271a	
248.	961-22-8	Phosphorothioic acid, *O,O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl) methyl] ester {Azinphos-Methyl-Oxon®} 	419, 3302, 4249	419, 4249	
249.	20300-00-9	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfinyl]ethyl] ester {Vamidothion sulfoxide®}		3992a, 4249	
250.	2275-23-2	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester {Vamidothion®}		822a, 2650a, 3633, 4249	
251.	70898-34-9	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-[[1-methyl-2-(methylamino)-2-oxoethyl] sulfonyl]ethyl] ester {Vamidothion sulfone®}		4249, 4917	
252.	122-14-5	Phosphorothioic acid, *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester {Fenitrothion®}		3633, 3973, 4249, 4271a, 4917	
253.	55-38-9	Phosphorothioic acid *O,O*-dimethyl *O*-(4-methylthio)-3-methylphenyl ester {Fenthion®}		3633, 4271a	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

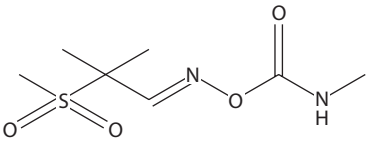
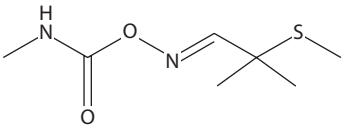
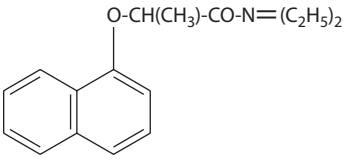
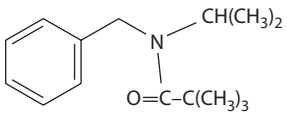
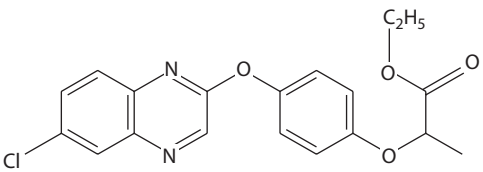
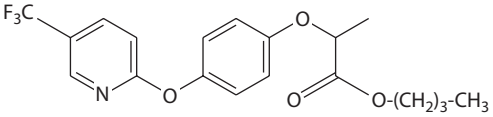
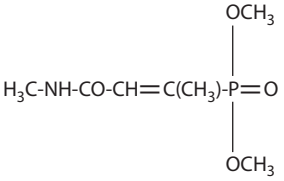
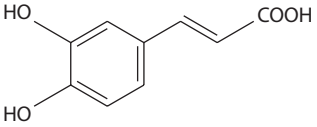
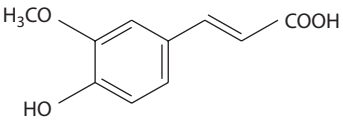
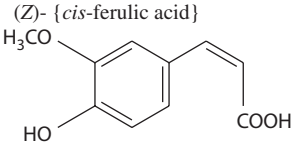
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
254.	29232-93-7	Phosphorothioic acid, *O,O*-dimethyl *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] ester {Pirimiphos-methyl®}		4249	
255.	40626-35-5	Phosphorothioic acid, O-ethyl O-phenyl S-propyl ester {Heterophos®}	5811, 5811a, 5811b		
256.	1646-87-3	Propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb sulfoxide}		1280, 2650a, 4249, 4271a, 5811b	
257.	1646-88-4	Propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino)carbonyl]oxime {Aldoxycarb®} 		1280, 3585d, 4249, 5811b	
258.	116-06-3	Propanal, 2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb®} 	4249	1280, 1451, 2650a, 3585d, 3633, 3634, 3646a, 3973, 4249, 4271a, 5811b	
259.	15299-99-7	Propanamide, diethyl-2-(1-naphthyloxy)- {Napropamide®, Devrinol®} 		1219b, 1219c, 2913a, 3633, 3973, 4271a	
260.	35256-85-0	Propanamide, dimethyl-*N*-(1-methylethyl)-*N*-(phenylmethyl) {Butam®} 		4271a	
261.	96-12-8	Propane, 1,2-dibromo-3-chloro- {DBCP®}		3188a, 3633	
262.	78-87-5	Propane, 1,2-dichloro-		3633, 3634, 3646a, 4249	
263.	142-28-9	Propane, 1,3-dichloro-		3633, 3634, 3646a, 4249	
264.	76578-14-8	Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl) oxy]phenoxy]-, ethyl ester {Quizalofop-Et®} 		3633	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
265.	69806-50-4	Propanoic acid, 2-(4-(5-trifluoromethyl-2-pyridyloxy)phenoxy)-, butyl ester {Fluazifop-butyl®} 		3633, 4271a	
266.	26952-23-8	1-Propene, 1,2-dichloro- {Telone®}		4271a	
267.	542-75-6	1-Propene, 1,3-dichloro- {1,3-D}		3633, 3634, 3646a, 3973, 4249, 5811b	
268.	2157-98-4	1-Propene, 1-methyl-3-(methylamino)-3-oxo-, dimethyl phosphate {Monocrotophos®} 		2058a, 2650b, 3633, 3973, 4271a	
269.	331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid} 	1626, 1743, 1744, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3300, 3308, 3712, 3714, 3797, 4036, 4113, 4163, 4249, 4376, 5079, 5389, 5512, 5811b, 4A01	72, 120, 722, 835, 890, 1102, 1626, 1981, 2154, 2216, 2270, 2514, 2939, 2954, 3029, 3103, 3161, 3462, 3476, 3655b, 3660, 3700, 3748, 3749, 3751, 3973, 3974a, 4249, 4999, 5079, 5126, 5385, 5389, 4A01, 5591, 5652, 5672, 5673, 5705, 5713, 5722, 5809, 5810, 5811b, 5830, 5831, 5900, 5908	
270.	1135-24-6	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)- {cinnamic acid, 3-hydroxy-4-methoxy-, ferulic acid}	3712, 5811b	5811b	
271.	537-98-4	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid} 	1626, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3555, 3749, 3797, 4249, 4377, 5811b	404, 1102, 1626, 1884, 2216, 2389, 2544, 2939, 2954, 3103, 3161, 3555, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 4377	
272.	1014-83-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid} 	1626, 1842, 2216, 2939, 3255, 3257, 3302, 3712, 3741, 3743, 3749, 4249, 4377	1102, 1626, 2216, 2389, 2544, 2939, 2954, 3103, 3161, 3748, 3749, 3751, 3797, 3973, 3974a, 4249	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

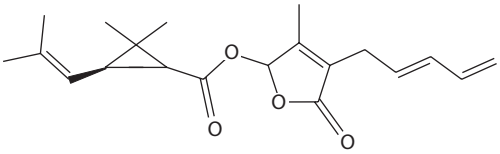
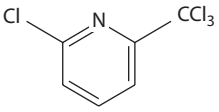
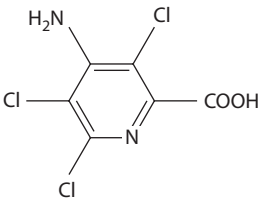
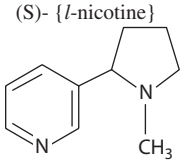
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
273.	7400-08-0	2-Propenoic acid, 3-(4-hydroxyphenyl)- {coumaric acid}	101, 1626, 1842, 2543, 2939, 3302, 3308, 3712, 4113, 4163, 4249, 4377, 5811b	120, 908, 1102, 1626, 2386, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3973, 3974a, 4163, 4249, 4377, 4677	
274.	107-18-6	2-Propen-1-ol {allyl alcohol} $H_2C{=}CH\text{-}CH_2OH$	37, 38, 172, 299, 568b, 1365, 2559, 2559a, 3255, 3530, 3553, 4249, 5811b	38, 568b, 3633, 4249	3401
275.	121-21-1 4466-14-2 25402-06-6 121-21-9 1171-63-0 121-29-9 121-20-0	Pyrethrins (natural) 		3634	
276.	123-33-1	3,6-Pyridazinedione, 1,2-dihydro- {maleic hydrazide, MH, MH-30}	715, 716, 1333, 1470, 1507, 1580, 1741, 1884, 2384, 2385, 3300, 3493, 4249, 4274, 5512, 21A19	479, 480, 691,704, 715, 716, 905, 1147, 1333, 1473, 1474, 1580, 1884, 2277, 2383, 2385, 2906, 2907, 2939, 3493, 3585c, 3633, 3723, 3725, 3728, 3767a, 3811a, 3973, 3974b, 3977, 3998, 4236, 4249, 4269, 4271a, 4274, 5016, 5553, 5568, 5586, 5605, 5642, 5667, 5686, 5687, 5717, 5774, 5811b, 21A19	
277.	1929-82-4	Pyridine, 2-chloro-6-(trichloromethyl)- {Nitrapyrin®} 		3973, 4249	
278.	1918-02-1	2-Pyridinecarboxylic acid, 4-amino-3,5, 6-trichloro- {Picloram®} 		3973, 4249	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
279.	54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} 	14, 29–31, 41–43, 50, 83, 85a, 86–89, 95, 96, 106, 107, 117, 119, 123, 126, 126a, 126b, 126c, 160, 171, 172, 173a, 174b, 174c, 175, 178, 187, 188, 196–198, 207, 209, 211, 218, 222–224, 237, 239, 270, 274–276, 282, 288, 292b, 293, 294, 302, 306, 308, 337–339, 352, 353, 355, 357a, 357b, 362–365, 375, 376, 378, 382, 388, 395, 409, 410, 413, 424, 427–429, 429e, 437, 438, 441, 442, 445, 446, 456, 462, 469a, 473, 480, 488, 489, 491, 492, 499, 521, 527, 559, 568b, 575, 576, 578, 590, 603, 636, 638, 677b, 678, 679, 681, 686, 688, 723, 761, 765, 767, 768, 804, 824, 830a, 849, 850, 852, 866, 887, 888, 916, 918a, 919, 921, 953, 959, 962, 966, 973, 975, 988a, 989, 998, 999, 1006a, 1007, 1011, 1016, 1022, 1031, 1051, 1063–1075, 1078, 1083, 1084, 1088, 1089a, 1097, 1099, 1100, 1107, 1112, 1118, 1128b, 1129, 1134, 1137, 1138, 1162, 1166–1170, 1177b, 1187, 1188, 1199, 1203, 1215, 1225, 1232, 1263, 1271, 1275, 1283, 1284, 1293, 1301, 1314, 1317–1319, 1320, 1323, 1329–1334, 1334a, 1336, 1338, 1339, 1341, 1348–1350, 1354, 1360–1363, 1366, 1368, 1371–1375, 1375a, 1375b, 1376, 1377, 1378, 1380, 1384–1386, 1388–1390, 1423, 1427, 1437, 1442–1445, 1449, 1450, 1464, 1466, 1469, 1483, 1484, 1491, 1492, 1497, 1502, 1519, 1523, 1536, 1542, 1546, 1567a, 1568, 1580, 1584, 1586, 1589, 1606, 1607, 1614, 1615, 1637, 1639, 1642, 1673, 1674, 1686, 1687, 1692, 1695, 1696, 1700, 1702, 1709, 1719, 1725, 1730, 1736, 1738, 1741, 1743, 1744,	29, 64, 69, 120, 174c, 207, 212, 256, 261, 262, 306, 308, 324, 337, 339, 374, 404, 410, 427–429, 429e, 468, 480, 499, 504, 506–508, 515, 548–550, 555, 555a, 557, 559, 568b, 647, 654, 660, 667, 677b, 678, 679, 685, 687, 689, 722, 792, 830a, 856, 866, 867, 888, 910, 914, 915a, 915b, 959, 963, 984–986, 989, 995, 997, 998, 1003, 1004, 1007, 1015, 1020, 1033, 1035, 1036, 1063–1066, 1068–1074, 1086, 1088, 1090, 1101, 1107, 1113, 1114, 1118, 1176, 1189, 1193–1199, 1203, 1220–1226, 1276, 1324, 1327, 1329, 1330, 1332, 1333, 1361, 1384, 1385, 1388–1390, 1393, 1464, 1492, 1546, 1549, 1550, 1564, 1567a, 1568, 1575, 1577, 1580, 1584, 1606, 1608–1613, 1615, 1624, 1676, 1686, 1702, 1709, 1712, 1719, 1725, 1730, 1746, 1749, 1774, 1811, 1812, 1814, 1836, 1837, 1848, 1853b, 1860a, 1927, 1933a, 1962a, 1990, 2006, 2079, 2104–2111, 2118, 2139, 2146–2150, 2152, 2153, 2164, 2166, 2167, 2191, 2212, 2226, 2263, 2270, 2272, 2273, 2282, 2283, 2290,	50 (0), 1330 (0), 1332 (0), 1354, 1360, 1375a (0), 1377 (0), 1378 (0), 2387, 2506 (0), 2507 (0)

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	1749, 1760, 1761, 1764, 1766, 1797, 1807a, 1810–1812, 1814, 1818, 1827, 1836, 1837, 1842, 1848, 1860a, 1878,1882, 1887a, 1890, 1891, 1901, 1908, 1909, 1912, 1913, 1921, 1928, 1933, 1942, 1950, 1966, 1984–1996, 1989, 1990, 2006, 2007, 2012, 2055, 2061, 2062, 2079, 2088, 2097, 2100, 2103, 2110, 2111, 2133, 2134a, 2142, 2144, 2146–2153, 2164, 2166, 2167, 2170, 2171, 2181, 2191, 2211, 2212, 2223, 2225–2229, 2231, 2247, 2254, 2261, 2263, 2267, 2269, 2270–2272, 2294, 2303, 2313, 2313b, 2324, 2327c, 2337, 2338, 2349, 2353a, 2371, 2372, 2374–2378, 2400d, 2401, 2408, 2410, 2412, 2416, 2482, 2488, 2493, 2503, 2504, 2506, 2507, 2517, 2523, 2524, 2524a, 2528, 2535, 2543, 2546, 2549, 2557a, 2570, 2601a, 2603, 2606, 2610, 2612, 2613, 2622, 2628, 2632, 2635, 2652, 2653, 2658, 2668–2673, 2683, 2688, 2690–2695, 2696, 2717, 2719, 2724, 2737, 2739, 2740, 2744, 2761, 2762, 2767, 2774, 2777, 2792, 2793, 2799a, 2800, 2827–2829, 2831, 2832, 2835–2837, 2839, 2840, 2842–2845, 2848, 2857, 2863, 2869, 2874, 2877, 2878a, 2879, 2880, 2899, 2912, 2919, 2920, 2921, 2924–2927, 2936–2939, 2947, 2951, 2958, 2959, 2966, 2967a, 2969, 2970, 2973–2976, 2980, 2982, 2984–2986, 2998, 3008–3016, 3019, 3021, 3022, 3024, 3025, 3027–3029, 3035, 3040, 3041, 3044, 3045, 3054, 3056, 3057, 3059, 3072b, 3078, 3087–3089, 3116, 3121a, 3133, 3137, 3139, 3140, 3142, 3143, 3148a, 3156, 3190, 3214, 3227, 3228, 3254, 3255, 3257, 3258, 3265, 3274,	2294, 2331a, 2332, 2334, 2337, 2338, 2339a, 2349, 2359, 2372, 2374, 2389, 2417, 2446, 2488, 2503, 2504, 2528, 2529, 2532, 2534, 2543–2545, 2557a, 2606, 2611, 2682, 2688, 2689, 2724, 2761, 2762, 2765, 2766, 2786, 2792, 2841, 2844, 2913, 2914, 2917a, 2919, 2920, 2921, 2924–2926, 2938, 2939, 2954 2979–2982, 2989, 3016, 3019, 3022, 3024, 3027, 3028, 3034, 3035, 3041, 3044, 3056, 3059, 3063, 3073, 3074, 3087, 3155, 3188, 3214, 3219, 3254, 3329, 3333, 3375, 3420, 3430, 3444, 3459, 3460, 3476, 3477, 3482, 3491, 3499, 3511, 3512, 3517, 3543, 3549, 3560, 3561, 3570, 3571, 3608a, 3614, 3633, 3634, 3670a, 3705, 3707, 3767a, 3797, 3816, 3905, 3925, 3926, 3928, 3942, 3943b, 3950, 3961, 3972–3974, 3974a, 3974b, 3976, 3980, 3983a, 3999, 4009–4011, 4016, 4017, 4043, 4045, 4047, 4051, 4071, 4073, 4103, 4127, 4159, 4169–4173, 4189, 4207, 4210,4213, 4218, 4236, 4249, 4266a, 4267, 4370, 4418, 4420, 4529, 4744, 4745, 4817, 4885,	

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	3300, 3302, 3308, 3333, 3370, 3373, 3375, 3378, 3386, 3397, 3398, 3406, 3407, 3410, 3415, 3426, 3443–3446, 3457, 3461, 3454, 3477, 3482, 3491, 3493, 3499, 3505, 3516, 3517, 3521, 3548, 3553, 3557–3559, 3562, 3563, 3570–3572, 3576, 3577, 3585, 3623, 3640, 3658, 3659, 3662, 3670–3672, 3682, 3722, 3731, 3739–3742, 3782–3784, 3790, 3796, 3797, 3803, 3822, 3826, 3833, 3844, 3876, 3884, 3896, 3909, 3910, 3921, 3926, 3928, 3930, 3934, 3936–3939, 3942, 3943, 3952, 3955–3959, 3961, 3972, 3980, 3984, 3990, 3992, 3999, 4009–4011, 4016, 4017, 4039, 4045, 4064, 4065, 4072, 4075, 4076, 4078, 4082, 4103, 4116, 4119–4122, 4127, 4132, 4134, 4137, 4138, 4140–4143, 4162, 4167–4176, 4178–4183, 4189–4191, 4194, 4197, 4198, 4202–4207, 4210, 4211, 4213, 4240, 4248, 4249, 4259, 4264, 4267, 4268, 4273, 4275a, 4285, 4291, 4309, 4310, 4319, 4330, 4363, 4366, 4370, 4385, 4398, 4418, 4529, 4570a, 4636, 4745, 4921, 4994, 5000, 5008, 5013, 5017, 5034, 5035, 5041, 5045, 5047, 5052, 5065, 5068, 5069, 5071, 5079, 5082, 5084, 5099, 5100, 5104, 5112, 5118, 5124, 5129, 5130, 5140, 5159, 5163, 5175, 5166, 5179, 5183, 5189, 5207, 5210, 5211, 5219, 5225, 5226, 5236, 5258, 5259, 5263, 5325, 5343, 5346, 5351, 5390, 5401, 5412, 5414, 5427, 5431, 5443, 5452, 5458–5461, 5470–5473, 5475, 5476, 5480, 5489, 5507, 5508, 5512, 5520, 5529, 5531, 5532, 5544–5546, 5554, 5558, 5563, 5565, 5643a, 5679, 5706, 5770, 5811b, 5836, 25A84, 25A85	4921, 5000, 5001, 5005, 5018, 5020, 5024, 5033, 5040, 5053, 5079, 5083, 5106, 5107, 5112, 5121, 5122, 5126, 5131, 5133, 5140, 5144, 5146, 5150, 5159, 5161, 5162, 5165, 5171, 5172, 5174, 5189, 5198, 5209, 5213, 5214, 5223, 5229, 5244, 5247, 5258, 5259, 5263, 5267, 5294, 5324, 5331, 5335, 5336, 5339, 5349, 5351, 5366, 5382, 5389, 5390, 5390a, 5391, 5404, 5405, 5416, 5419, 5427, 5430, 5439a, 5444, 5445, 5451–5453, 5463, 5469, 5474, 5477, 5481, 5482, 5487, 5488, 5498, 5499, 5508, 5512, 5528, 5535, 5536, 5542, 5561, 5573, 5582, 5622, 5623, 5634, 5652, 5654–5656, 5663, 5664, 5667, 5676, 5681, 5685, 5701, 5702, 5712, 5725, 5726, 5734, 5735, 5765, 5771, 5772, 5774, 5775, 5790, 5803, 5811b, 5824, 5828, 5848, 5853, 5884, 5886, 5895, 5896, 5901, 5905, 17B05, 17B06, 17B08, 17B11, 17B14, 17B18, 17B20, 17B29, 17B42, 17B43, 17B44, 17B48, 17B61, 17B62, 17B64, 21A07, 21A08, 21A40–21A42	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

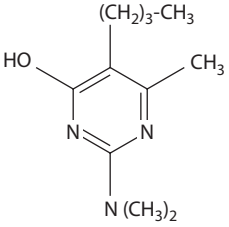
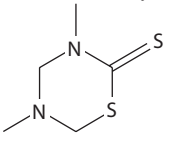
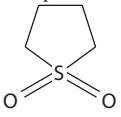
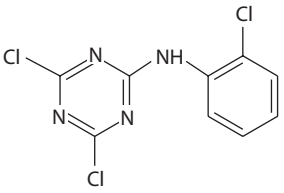
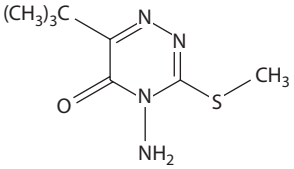
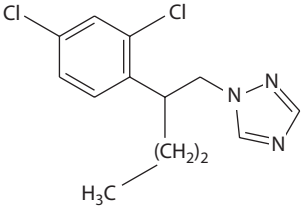
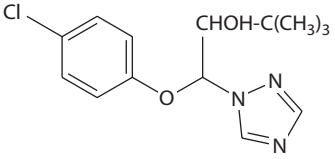
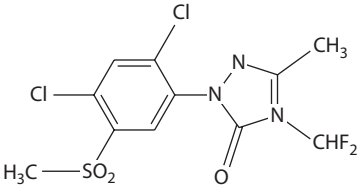
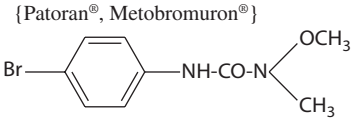
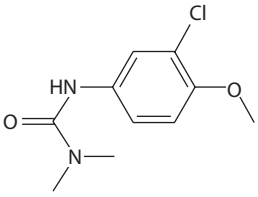
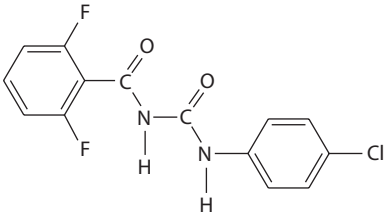
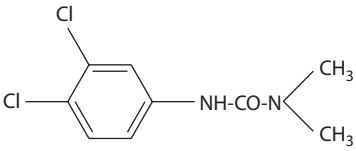
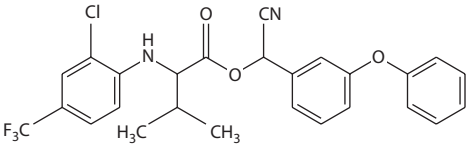
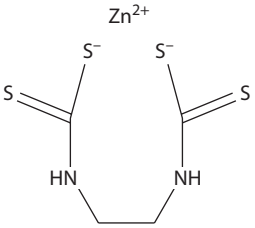
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
280.	65-30-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate (2:1)		3633, 3634, 3874c, 4249	
281.	6505-86-8	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate		3633, 3634, 3874c, 4249	
282.	5221-53-4	Pyrimidine, 5-butyl-2-dimethylamino-4-hydroxy-6-methyl- {Dimetherimol®} 		3633, 4249	
283.	5979-94-2	Pyrrolidine, 1-acetyl-2-(3-pyridinyl)-, (S)- {*N*′-acetylnornicotine}	568b, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 2761, 2762, 2765–2767, 2777, 3410, 3553, 3739–3741, 4249, 5811b	64, 568b, 993, 2359, 3550, 3260a, 3973, 4133, 4236, 4249, 5811b	1360, 1375a
284.	86900-39-2	Pyrrolidine, 1-ethyl-2-(3-pyridinyl)- {*N*′-ethylnornicotine}		2917a, 4249	
285.	91907-45-8	Pyrrolidine, 1-propyl-2-(3-pyridinyl)- {*N*′-propylnornicotine}		2917a	
286.	38840-03-8 3000-81-5	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)- {*N*′-formylnornicotine}	568b, 830a, 1063–1066, 1068–1074, 1360, 1365, 1371, 1375a, 1586, 2601a, 2761, 2762, 2765–2767, 2777, 3255, 3410, 3553, 3739–3742, 4249, 4407, 5811b	64, 568b, 689, 994, 2359, 2952, 3491, 3549, 3550, 3742, 3973, 4133, 4249, 5811b	1360, 1375a
287.	57-92-1	Streptomycin		3633, 3661a	
288.	7704-34-9	Sulfur	50, 641, 1240, 1933b, 2270, 2524a, 3302, 4229, 4230, 4249, 5811b	116, 193, 1128b, 1240, 2079, 2270, 2283, 2338, 2393, 3476, 3633, 3797, 3973, 3974b, 4249, 5079, 5113, 5189, 5220, 5282, 5378, 5448, 5670, 5715, 5811b	50, 641, 4249
289.	7664-93-9	Sulfuric acid		3476, 3633	
290.	7758-98-7	Sulfuric acid, copper salt		3633	
291.	533-74-4	1,3,5-Thiadiazine, 2-thio-3,5-dimethyl-tetrahydro- {Dazomet®, Mylone®} 		3633, 3646a, 3973	
292.	137-26-8	Thioformamide, 1,1′-dithiobis(*N,N*-dimethyl {Thiram®}		3633, 5811b	
293.	126-33-0	Thiophene, tetrahydro-, 1,1-dioxide {Sulfolan®} 	568b, 1360, 1375a, 2761, 2762, 3553, 4249, 5811b		1360, 1375a, 4249

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
294.	101-05-3	1,3,5-Triazin-2-amine,4,6-dichloro-*N*-(2-chlorophenyl)- {Anilazine®, Dyrene®} 	1884	1884, 3633, 3661a, 3797, 4271a	
295.	21087-64-9	1,2,4-Triazin-5(4*H*)-one, 4-amino-6-*tert*-butyl-3-(methylthio)- {Metribuzin®} 		2913a, 4249	
296.	66246-88-6	1,2,4-Triazole, 1-(2-(2,4-dichlorophenyl)pentyl)- {Penconazole®} 		3633, 4249	
297.	55219-65-3	1*H*-1,2,4-Triazol-1-ethanol, 8-(4-chlorophenoxy)-α-(1,1-dimethylethyl)- {Triadimenol®} 		928a	
298.	122836-35-5	1*H*-1,2,4-Triazol-1-yl)phenyl)methane-sulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4, 5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)phenyl)-; Sulfentrazone®} 		2913a	
299.	76-87-9	Triphenylstannium hydroxide $(C_6H_5)_3$≡Sn-OH {Fentin hydroxide®}		3633, 4271a	

(*continued*)

TABLE 21.3 (continued)
Synthetic and Natural Pesticides and Plant Growth Regulators in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
300.	3060-89-7	Urea, *N′*-(4-bromophenyl)-*N*-methoxy-*N′*-methyl- {Patoran®, Metobromuron®} 	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
301.	19937-59-8	Urea, *N′*-(3-chloro-4-methoxyphenyl)-*N,N*-dimethyl- {Metoxuron®} 		622, 3633, 4249, 4271a	
302.	1746-81-2	Urea, *N′*-(4-chlorophenyl)-*N*-methoxy-*N*-methyl- {Linuron®, 30% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
303.	35367-38-5	Urea, 1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)- {Diflubenzuron®} 	21A19	4911, 21A19	
304.	330-55-2	Urea, *N′*-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methyl- {Monolinuron®, 20% of Molipan®}	822, 4249, 21A19	822, 3633, 4249, 4271a, 21A19	
305.	150-68-5	Urea, 1,1-dimethyl-3-(4-chlorophenyl) {Monuron®}		3633, 4271a	
306.	330-54-1	Urea, 1,1-dimethyl-3-(3,4-dichlorophenyl) {Diuron®} 		3973	
307.	102851-06-9	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®} 		904, 2346, 3585e	
308.	12122-67-7	Zinc, [[1,2-ethanediylbis[carbamodithioato]] (2-)]- {Zineb®} 		3481, 3491, 3513, 3633, 4249, 4271a, 4645, 4757, 5629, 5811b, 21A19	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

22 Genes, Nucleotides, and Enzymes

Prior to discussing genes, nucleotides (DNA/RNA strands), and enzymes identified in tobacco, a general discussion of genetics, genes, nucleotides, and enzymes is appropriate (3973). There are numerous excellent reference texts that the reader can access for more detailed information on genetics [910a, 3973, Acquaah (22A01), Bernardi (22A03), Griffiths et al. (22A12), Hartl and Jones (22A14)] and several sources of encyclopedic information (22A05, 22A17, 22A34). The general discussion will be followed by a review of work accomplished over many decades toward an understanding of the mysteries of tobacco genetics.

22.1 GENERAL DISCUSSION OF GENETICS

Genetics is the science of heredity and variation in living organisms (22A12, 22A14, 22A17). Knowledge that desired characteristics were inherited has been implicitly used since prehistoric times for improving crop plants and animals through selective breeding. The science originated from human experience to improve crop and animals through the use of varied methods, such as domestication. However, the modern science of genetics, which seeks to understand the mechanisms of inheritance, only began with the work of Gregor Mendel in the mid-1800s (3973, 22A32).

Inheritance is fundamentally a discrete process with specific traits that are passed on in an independent manner. These basic units of inheritance are now known as genes. In the cells of organisms, genes exist physically in the structure of the molecule DNA, and the information contained in the genes is used to create and control the components of cells. Although genetics plays a large role in determining the appearance and behavior of organisms, it is the interaction of genetics with the environment an organism experiences that determines the ultimate outcome. For example, *Nicotiana tabacum* seeds planted and cultivated in different soils and under different climatic and agronomic conditions can produce different types of tobacco that have vastly different appearances and chemical composition, e.g., Maryland vs. Virginia tobacco (3973).

A gene is a set of segments of nucleic acid. A nucleic acid is a complex, high-molecular-weight biochemical macromolecule composed of nucleotide chains that convey genetic information. The most common nucleic acids are deoxyribonucleic acid (DNA) and ribonucleic acid (RNA).

Genes are arranged linearly in long chains of DNA sequences, called chromosomes. In eukaryotic organisms (which include plants and animals), each cell has its DNA arranged in multiple linear chromosomes. These DNA strands are often extremely long. The largest human chromosome, for example, is about 140 million base pairs in length (22A11).

Certain segments of nucleic acid contain the information necessary to produce a functional RNA product in a controlled manner. They contain regulatory regions dictating under what conditions this product is made, transcribed regions dictating the sequence of the RNA product, and/or other functional sequence regions (22A23, 22A24). The physical development and phenotype, i.e., a measurable characteristic, such as color or disease resistance, of organisms can be thought of as a product of genes interacting with each other and with the environment, and genes can be considered as units of inheritance.

In cells, genes consist of a long strand of DNA that contains a promoter, which controls the activity of a gene, and coding sequences, which determine what the gene produces. When a gene is active, the coding sequence is copied in a process called transcription, producing an RNA copy of the gene's information. This RNA can then direct the synthesis of proteins via the genetic code. The genetic code is the set of rules by which information encoded in genetic material (DNA or RNA sequences) is translated into proteins, i.e., amino acid sequences and enzymes, by living cells. However, RNAs can also be used directly, e.g., as part of the ribosome, which is a small, dense organelle in cells that assembles proteins. Molecules produced from gene expression, whether RNA or protein, are known as gene products.

Most genes contain noncoding regions that do not code for the gene products but can regulate gene expression. Additionally, there are large segments of the DNA that do not carry any genetic information. One single gene can lead to the synthesis of multiple proteins. The total complement of genes in an organism or cell is known as its genome. The estimated number of genes in the human genome has been repeatedly revised downward since the completion of the Human Genome Project, but current estimates place the human genome size at just under 3 billion base pairs and about 20,000–25,000 genes (22A15).

The vast majority of living organisms encode their genes in long strands of DNA. DNA consists of a chain made from four types of nucleotide subunits: adenosine (A), cytidine (C), guanosine (G), and thymidine (T). Each nucleotide subunit consists of three components: a phosphate group, a deoxyribose sugar ring, and a nucleobase. Thus, nucleotides in DNA or RNA are typically called bases; consequently, they are commonly referred to simply by their purine (adenine and guanine) or pyrimidine (cytosine and thymine) original base components. The most common form of DNA in a cell is a double helix structure in which two individual DNA strands twist around each other in a right-handed spiral. In this structure, the base pairing rules specify that guanine pairs with cytosine and adenine pairs with thymine (each pair contains

one purine and one pyrimidine). The base pairing between guanine and cytosine forms three hydrogen bonds, while the base pairing between adenine and thymine forms two hydrogen bonds. The two strands in a double helix must therefore be complementary, i.e., their bases must align such that the adenines of one strand are paired with the thymines of the other strand, and so on.

Due to the chemical composition of the pentose residues of the bases, DNA strands have directionality. One end of a DNA polymer contains an exposed hydroxyl group on the deoxyribose; this is known as the 3′ end of the molecule. The other end contains an exposed phosphate group; this is the 5′ end. The directionality of DNA is vitally important to many cellular processes, since double helices are necessarily directional (a strand running 5′-3′ pairs with a complementary strand running 3′-5′) and processes such as DNA replication occur in only one direction. All nucleic acid synthesis in a cell occurs in the 5′-3′ direction because new monomers are added via a dehydration reaction that uses the exposed 3′ hydroxyl as a nucleophile.

The expression of genes encoded in DNA begins by transcribing the gene into RNA, a second type of nucleic acid that is very similar to DNA, but monomers of which contain the sugar ribose rather than deoxyribose. RNA also contains the base uracil (U) in place of thymine. Genes that encode proteins are composed of a series of three-nucleotide sequences called codons. A codon is a set of any three adjacent bases in the DNA or RNA. There are 64 different codons of which 61 specify the incorporation of an amino acid into a polypeptide chain while the remaining 3 are stop codons that signal the end of a polypeptide. For example, the DNA codon ACG via its complementary RNA codon CGU specifies the amino acid arginine. For another example, the DNA codon TAC via its complementary RNA codon GUA specifies the amino acid valine. There are three stop codons: uracil–adenosine–adenosine (UAA), uracil–adenosine–guanosine (UAG), and uracil–guanosine–adenosine (UGA). They are also called termination codons or nonsense codons. The genetic code specifies the correspondence during protein translation between codons and amino acids. The genetic code is nearly the same for all known organisms.

Many molecular definitions of a gene relate to their role in directing the production of specific proteins. Production of protein itself is made possible via certain enzymes known as polymerases. Various DNAs and RNAs could not be produced without these polymerases, and therefore, they are of primary importance. Numerous other enzymes are produced that control metabolic and catabolic processes (enzymatically), provide structural components, and perform regulatory functions in cells.

A single gene can encode multiple enzymes, and an enzyme can have multiple genes. For example, ribulose bisphosphate carboxylase–oxygenase in *N. tabacum* is a multimeric protein of 16 peptides, 8 small subunits (nuclear encoded) and 8 large subunits (chloroplast encoded); thus, 2 genes are responsible for this enzyme (3974c, 22A27, 22A35).

Metabolic and catabolic enzymes are specialized proteins that catalyze chemical reactions. In enzymatic catalyzed reactions, the molecules at the beginning of the process are called substrates, and the enzyme converts them into different molecules or products. Almost all processes in a biological cell need enzymes in order to occur at significant rates. Since enzymes are extremely selective for their substrates and accelerate only a few reactions from among many possibilities, the set of enzymes made in a cell determines which metabolic pathways occur in that cell (3973).

Each type of enzyme is generally geared to interact chemically with only one particular substance or type of substance, termed a substrate. The two parts fit together, according to a widely accepted theory introduced in the 1890s by the German chemist Emil Fischer (1852–1919), as a key fits into a lock. Each type of enzyme has a specific 3D shape that enables it to fit with the substrate, which has a complementary shape.

The link between enzymes and substrates is so strong that enzymes often are named after the substrate involved, simply by adding *ase* to the name of the substrate. For example, lactase is the enzyme that catalyzes the breakdown of lactose, while urease catalyzes the chemical breakdown of urea. Enzymes bind their reactants or substrates at special folds and clefts, named active sites, in the structure of the substrate. Because numerous interactions are required in their work of catalysis, enzymes must have many active sites and therefore can have molecular weights as high as one million.

22.2 TOBACCO GENETICS

Tobacco has been used in one form or another in civilized society for nearly five centuries. Eventually in the late nineteenth century, investigations as to its composition began, but they were not particularly numerous. The major driving force in the escalation in the mid-twentieth century of studies on tobacco composition was the attempt to define (1) its components that contributed to the consumer acceptability of the taste and aroma of tobacco itself and its smoke and (2) the precursors in tobacco of the toxicants in its smoke (3973, 22A30).

In 1972, Tso (22A30) remarked

> The characteristics of cigarette smoke are functions of the physical and chemical properties of leaf tobacco which make the cigarette. Smoke constituents may be modified by changing leaf characteristics. The questions are: What kinds of changes are needed? and, how can these changes be achieved?

Tobacco genetics is a rather new field of study although research on tobacco to understand its physical and chemical makeup has been a goal of tobacco scientists for over a hundred years. The initial problem in undertaking the goal of trying to understand the origins of the chemical and physical essence of tobacco was that our understanding of life processes, in general, was inadequate prior to the discovery of the structure and function of DNA. Additionally,

the life processing functions of numerous DNAs and RNAs in tobacco were not understood. Although scientists had an empirical knowledge of how the genetics worked via the tobacco breeding program, basic fundamental knowledge was lacking until technology was developed to execute the search for information on the genetic code for tobacco (3973).

Regardless, research directed toward the ultimate goal of understanding of the fundamental life processes of tobacco began. The early genetic research was conducted in the areas of tobacco breeding (as a means to improve leaf characteristics, quality, and disease resistance) and the chemical composition of tobacco via identification of extractable material in tobacco, e.g., amino acids, various proteins, enzymes (424a, 2341a, 3972, 3973, 22A06, 22A29, 22A30). It was not until the 1970s and 1980s with the development of new analytical and genetic tools, e.g., HPLC, GC/MS, instrumental polymerase chain reaction (PCR), plant transformation, genetic mapping with molecular markers, gene tagging, and positional cloning, that significant progress was possible in the understanding of tobacco genetics directed toward improved pest resistance, yield, and quality (424a).

The chemical composition of tobacco smoke is highly dependent upon the physical and chemical properties of the leaf tobaccos used in cigarette manufacture. It is a basic tenet that the biological properties of cigarette mainstream smoke (MSS) and cigarette smoke condensate (CSC) can be improved through changes in the genetics of tobacco. Numerous types of chemical and physical modifications performed on tobacco, e.g., tobacco extraction, tobacco reconstitution, tobacco expansion, inclusion of tobacco substitutes, have indicated that this tenet is possible (1375a, 1375b). Thousands of genes, nucleotides, and enzymes have been identified in tobacco. Although they do not transfer intact to MSS, hundreds of decomposition products from their combustion and pyrolysis products have been identified. Many of the combustion and pyrolysis products found in MSS and CSC have been called "Hoffmann analytes" because of their alleged adverse biological effects, e.g., quinoline, HCN, and several other undesirable nitrogenous compounds, certain PAHs, aza-arenes, and phenolics (3974c). It is hoped that through genetic modifications, precursors in tobacco of the toxicants in its smoke can be altered significantly to improve the safety of tobacco products (3794b, 3974c, 3975, 3976, 3984, 22A30).

22.3 GENES, NUCLEOTIDES, AND ENZYMES IDENTIFIED IN TOBACCO

The 65 species related to *N. tabacum* represent sources of a divergent germplasm for biochemical and physical variations (3793, 22A19, 22A30). These species differ widely in growth habit and in chromosome numbers (3793). Tobacco breeding via interspecific hybridization has been the major tool for agricultural scientists to improving the health and quality of tobacco (22A30). Possible approaches that plant scientists can take to modify tobacco leaf have been reviewed by Tso (22A31). Modifications discussed by Tso (3973, 22A31) involved genetic and cultural modification, nitrogen fertilization technology, leaf and plant population, the physiological stage of topping, and pesticide treatments. Postharvest modifications were also discussed (22A31), as leaf composition is markedly affected by the curing process, aging, or other treatment of cured leaves (4005).

The U.S. *Nicotiana* Germplasm Collection was initiated by the U.S. Department of Agriculture (USDA) in 1934 as a resource for tobacco breeders. The collection currently consists of approximately 1244 tobacco introductions, 656 cultivars, and 224 accessions representing 59 *Nicotiana* species, 50 interspecific hybrids, and a newly introduced set of mutants (22A19). The gene pool of the *Nicotiana* Germplasm Collection represents enormous possibilities for researchers in plant pathology, plant molecular biology, and biotechnology to modify and improve the quality, yield, and safety of tobacco. It has been estimated that the genetic makeup of tobacco includes 25,000–50,000 genes (22A22). *N. tabacum* has a very large genome size compared with other cultivated solanaceous plants (22A13, 22A21, 22A22). At approximately 4.5 billion base pairs, it is 1.5 times the size of the human genome (22A13, 22A21, 22A22).

There are at least two major (and several minor) initiatives to sequence the tobacco genome: the Tobacco Genome Initiative (TGI) and the European Sequencing of Tobacco Project (ESTobacco). Both projects have an ultimate goal of sequencing the greater part of the tobacco genome. Although tobacco has been cultivated for more than 500 years and is a crop of great economic significance, relatively little information exists on its genome structure and organization.

The overall goal of the TGI is to sequence and annotate more than 90% of the open reading frames in the genome of cultivated tobacco, *N. tabacum*. *N. tabacum* is an amphiploid species ($2n = 48$) likely resulting from an interspecific cross between *Nicotiana sylvestris* ($2n = 24$) and *Nicotiana tomentosiformis* ($2n = 24$) and, at approximately 4.5 billion base pairs, has a very large genome size compared with other cultivated solanaceous plants. A complete gene catalog will provide the raw information to investigate physiological and genetic processes in the tobacco plant, a widely used model in plant biotechnology. Tobacco genomics may lead to the elucidation of genetic factors that impact constituents associated with tobacco consumption. Improving our understanding of these processes may potentially contribute to achieving the goal of reducing the harm associated with cigarette smoking. In addition, important agronomic traits such as disease and pest resistance genes could be identified and thus could be available for use in traditional and molecular breeding projects, the goal of which is to enhance the performance of tobacco as a crop in different environments. Finally, *N. tabacum* is a member of the agriculturally important *Solanaceae* family, which also includes tomato, potato, eggplant, and pepper crop plants. All of these plants may benefit from gene discovery in tobacco. The TGI is housed in the laboratories of the Plant Pathology Department of the North Carolina State University (NCSU) Centennial Campus, College of Agricultural and Life Sciences

(Raleigh, NC). NCSU will make the TGI data available to authorized academic researchers. The TGI is supported by Philip Morris USA, Inc. (22A13, 22A21, 22A22).

The TGI has identified a large percentage of genes in *N. tabacum* by utilizing a combination of strategies. Researchers at TGI have employed a methyl filtration approach to identify gene-rich regions in *N. tabacum* in order to expedite the gene discovery process. As of 2006, TGI had sequenced 1,700,000 lanes of methyl-filtered clones and observed a dramatic increase in gene discovery in filtered vs. nonfiltered libraries. TGI has also performed expressed sequence tag (EST) sequencing from various *Nicotiana* libraries and to date has sequenced over 80,000 ESTs. Genes tagged by these two strategies have been used as probes to identify bacterial artificial chromosome (BAC) clones for more targeted sequencing. Numerous BACs have been sequenced, revealing information about both gene structure and genome organization in *Nicotiana* species (22A13, 22A21). The TGI has a projected completion date in late 2007.

The second major tobacco genomic project is centered in Europe and was started in 2006. It is known as the European Sequencing of Tobacco Project or ESTobacco. This project is being conducted by Advanced Technologies (Cambridge) Ltd. (a wholly owned subsidiary of British American Tobacco) and Institut du Tabac de Bergerac (part of the Altadis Group). The aim of the ESTobacco project is to be complementary to other projects currently underway concerning the tobacco genome. The strategy of ESTobacco is to sequence only genes expressed in tobacco and not the whole genome. They believe that the size of the tobacco genome is too large to be totally sequenced. The tobacco genome is thought to be about 29 times larger than *Arabidopsis thaliana* (Table 22.1).

The plan of the ESTobacco project is to investigate three commercial varieties of tobacco used throughout the world: K326 for the flue-cured type, Burley 21 and TN86 for the burley types. To obtain the major genes, the organs of the plant (seeds, roots, stems, midribs, laminae, and flowers) prepared at different stages of development (germination, young seedlings, before and after topping, maturity) will be used as a basis for this work. A large tobacco EST data set was obtained from 11 normalized cDNA libraries comprising 56,000 clones. It is envisioned that a DNA array designed with these sequences will allow the large-scale study of the genes expressed in tobacco. This new tool should lead to the acceleration of programs already underway concerning the origins of risks associated with tobacco and provide strategies for harm reduction. To encourage a wide range of initiatives on tobacco plant genetic, as with other crops, the resulting sequences obtained during the ESTobacco project will be available to the worldwide scientific community through public access databases (22A08, 22A26).

TABLE 22.1
Relative Size of Genomes and Number of Genes by Species

Species	Genome Size (Mb)	Number of Genes
A. thaliana	125	25,500
Homo sapiens	3000	20,000–25,000
N. tabacum	3500–4500 (est.)	25,000–50,000 (est.)

As whole gene sequences and nucleotide sequences (DNA and RNA sequenced strands) become available, they are being entered into GenBank (22A10). GenBank is the National Institute of Health (NIH) genetic sequence database, an annotated collection of all publicly available DNA sequences (22A02). There were approximately 65,369,091,950 bases in 61,132,599 sequence records in the traditional GenBank divisions and 80,369,977,826 bases in 17,960,667 sequence records in the whole-genome shotgun (WGS) division as of August 2006. GenBank is part of the International Nucleotide Sequence Database Collaboration, which comprises the DNA DataBank of Japan (DDBJ), the European Molecular Biology Laboratory (EMBL), and GenBank at the National Center for Biotechnology Information (NCBI). Information located in GenBank can be accessed on the Internet (1282a).

Within the next few years, our understanding of the tobacco genome will be greatly improved. It is anticipated or predicted that advances in tobacco genomic will lead to the next major improvement in safety and health associated with cigarette smoking via genetic modifications of various *Nicotiana* species. The symposium at the *61st Tobacco Science Research Conference* featured presentations from representatives from the TGI and the ESTobacco projects. Updates on both projects were given as well as how new types of biotechnologies are being employed to provide both fundamental and practical information of genes that could be used to improve pest resistance, quality, yield of tobacco, and the safety of tobacco products (22A09, 22A20).

In the late 1950s and through the 1960s, enormous breakthroughs in DNA enzymology took place. For example, in 1955, Kornberg et al. (22A18) isolated DNA polymerase, Weiss and Richardson (22A33) isolated DNA ligase in 1967, and Smith and Wilcox (22A28), and Kelley and Smith (22A16) isolated and characterized the first sequence specific restriction nuclease in 1970. These enzymes, respectively, play roles in the synthesis of DNA molecules, the attachment of two or more DNA molecules to one another, and the breaking of DNA molecules into fragments. Importantly, these enzymes make it possible to create entirely new kinds of DNA molecules and, equally important, to manipulate the functioning of the genes located on these new molecules. The types of enzymes that Smith, Wilcox, and Kelley (22A16, 22A28) discovered are called restriction enzymes. Restriction enzymes recognize and cut specific short sequences of DNA. They are found in bacteria, which use the enzymes to digest invading DNA. The bacteria add methyl groups to their own DNA to protect them from digestion. Molecular biologists began using these enzymes, along with DNA polymerase and DNA ligase in the early 1970s to cut, manipulate, and analyze pieces of DNA in a predictable and reproducible way. The enzymes became an important, early tool for mapping genomes. There are over 900 types of restriction enzymes

that have been isolated from over 230 strains of bacteria; some of these enzymes provide specific sequence segments of DNA and some do not. About 180 restriction enzymes are commercially available.

There have been hundreds of thousands of nucleotide sequences (DNA and RNA sequenced strands) that have been produced via restriction enzymes from various forms of DNA and RNA in tobacco (22A13, 22A21). Not every DNA strand though holds or is encoded with genetic information. There are considerable lengths of DNA that contain no genetic information or the function of which has yet to be identified. These segments are called "junk" or "noncoding" DNA. For example, about 97% of the human genome has been designated as "noncoding" (22A24). So, of the hundreds of thousands of nucleotide sequences that have been produced from various forms of DNA and RNA in tobacco, only a small percentage contains the essential genetic information needed to direct its life processes. However, all of these DNA and RNA strands serve a very important purpose during the construction of genomes. By employing sophisticated computer programs that can identify patterns in the bases in the DNA fragments, DNA fragments can be sequenced. "Fingerprinting" of large insert genomic fragment libraries, also known as bacterial artificial chromosomes (BAC) clones, can lead to the construction of a physical map of a genome. These maps are critical to genome sequencing, positional cloning, and understanding the relative organization of genes and markers. When BAC libraries are arranged into maps that reflect the DNA sequence in a chromosome, they provide maximal information and utility. Generally, these BAC libraries are deposited in the GenBank. For example, BAC clone libraries for *N. tabacum*, currently being compiled as part of the TGI and ESTobacco projects, are being deposited in the GenBank.

There are vast arrays of enzymes that have been identified in tobacco (429b,c, 3973). Plant enzymes perform valuable functions almost as soon as seeds are planted and continue to be important even through the tobacco-curing process. Enzymes are in fact essential molecules that assimilate carbon dioxide from air (via photosynthesis) and nitrogen by roots from the soil and utilize hydrogen liberated by dehydrogenation from the components of the Krebs tricarboxylic acid (TCA) cycle to produce a variety of organic acids, e.g., oxaloacetic, α-ketoglutaric acids. The net result of nitrogen assimilation is the utilization of a portion of newly photosynthesized carbon chains into the nitrogenous pool. When the nitrogen supply is abundant, there will be more synthesis of amino acids, e.g., aspartic and glutamic acids, and nicotine and less sugars and starch. If the nitrogen supply is limited, there will be an excess accumulation of acetate in the TCA cycle which results in higher production of carbohydrates, fats, volatile oils, resins, and polyterpenes. Tobacco enzymes efficiently and effectively control and regulate the type and level of tobacco constituents available to the plant for growth. The variations in leaf characteristics, texture, color, porosity, and combustibility; quality, e.g., aroma and flavor based on chemical composition; and yield (poundage per acre/hectare) are a reflection of the genetic makeup of the plant, agronomic practices, soil types, and environmental conditions (3972, 3973, 22A29, 22A30).

Enzymes can either work individually or in teams. In a metabolic pathway (like the TCA cycle), several enzymes work together in a specific order; one enzyme takes the product of another enzyme as a substrate. Two sources of information on hundreds of enzymes that have been identified in tobacco are Brenda and Kegg (429b,c). Brenda is the comprehensive enzyme information system and is a database of enzymes and enzyme pathways. It was developed and is maintained at the Institute of Biochemistry at the University of Cologne and is available through the Internet at http://www.brenda.uni-koeln.de//. Kegg stands for the Kyoto Encyclopedia of Genes and Genomes. Kegg is a bioinformatics resource that was developed and is maintained as part of the research projects of the Kanehisa Laboratories in the Bioinformatics Center of Kyoto University and the Human Genome Center of the University of Tokyo.

The phase of plant growth that extends from maturity to actual death (called senescence) is characterized by an accumulation of metabolic products, increase in respiratory rate, and a loss of dry matter (3973). At the senescence stage, enzyme activities (especially hydrolytic and other degradative enzyme systems) are intensified. These systems are responsible for breakdown of functional and structural components of the cell, such as proteins, nucleic acids, carbohydrates, and lipids. The latter stage of senescence resembles the early stage of leaf curing. Curing is a vital process which falls into the category of starvation phenomena or inanition of excised plant parts (3972, 3973).

The most conspicuous chemical conversions during curing involve two phases. The first phase is dominated by hydrolytic enzymes and occurs in either flue curing or air curing. In this phase, disaccharides and polysaccharides are hydrolyzed to simple sugars; proteins are hydrolyzed to amino acids which undergo oxidative deamination; and the pectins and pentosans are hydrolyzed to pectic acid, uronic acid, and methyl alcohol. The second phase is dominated by oxidative reactions and takes place mostly in air-curing processes. Among the conversions are the following: oxidation of simple sugars to acids, oxygen, and water; the increased oxidative deamination of amino acids leads to the formation of ammonia and amides, particularly asparagine; changes in organic acids, including conversion of malic to citric acid and also decarboxylations; and the oxidative and polymerization of phenols to brown products. There is a small decrease in alkaloids and some loss of dry weight (3972, 3973).

Although not discussed specifically, the tobacco plant contains many thousands of different proteins that are produced by the plant to perform both structural and functional roles. The abundance and types of proteins differ according to the plant organ and cell type being considered. And at the cellular level, proteins with functional roles in chloroplasts and mitochondria may be encoded by the small DNA genomes of those organelles or may be specified by nuclear genes and imported into those organelles.

A significant percentage of proteins in the tobacco leaf are those involved in photosynthesis. This complex process is mediated by the action of hundreds of enzymes involved in the capture of energy from sunlight and the use of that energy to assimilate carbon dioxide from the atmosphere. A key enzyme responsible for this process is ribulose-1,5-bisphosphate carboxylase–oxygenase (sometimes referred to as RuBP carboxylase or simply "Rubisco") (22A35). It is an enzyme that has a dual function in that it catalyzes the carboxylation and oxygenation of ribulose-1,5 bisphosphate. Therefore, it catalyzes the crucial reactions of both photosynthesis and photorespiration; the ratio of these two processes determines plant productivity (3973, 3974c). This important enzyme is the most abundant individual leaf protein and has been proposed as the most important and abundant single protein in nature. On the other hand, the majority of nicotine biosynthesis occurs in root tissues, so the enzymes involved in that process are expressed most abundantly in roots.

Before the advent of modern plant biochemistry and molecular biology, tobacco leaves, as well as the leaves of other higher plants, were considered to possess two broad classes of proteins based on their solubility properties during extraction. Of the total tobacco leaf proteins, approximately half are "soluble" and half "insoluble." The most abundant soluble protein came to be known as "Fraction-1 protein" (F-1 protein, shown to be primarily RuBP carboxylase), a material that can constitute as much as 50% of the total soluble tobacco leaf protein. During the 1980s, this material was considered as a potential source of food protein and for a number of other food applications due to its abundance and a number of other favorable properties. The remaining leaf protein consisting of multitude of smaller soluble proteins and unfractionated protein in the cytoplasm and chloroplast was referred to as "Fraction-2 protein" (F-2 protein) (3973, 3974c). In addition to tobacco proteins having functional roles such as RuBP carboxylase, tobacco and other plants contain proteins, the primary role of which is structural. For example, extensins, a family of glycoproteins rich in hydroxyproline residues, may constitute as much as 15% of the primary cell wall. Extensins are incorporated into the carbohydrate structure of cell walls and are thought to help provide structural support as cell walls develop.

Contemporary research has tended to concentrate on the identification and function of individual proteins that play key roles in plant growth, development, and response to environmental cues. While much of this research has shifted from tobacco to the more easily manipulated model plant system *A. thaliana*, tobacco continues to be the subject of considerable research due to the historical database of tobacco-specific information, its ease of genetic manipulation, and its interesting biochemical pathways for alkaloid biosynthesis. This research has shown tobacco to possess an amazing diversity of proteins, the roles of which continue to be elucidated.

Tobacco "leaf protein" by itself contributes little to smoking quality, but it is a major precursor of hundreds of tobacco smoke components, e.g., numerous nitrogenous compounds and amino acids. Similarly, other major tobacco components such as the carbohydrates, carboxylic acids, pigments, polyphenols, fatty compounds, phytosterols, and many primary or secondary compounds play a significant role in producing a myriad of tobacco smoke compounds (3972–3974c).

> Plant material and smoke composition are closely interrelated. Properties of leaf material can be modified through genetic and biochemical manipulation from seed to curing (22A30).

In dealing with an organic material as complex as tobacco, there are limitations in the range of possible changes that can be made to improve the biological interaction and metabolic balance within a plant system and at the same time improve or alter the smoke composition and ultimately the biological activity of the smoke. The challenge that faces the tobacco industry today in light of the numerous possibilities that will come from the genetic mapping of *N. tabacum* is the development of new tobacco types that can satisfy farmers, manufacturers, regulators, and consumers in quality and tobacco safety.

Solutions to the questions posed by Tso in 1972 (22A30) as to: What kinds of changes are needed [to produce safer tobacco products]? and [H]ow can these changes be achieved? may be attainable in the future with the newfound knowledge from the genetic mapping of the tobacco genome.

Table 22.2 is a catalog of the genes, nucleotides (DNA/RNA strands), enzymes, and a few major proteins identified to date in tobacco. The format of this table differs from those in most other chapters since all listed are tobacco components. As a result, the Tobacco Smoke column was deleted from Table 22.2. The catalog contains 580 entries. The increase in this number from the 491 cited in our First Edition is primarily due to the inclusion in Table 22.2 of a number of bacteria recently described as tobacco components (5169, 5369, 5498). However, this number of entries represents only a very small fraction of the genes identified and nucleotides created recently during the tobacco genome projects. As more time passes, the totality of the genes and nucleotides identified in the tobacco genome will be published or made available in databases for researchers to access. The majority of the known enzymes identified in tobacco are contained in Table 22.2.

ACKNOWLEDGMENTS

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TABLE 22.2
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
1.	9012-33-3	β-Acetylglucosaminidase	5811, 5811b
2.		Acetylserine sulfhydrylase	4249, 4896
3.	9040-07-7	Acetyltransferase, chloramphenicol	3912a, 4249
4.		*Acinetobacter*	5369, 5498
5.		*Actinobacteria, Actinobacteria*	5369
6.	141733-40-6	Acyltransferase, glycerol phosphate (*A. thaliana* clone BX3.6/BB2.6 reduced)	922d, 2663a, 4249
7.	9012-52-6	Adenosyltransferase, methionine	429b, 922d, 4249
	9012-39-9	Adenylyltransferase, sulfate	429b, 922d, 3973, 4249, 4853, 5811b
8.	9006-50-2	Albumin	2529, 4249, 4561
9.	9048-46-8	Albumins, blood serum	429b
10.	9024-52-6	Aldolase, fructose diphosphate	429b, 4249, 4586
11.	9026-94-2	Aldolase, phospho-2-keto-3-deoxyheptonate	429b, 4249
12.	145137-43-5	Aldolase, phospho-2-keto-3-deoxyheptonate (tobacco clone NtDAHPS-1 precursor reduced)	2380b, 4249
13.	9031-85-0	Aminoacyltransferase	429b, 922d, 4249, 4557
14.	9031-94-1	Aminopeptidase	4249, 4646, 22A25
15.	9001-61-0	Aminopeptidase, cytosol	429b, 4249
16.	9054-63-1	Aminopeptidase, leucine	923, 4249
17.	37277-82-0	Aminopropyltransferase, putrescine	429b, 922d, 4249
18.	9031-66-7	Aminotransferase	429b, 922d, 4249
19.	9000-86-6	Aminotransferase, alanine	429b, 922d, 2058d, 4249
20.	9000-97-9	Aminotransferase, aspartate	429b, 922d, 4249, 4592
21.	50812-10-7	Aminotransferase, glutamate–glyoxylate	429b, 922d, 4249, 4705
22.	9030-42-6	Aminotransferase, ornithine ketoacid	429b, 922d, 3973, 4249
23.	37259-57-7	Aminotransferase, serine–glyoxylate	429b, 922d, 4249, 4734
24.	9024-28-6	Ammonia-lyase, phenylalanine {tyrase}	1102, 4221, 4249, 4438a, 4605, 5811b
25.	9000-92-4	Amylase {diastase}	922d, 923, 3973, 4249, 5079, 5099, 5100, 5129, 5189, 5194, 5263, 5359, 5382, 5389, 5811b
26.	9000-90-2	Amylase, α-	1052, 2914, 3772, 3973, 4249, 4464, 5811b
27.	9000-91-3	Amylase, β-	3973, 4249, 4464
28.	9067-73-6	Amylase, iso-	429b, 4249, 4684
29.	9001-03-0	Anhydrase, carbonate	4249, 4601
30.	9000-95-7	Apyrase	429b, 4249, 4593
31.		*Atopobium*	5369
32.		*Aurantimonas altamirensis*	5369
33.	9024-08-2	*Bacillus pumilus* {racemase, glutamate}	5369
34.	68038-71-1	*Bacillus thuringiensis* {Dipel®}	3633, 3634, 5237, 5238
35.	9012-49-1	Carbamoyltransferase, aspartate	429b, 4249, 4900
36.		*Bacteroidetes, Bacteroidetes*	5369
37.		*Bacteroidetes, Sphingobacteria*	5369
38.		*Burkholderia*	5369
39.		*Campylobacter*	5369
40.	9031-55-4	Carboxylase	429b, 2153b, 4249
41.	9067-77-0	Carboxylase, phosphoenolpyruvate (phosphate)	429b, 4249, 4639
42.	37341-54-1	Carboxylase, phosphopyruvate	429b, 4249, 4705
43.	131201-61-1	Carboxylase, ribulose diphosphate (*N. sylvestris* clone NySS4 small subunit precursor reduced)	2236a, 3973, 4249
44.	9031-98-5	Carboxypeptidase	1662, 4249, 4287
45.	9001-05-2	Catalase	1127b, 3433, 3434, 4249, 4464, 5079, 5137, 5165, 5188, 5189, 5231, 5275, 5301, 5739, 5791, 5811b
46.	9012-54-8	Cellulase	429b, 4249, 5079, 5123, 5421

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
47.	9001-06-3	Chitinase	1102, 4249, 5811b
48.	131554-01-3	Chitinase (*N. tabacum* samsun isoenzyme reduced)	2687a, 4249
49.	148348-37-2	Chitinase (*N. tabacum* xanthi clone pBSCL226 isoenzyme III precursor reduced)	2318a, 4249
50.	152619-17-5	Chitinase (tobacco basic isoenzyme III precursor reduced)	3370d, 4249
51.	128285-05-2	Chitinase (tobacco clone lambda CHN17 basic isoenzyme precursor reduced)	4249, 22A04
52.	128285-06-3	Chitinase (tobacco clone lambda CHN17 basic isoenzyme reduced)	387a, 4249
53.	159520-75-9	Chitinase (tobacco clone 59 gene chi-V precursor reduced)	2527b, 4249
54.		*Chloroflexi*, *Chloroflexi*	5369
55.		*Chlorogloeopsis*	5369
56.	9025-96-1	Chlorophyllase	3632, 3678, 4249, 4473
57.	9001-12-1	*Clostridium*	5369
58.	85-61-0	Coenzyme A	429b, 4249
59.	604-98-8	Coenzyme A, *S*-(hydrogen butanedioate)	429b, 4249, 4524
60.	303-98-0	Coenzyme Q_{10}	5085
61.		*Comamonas testosteroni*	5369
62.		*Corynebacterium xerosis*	5369
63.	115742-70-6	Cryptogein	1111, 2068a
64.		*Cyanobacteria, Cyanobacteria*	5369
65.		*Cyanobacteria, Cyanophyceae*	5369
66.	94185-89-4	Cyclase, farnesyl pyrophosphate	429b, 4249
67.	9044-61-5	Cytochrome b 559	2079, 4249
68.	9035-46-5	Cytochrome c 6	429b, 4249, 4631
69.	62168-75-6	Deacylase	4249, 4650a, 22A07
70.	9027-22-9	Decarboxylase	3973, 4249, 4650
71.	9036-20-8	Decarboxylase, adenosylmethionine	429b, 920a, 4249
72.	9024-77-5	Decarboxylase, arginine	3973, 4249, 5811b
73.	9024-58-2	Decarboxylase, glutamate	429b, 920a, 4249, 4834
74.	37259-67-9	Decarboxylase, glycine	429b, 920a, 4249, 4705
75.	37205-42-8	Decarboxylase, α-ketoglutaric acid	5079, 5123
76.	9024-60-6	Decarboxylase, ornithine	3973, 4249, 4792, 5811b
77.	9001-04-1	Decarboxylase, pyruvate	429b, 920a, 4249, 4650
78.	9024-70-8	Decarboxylase, uroporphyrinogen	429b, 920a, 4249, 4538
79.	9001-03-0	Dehydratase, carbonate	429b, 4249
80.	9024-34-4	Dehydratase, threonine	429b, 4249
81.	9035-82-9	Dehydrogenase	3973, 4249, 4490a
82.	9031-72-5	Dehydrogenase, alcohol	5811
83.	9001-40-5	Dehydrogenase, glucose 6-phosphate	922d, 2954, 3973, 4249, 4501, 5811b
84.	9029-12-3	Dehydrogenase, glutamate (nicotinamide adenine dinucleotide (phosphate))	922d, 4249, 4565
85.	9001-46-1	Dehydrogenase, glutamic acid	429b, 922a, 4249, 4426
86.	9026-38-4	Dehydrogenase, glutathione (ascorbate)	429b, 922a, 4249, 4834
87.	9001-50-7	Dehydrogenase, glyceraldehyde phosphate	922d, 4249, 4472
88.	9028-13-1	Dehydrogenase, homoserine	429b, 922a, 4249
89.	9001-58-5	Dehydrogenase, isocitrate	429b, 922a, 4249, 4490
90.	9028-48-2	Dehydrogenase, isocitrate (nicotinamide adenine dinucleotide phosphate)	922d, 4249, 4565, 5811b
91.	9001-64-3	Dehydrogenase, malate	922d, 3677, 4249, 4426, 5811b
92.	56941-16-3	Dehydrogenase, malate (decarboxylating) (nicotinamide adenine dinucleotide (phosphate))	922d, 4249, 4565
93.	37250-19-4	Dehydrogenase, malate (nicotinamide adenine dinucleotide phosphate)	922d, 4249
94.	9028-47-1	Dehydrogenase, malate (oxalacetate decarboxylating) (nicotinamide adenine dinucleotide phosphate)	429b, 922a, 4249
95.	9029-14-5	Dehydrogenase, methylenetetrahydrofolate	429b, 922a, 4249, 4969
96.	37256-31-8	Dehydrogenase, nicotine	429b, 922a, 4249
97.	9001-82-5	Dehydrogenase, phosphogluconate	429b, 922a, 4249, 4834
98.	9073-95-4	Dehydrogenase, phosphogluconate (decarboxylating)	922d, 4249, 5811b
99.	9050-70-8	Dehydrogenase, proline	429b, 922a, 4249, 4808

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
100.	9028-28-8	Dehydrogenase, quinate	429b, 922a, 4249, 4483
101.	9079-67-8	Dehydrogenase, reduced nicotinamide adenine dinucleotide	429b, 922a, 4249, 4834
102.	9032-20-6	Dehydrogenase, reduced nicotinamide adenine dinucleotide (phosphate) (quinone)	429b, 922a, 4249,4834, 4983
103.	37256-36-3	Dehydrogenase, reduced nicotinamide adenine dinucleotide (quinone)	429b, 922a, 4249, 4834
104.	37256-37-4	Dehydrogenase, reduced nicotinamide adenine dinucleotide phosphate (quinone)	429b, 922a, 4249
105.	9001-68-7	Dehydrogenase, reduced nicotinamide adenine dinucleotide phosphate	429b, 922a, 4249
106.	9026-87-3	Dehydrogenase, shikimate	429b, 922a, 4249, 4483
107.	9002-02-2	Dehydrogenase, succinate	922a, 3677, 4249, 4660
108.	9054-84-6	Dehydrogenase, xanthine	429b, 922a, 4249, 4783
109.		*Deinococcus-Thermus*, *Thermus*	5369
110.	97162-77-1	Demethylase, nicotine	4885a, 5033, 5487, 5488, 5531
111.	9007-49-2	Deoxyribonucleic acid	5079, 5395
112.	159844-35-6	Deoxyribonucleic acid (*A. thaliana* clone TAY029 gene UbcAt3 ubiquitin-carrier enzyme E 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 1282b, 4249
113.	141712-74-5	Deoxyribonucleic acid (*A. thaliana* strain Heynhold glycerol phosphate acyltransferase messenger RNA complementary)	950b, 2791a, 4249
114.	140812-74-4	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* gene pma1 plus 5′- and 3′-flanking region fragment)	950b, 4249
115.	130061-32-4	Deoxyribonucleic acid (*N. sylvestris* clone NySS4 ribulose diphosphate carboxylase small subunit gene)	950b, 1919a, 4249, 5811, 5811b
116.	144997-82-0	Deoxyribonucleic acid (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa protein D 2 messenger RNA complementary)	950b, 4249, 4366a
117.	155317-25-2	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A11 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
118.	155317-10-5	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A13 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
119.	155317-11-6	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A14 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
120.	155317-12-7	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A15 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
121.	155317-13-8	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A6 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
122.	155317-14-9	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A7 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
123.	155317-15-0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A9 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2878c, 4249
124.	160074-66-8	Deoxyribonucleic acid (*N. tabacum* clone Ubi.U4 gene Ubi.U4 polyubiquitin plus 5′ and 3′ flanking region fragment)	950b, 2969a, 4249
125.	160075-53-6	Deoxyribonucleic acid (*N. tabacum* cv. SR1 leaf clone Ntfad3 ω-3 fatty acid desaturase mRNA complementary plus 5′ and 3′ flanking region fragment)	950b, 1492a, 4249
126.	131553-16-7	Deoxyribonucleic acid (*N. tabacum* samsun 16.5 kDa protein messenger RNA complementary)	950b, 2687a, 4249
127.	131553-15-6	Deoxyribonucleic acid (*N. tabacum* samsun chitinase isoenzyme messenger RNA complementary)	950b, 4039a, 4249
128.	143514-65-2	Deoxyribonucleic acid (*N. tabacum* samsun clone NeIF-5A3 protein formation initiation factor eIF 5A isoform gene)	950b, 4249
129.	141093-81-4	Deoxyribonucleic acid (*N. tabacum* samsun clone pMOG404 osmotin messenger RNA complementary)	950b, 4249, 4273a
130	143638-33-9	Deoxyribonucleic acid (*N. tabacum* samsun clone pTOL1 osmotin messenger RNA complementary)	950b, 3863b, 4249
131.	143341-52-0	Deoxyribonucleic acid (tobacco 1-109-extensin-like protein precursor specifying)	950b, 4249
132.	152619-15-3	Deoxyribonucleic acid (tobacco chitinase acidic isoenzyme III messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 3370d, 4249

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
133.	152619-16-4	Deoxyribonucleic acid (tobacco chitinase basic isoenzyme III messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 3370d, 4249
134.	142978-98-1	Deoxyribonucleic acid (tobacco chloroplast clone L27-1 ribosome protein L 27 messenger RNA complementary)	950b, 1124b, 4249
135.	139872-58-5	Deoxyribonucleic acid (tobacco clone lambda 5A gene RB7 plus 5′- and 3′-flanking region fragment)	790e, 950b, 4249
136.	139872-57-4	Deoxyribonucleic acid (tobacco clone lambda 5A gene RB7)	790e, 950b, 4249
137.	128284-58-2	Deoxyribonucleic acid (tobacco clone lambda CHN17 chitinase basic isoenzyme gene)	950b, 1256b, 4249
138.	156553-68-3	Deoxyribonucleic acid (tobacco clone 59 gene chi-V chitinase plus 5′- and 3′-flanking region fragment)	950b, 1848a, 4249
139.	156553-69-4	Deoxyribonucleic acid (tobacco clone cA-3 gene chi-V chitinase messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 1848a, 4249
140.	155663-09-5	Deoxyribonucleic acid (tobacco clone cpb20-52 antifungal protein CPB 20 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2972a, 4249
141.	124757-79-5	Deoxyribonucleic acid (tobacco clone E22 protein PR 5 gene)	950b, 4038a, 4249
142.	148757-18-0	Deoxyribonucleic acid (tobacco clone G27.1/G27.2 gene Npg1 plus 5′- and 3′-flanking region fragment)	950b, 3874b, 4249
143.	158928-85-9	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 1 fragment)	950b, 2072a, 4249
144.	158928-86-0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 2 fragment)	950b, 2072a, 4249
145.	158928-87-1	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 3 fragment)	950b, 2072a, 4249
146.	145137-42-4	Deoxyribonucleic acid (tobacco clone NtDAHPS-1 phospho-2-keto-3-deoxyheptonate aldolase messenger RNA complementary)	950b, 2380b, 4249
147.	151876-45-8	Deoxyribonucleic acid (tobacco clone OMT3.4 catechol methyltransferase isoenzyme II messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2481c, 4249
148.	128512-15-2	Deoxyribonucleic acid (tobacco clone pBSGlu39.1 endo-1,3-β-glucanase isoenzyme gene coding region)	950b, 3370c, 4249
149.	128512-16-3	Deoxyribonucleic acid (tobacco clone pBSGlu39.3 endo-1,3-β-glucanase isoenzyme gene coding region)	950b, 3370c, 4249
150.	147626-92-4	Deoxyribonucleic acid (tobacco clone pcGS2-17 glutamine synthetase isoenzyme 2 messenger RNA complementary)	225a, 950b, 4249
151.	128512-19-6	Deoxyribonucleic acid (tobacco clone pGL31 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)	950b, 3370a, 4249
152.	128512-20-9	Deoxyribonucleic acid (tobacco clone pGL36 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)	950b, 3370a, 4249
153.	128512-21-0	Deoxyribonucleic acid (tobacco clone pGL43 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)	345c, 950b, 4249
154.	103469-25-6	Deoxyribonucleic acid (tobacco clone PROB12 protein TL messenger RNA complementary)	293a, 950b, 4249
155.	158928-82-6	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 1 fragment)	950b, 4129a, 4249
156.	158928-83-7	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 2 fragment)	950b, 4129a, 4249
157.	158928-84-8	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 3 fragment)	950b, 4129a, 4249
158.	141002-75-7	Deoxyribonucleic acid (tobacco clone pVK5 osmotin messenger RNA complementary)	950b, 2235a, 4249
159.	150001-42-6	Deoxyribonucleic acid (tobacco clone TSC81 ribosome protein L 17 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 1274a, 4249
160.	128512-25-4	Deoxyribonucleic acid (tobacco endo-1,3-β-glucanase isoenzyme messenger RNA complementary)	950b, 3772a, 4249
161.	143341-55-3	Deoxyribonucleic acid (tobacco extensin-like protein 107-amino acid fragment specifying)	950b, 1024a, 4249
162.	143341-56-4	Deoxyribonucleic acid (tobacco extensin-like protein 81-amino acid fragment specifying)	702a, 950b, 4249
163.	160936-44-7	Deoxyribonucleic acid (tobacco leaf curl virus coat protein gene)	950b, 2911a, 4249
164.	141004-11-7	Deoxyribonucleic acid (tobacco ribosome protein L 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2481b, 4249

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
165.	143513-68-2	Deoxyribonucleic acid (tobacco strain NK326 gene oee2-A plus 5′- and 3′-flanking region fragment)	950b, 3625, 4249a
166.	143513-69-3	Deoxyribonucleic acid (tobacco strain NK326 gene oee2-A)	950b, 3625a, 4249
167.	149309-58-0	Deoxyribonucleic acid (tobacco thioredoxin h2 gene plus 5′- and 3′-flanking region fragment)	452, 950b, 4249
168.	140114-22-3	Deoxyribonucleic acid (tobacco thioredoxin messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2934a, 4249
169.	141712-75-6	Deoxyribonucleic acid (*A. thaliana* strain Heynhold glycerol phosphate acyltransferase messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2791a, 4249
170.	148037-15-4	Deoxyribonucleic acid (*A. thaliana* thioredoxin h messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 2254a, 4249
171.	147533-09-3	Deoxyribonucleic acid (*Nicotiana alata* clone NaPRP3g12 proline-rich protein PRP 3 gene plus 5′- and 3′-flanking region fragment)	685a, 950b, 4249
172.	139860-37-0	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A2 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′-and 3′-flanking region fragment)	950b, 2878b, 4249
173.	146150-24-5	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A2 protein formation initiation factor eIF 4A messenger RNA complementary)	950b, 2878b, 4249
174.	140095-89-2	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A3 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′-and 3′-flanking region fragment)	950b, 2878b, 4249
175.	146150-26-7	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A3 protein formation initiation factor eIF 4A messenger RNA complementary)	950b, 2878b, 4249
176.	140360-04-9	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-5A2 protein formation initiation factor eIF 5A isoform messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 4249
177.	143514-64-1	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-5A2 protein formation initiation factor eIF 5A isoform messenger RNA complementary)	669a, 950b, 4249
178.	141374-52-9	Deoxyribonucleic acid (*N. plumbaginifolia* clone pSOD3 copper–zinc superoxide dismutase messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 1623b, 4249
179.	143348-77-0	Deoxyribonucleic acid (*N. plumbaginifolia* clone pSOD3 copper–zinc superoxide dismutase messenger RNA complementary)	950b, 1623b, 4249
180.	144997-81-9	Deoxyribonucleic acid (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa protein D 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 4249, 4366a
181.	140110-39-0	Deoxyribonucleic acid (*N. tabacum* samsun clone NeIF-5A3 protein formation initiation factor eIF 5A isoform gene plus 5′- and 3′-flanking region fragment)	950b, 2878b, 4249
182.	141093-82-5	Deoxyribonucleic acid (*N. tabacum* samsun clone pMOG404 osmotin messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 4249, 4273a
183.	141093-84-7	Deoxyribonucleic acid (*N. tabacum* samsun clone pMOG4041-226-osmotin specifying plus 5′- and 3′-flanking region fragment)	950b, 4249, 4273a
184.	142978-99-2	Deoxyribonucleic acid (tobacco chloroplast clone L27-1 ribosome protein L 27 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 1124b, 4249
185.	145093-14-7	Deoxyribonucleic acid (tobacco clone EPSPS-1 5-enolpyruvoylshikimate 3-phosphate synthase messenger RNA complementary plus 5′- and 3′-flanking region fragment)	53a, 950b, 4249
186.	139837-73-3	Deoxyribonucleic acid (tobacco clone NtDAHPS-1 phospho-2-keto-3-deoxyheptonate aldolase messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 4249, 4398b
187.	128512-17-4	Deoxyribonucleic acid (tobacco clone pBSGlu39.1 endo-1,3-β-glucanase isoenzyme gene coding region plus 5′- and 3′-flanking region fragment)	950b, 3370c, 4249
188.	128512-18-5	Deoxyribonucleic acid (tobacco clone pBSGlu39.3endo-1,3-β-glucanase isoenzyme gene coding region plus 5′- and 3′-flanking region fragment)	950b, 3370c, 4249
189.	145735-56-4	Deoxyribonucleic acid (tobacco clone pcGS2-17 glutamine synthetase isoenzyme 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)	225a, 950b, 4249
190.	128512-22-1	Deoxyribonucleic acid (tobacco clone pGL31 endo-1,3-β- glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 4249

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
191.	128512-23-2	Deoxyribonucleic acid (tobacco clone pGL36 endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 3370a, 4249
192.	128512-24-3	Deoxyribonucleic acid (tobacco clone pGL43 endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)	345c, 950b, 4249
193.	143341-58-6	Deoxyribonucleic acid (tobacco clone pMG15 extensin-like protein messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 1320a, 4249
194.	128512-26-5	Deoxyribonucleic acid (tobacco endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)	950b, 3772a, 4249
195.	143341-53-1	Deoxyribonucleic acid (tobacco extensin-like protein 171-amino acid C-terminal fragment specifying plus 3′-flanking region fragment)	848a, 950b, 4249
196.	143341-54-2	Deoxyribonucleic acid (tobacco extensin-like protein 264-amino acid C-terminal fragment specifying plus 3′-flanking region fragment)	950b, 2534b, 4249
197.	143341-57-5	Deoxyribonucleic acid (tobacco extensin-like protein 393-amino acid C-terminal fragment specifying plus 3′-flanking region fragment)	950b, 2113a, 4249
198.	139637-37-9	Deoxyribonucleic acid, d(A-T-G-T-T-C-T-C-T-C-T-T-T-T-T-A-A-T-G-G-T-G-G-T-T-C-T-T-T-A-G)	950b, 4249
199.	152789-83-8	Deoxyribonucleic acid, d(C-A-T-C-A-C-G-T-G-A-G-A-T-A-A-G-A-G-C-C-G-C-C-A), double-stranded complementary	950b, 4249
200.	152789-84-9	Deoxyribonucleic acid, d(T-A-A-A-G-T-C-A-A-A-G-A-A-T-T-T-C-A-A-T-G-T-C-A-C-A), double-stranded complementary	950b, 4249
201.	67880-95-9	Desaturase, fatty acid ω3-	1859a, 4249
202.	159965-67-0	Desaturase, fatty acid ω3- (tobacco clone Ntfad3)	1492a, 4249
203.	107544-21-8	Desaturase, phytoene	429b, 4249
204.		*Dialister*	5369
205.	37340-89-9	Diaphorase	429b, 4249
206.	9025-33-6	Dipeptidase, prolyl	429b, 4249
207.	9054-89-1	Dismutase, superoxide	429b, 4249, 4748, 5811b
208.	143352-40-3	Dismutase, superoxide (*N. plumbaginifolia* clone pSOD3 copper–zinc protein moiety reduced)	1623b, 4249
209.	9007-57-2	Edestin	429b, 2079
210.		*Enterococcus gallinarum*	5369
211.	159844-36-7	Enzyme E 2 (*A. thaliana* clone TAY029 gene UbcAt3 ubiquitin-carrier)	1282b
212.		*Escherichia coli K12*	5369
213.	9013-79-0	Esterase	923, 4249, 4423, 5811b
214.	9025-98-3	Esterase, pectin {pectase}	922d, 4249, 5079, 5188, 5189
215.	9040-09-9	Ferredoxins	429b
216.		*Firmicutes, Bacilli*	5369
217.		*Firmicutes, Clostridia*	5369
218.	9001-57-4	β-Fructofuranosidase {β-fructosidase, invertase}	429b, 4069b, 4249, 4484, 4489, 4494, 5079, 5123, 5165, 5188, 5189, 5275, 5301, 5323, 5811b
219.	9033-47-0	Fructosidase {polyfructosidase}	429b, 1387a
220.	9001-34-7	Galactosidase	429b, 1837b, 4249, 4696
221.	152347-17-6	GenBank D16204	1282a, 4249
222.	152347-18-7	GenBank D16205	1282a, 4249
223.	152347-16-5	GenBank D16206	1282a, 1656b, 4249
224.	143787-54-6	GenBank L02124	1282a, 2131a, 4249
225.	150472-46-1	GenBank L13439	1282a, 4249
226.	150472-47-2	GenBank L13440	1282a, 4249
227.	150472-48-3	GenBank L13441	1282a, 4249
228.	150472-49-4	GenBank L13442	1282a, 4249
229.	150472-50-7	GenBank L13443	1282a, 4249
230.	149241-78-1	GenBank L14953	1282a, 4249
231.		GenBank M73791	1282a
232.	144680-39-7	GenBank M74102	1282a, 4249

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
233.	144680-37-5	GenBank M74103	1282a, 4249
234.	142693-30-9	GenBank M84650	1282a, 4249
235.	145767-36-8	GenBank M87838	1282a, 4249
236.	145767-40-4	GenBank M87839	1282a, 4249
237.	141683-31-0	GenBank M94135	1282a, 4249
238.		GenBank X58527	1282a
239.	139854-77-6	GenBank X60057	1282a, 4249
240.	140352-16-5	GenBank X61113	1282a, 4249
241.	140352-17-6	GenBank X61114	1282a, 4249
242.	139857-64-0	GenBank X61750	1282a, 4249
243.		GenBank X61826	1282a
244.	140360-05-0	GenBank X62339	1282a, 4249
245.	141005-27-8	GenBank X62368	1282a, 4249
246.	140104-46-7	GenBank X62395	1282a, 4249
247.		GenBank X62500	1282a
248.	142965-21-7	GenBank X63078	1282a, 4249
249.	145905-43-7	GenBank X63607	1282a, 4249
250.	139867-08-6	GenBank X64398	1282a, 4249
251.	139869-01-5	GenBank X64399	1282a, 4249
252.	140830-68-8	GenBank X64423	1282a, 4249
253.		GenBank X64621	1282a
254.	141164-37-6	GenBank X65117	1282a, 4249
255.	141164-36-5	GenBank X65118	1282a, 4249
256.	147904-32-3	GenBank X65982	1282a, 4249
257.	144031-18-5	GenBank X66145	1282a, 4249
258.	143341-50-8	GenBank X67158	1282a, 4249
259.	151468-68-7	GenBank X69971	1282a, 4249
260.	148757-17-9	GenBank X71015	1282a, 4249
261.		GenBank Z11803	1282a
262.	142914-46-3	GenBank Z12619	1282a, 4249
263.	142914-45-2	GenBank Z12623	1282a, 4249
264.	152651-60-0	GenBank Z14079	1282a, 2481a, 4249
265.	152651-59-7	GenBank Z14080	1282a, 2481a, 4249
266.	152651-58-6	GenBank Z14081	1282a, 2481a, 4249
267.	152651-57-5	GenBank Z14082	1282a, 4249
268.	152651-61-1	GenBank Z14085	1282a, 4249
269.	148544-79-0	GenBank Z16403	1282a, 4249
270.	148544-80-3	GenBank Z16404	1282a, 4249
271.	9007-83-4	Globulins, γ-	120, 4249, 4615, 5079, 5432
272.	9044-93-3	β-1,3-Glucanase	1111, 1430a, 4249, 4548
273.	9025-37-0	Glucanase, endo-1,3-β-	5811, 5811b
274.	128512-83-4	Glucanase, endo-1,3-β- (tobacco clone pGL31 isoenzyme)	1317a, 3370a, 4249
275.	128512-84-5	Glucanase, endo-1,3-β- (tobacco clone pGL36 isoenzyme)	1317a, 3370a, 4249
276.	128512-85-6	Glucanase, endo-1,3-β- (tobacco clone pGL43 isoenzyme)	345c, 1317a, 4249
277.	128512-86-7	Glucanase, endo-1,3-β- (tobacco isoenzyme)	1317a, 1824b, 4249
278.	62213-14-3	Glucanase, endo-1,3(4)-β-	429b, 1317a, 4249, 4799
279.	117277-96-0	Glucanase, preproendo-1,3-β-	5811, 5811b
280.	128475-00-3	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme signal peptide)	1317a, 3370b, 4249
281.	128475-01-4	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme signal peptide) 26-*L*-threonine-28-*L*-glutamic acid-	1317a, 2527a, 4249
282.	128512-87-8	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme protein moiety)	1317a, 2527a, 4249
283.	128512-88-9	Glucanase, preproendo-1,3-β- (tobacco clone pBSGluc39.3 isoenzyme protein moiety)	1317a, 2527a, 4249
284.	128512-89-0	Glucanase, preproendo-1,3-β- (tobacco clone pGL31 isoenzyme protein moiety)	1317a, 3370a, 4249

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
285.	128512-90-3	Glucanase, preproendo-1,3-β- (tobacco clone pGL36 isoenzyme protein moiety)	1317a, 3370a, 4249
286.	128512-91-4	Glucanase, preproendo-1,3-β- (tobacco clone pGL43 isoenzyme protein moiety)	345c, 1317a, 4249
287.	128512-92-5	Glucanase, preproendo-1,3-β- (tobacco isoenzyme protein moiety)	685b, 1317a, 4249
288.	117277-97-1	Glucanase, proendo-1,3-β-	5811, 5811b
289.	9001-42-7	Glucosidase, α-	1111, 4249
290.	9001-22-3	Glucosidase, β- {emulsin; amygdalase; synaptase}	429b, 4249, 5079
291.	9012-47-9	Glucosidase, amylo-1,6-	429b, 4249, 4920
292.	9031-48-5	Glucosyltransferase	429b, 4249, 4489
293.	9027-19-4	Glucosyltransferase, uridine diphosphoglucose-1,4-β-glucan	429b, 4249, 4827
294.	50812-18-5	β-*D*-Glucosyltransferase, uridine diphosphoglucose-flavonol 3-*O*-glucoside	429b, 4249
295.	9030-05-1	Glucosyltransferase, uridine diphosphoglucose-fructose	429b, 4249, 4489
296.	9030-06-2	Glucosyltransferase, uridine diphosphoglucose-fructose phosphate	429b, 4249, 4489
297.	146480-37-7 156859-11-9	Glucosyltransferase, uridine diphosphoglucose-salicylate 3-	689a, 4249, 5811b
298.	9001-45-0	Glucuronidase, β-	429b, 4249, 5811b
299.	9046-27-9	Glutamyltransferase, γ-	429b, 4249
300.	9061-41-0	Glutenin	429b, 4249, 4615
301.		Glycolase	5079, 5189
302.	83534-39-8	Glycosidase	4249, 4426
303.	9001-97-2	Glycosyltransferase, α-glucan branching	429b, 4249, 4920
304.	37347-76-5	Glyoxalase	429b, 2153b, 4249, 5079
305.	9024-25-3	Hydratase, aconitate	429b, 4249, 4438, 4628, 4634, 4886
306.	9032-88-6	Hydratase, fumarate	429b, 4249, 4838
307.	9014-08-8	Hydratase, phosphopyruvate	429b, 4249, 4873
308.	9027-05-8	Hydrogenase	429b, 4249, 4457
309.	9027-41-2	Hydrolase	429b, 922d, 1615a, 4249, 4808a
310.	120598-69-8	Hydroxycinnamoyltransferase, putrescine	429b, 4249
311.	73904-44-6	Hydroxycinnamoyltransferase, shikimate	429b, 4249, 4931
312.	128909-19-3	Hydroxycinnamoyltransferase, tyramine	1841a, 4249
313.	60321-02-0	Hydroxycinnamyl-CoA:quinate {hydroxycinnamoyl transferase, quinate}	429b, 4249, 4930
314.		Hydroxylase, glycine	4249, 4704
315.	9029-83-8	Hydroxymethyltransferase, serine	429b, 4249, 4705
316.	9025-67-6	Inulase	5079, 5323
317.	80449-01-0	Isomerase, deoxyribonucleate topo-	429b, 922d, 4249
318.	9001-41-6	Isomerase, glucose phosphate	429b, 922d, 4249, 4886
319.	9055-95-2	Isomerase, pentose phosphate	429b, 922d, 4249, 4937
320.	9023-83-0	Isomerase, ribose phosphate	429b, 922d, 4249, 4938
321.		Isoperoxidase A_3	3103
322.	9013-02-9	Kinase (phosphorylating), adenylate	429b, 2095b, 4249, 4879
323.	9012-50-4	Kinase (phosphorylating), aspartate	429b, 2095b, 4249
324.	9026-67-9	Kinase (phosphorylating), choline	429b, 2095b, 4249, 4912
325.	9030-51-7	Kinase (phosphorylating), fructo-	5811, 5811b
326.	9001-36-9	Kinase (phosphorylating), gluco-	429b, 2095b, 4249, 4919, 5811b
327.	9026-62-4	Kinase (phosphorylating), glucurono-	429b, 2095b, 4249
328.	9001-51-8	Kinase (phosphorylating), hexo-	429b, 2095b, 4249, 4888
329.	9032-66-0	Kinase (phosphorylating), nicotinamide adenine dinucleotide	429b, 2095b, 4249, 4977
330.	9001-80-3	Kinase (phosphorylating), phosphofructo-	429b, 2095b, 4249, 4759
331.	9032-96-6	Kinase (phosphorylating), phosphogluco-	429b, 2095b, 4249, 4919
332.	150656-38-5	Kinase (phosphorylating), protein (tobacco BY-2 cell isoenzyme ZmPK1 reduced)	429b, 1889, 2095b, 4249
333.	9001-59-6	Kinase (phosphorylating), pyruvate	429b, 2095b, 4249, 4487
334.	9027-40-1	Kinase (phosphorylating), pyruvate-phosphate di-	429b, 2095b, 4249, 4705
335.	9030-57-3	Kinase (phosphorylating), ribulo-	429b, 2095b, 4249, 4938
336.	9031-51-0	Kinase (phosphorylating), shikimate	429b, 2095b, 4249
337.		Kinase, protein	5062, 5491

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
338.		*Klebsiella oxytoca*	5369
339.	9031-11-2	Lactase	5079, 5123, 5188, 5323
340.		Limulus ameobocyte lysate (LAL)	5072
341.	9001-62-1	Lipase {lipase, triacylglycerol}	429b, 1971, 4249, 5079, 5188, 5189, 5323
342.		Lipopolysaccharide (LPS)	5072, 5215
343.	9029-60-1	Lipoxygenase	891
344.	9045-78-7	Lyase, isocitrate	429b, 922d, 4249, 4490
345.	9015-75-2	Lyase, pectate	429b, 922d, 4249, 4619
346.		*Lyngbya*	5369
347.	90803-60-4	M-1nkh	429b
348.	9025-42-7	Mannosidase, α-	429b, 4249, 4494
349.	9024-05-9	*Megasphaera* {racemase, lactate}	5369
350.	8049-97-6	Melanin	102, 3660, 3973, 5079
351.	50936-45-3	Methyltransferase, caffeate	429b, 4249, 4725
352.	9012-25-3	Methyltransferase, catechol	429b, 4249, 5811b
353.	152288-82-9	Methyltransferase, catechol (tobacco clone OMT3.4 isoenzyme II reduced)	429b, 2481c, 4249
354.	9012-40-2	Methyltransferase, homocysteine {transmethylase}	429b, 4249
355.	9027-77-4	Methyltransferase, methionine *S*-	429b, 4249
356.	9055-07-6	Methyltransferase, protein (arginine)	429b, 4249
357.	9075-39-2	Methyltransferase, putrescine	429b, 4249, 5090
358.		*Microcystis*	5369
359.	9047-56-7	Mutase	429b, 2702a, 4249, 1971, 5079
360.	9033-12-9	Mutase, ketone–aldehyde	5079, 5189
361.		Mycorrhiza	5051
362.		*Myobacterium avium*	5169
363.		*Novosphingobium aromaticivorans*	5369
364.	9026-81-7	Nuclease	429b, 4249, 4494
365.	9003-98-9	Nuclease, deoxyribo-	429b, 4249, 4496
366.	9055-11-2	Nuclease, endo-	429b, 4249
367.	59977-50-3	Nuclease, mammalian deoxyribonucleate-nicking endo-	345, 4249
368.	9025-44-9	Nucleosidase	429b, 4249, 4657
369.	9033-33-4	Nucleotidase	429b, 4249, 4824
370.	9012-90-2	Nucleotidyltransferase, deoxyribonucleate {polymerase, nucleic acid deoxyribo}	429b, 4249, 4505, 4898
371.	9068-38-6	Nucleotidyltransferase, deoxyribonucleate, RNA dependent	429b, 4249
372.	9014-24-8	Nucleotidyltransferase, ribonucleate	429b, 4249, 4505
373.	9026-28-2	Nucleotidyltransferase, ribonucleate, RNA dependent	429b, 4249, 4962
374.	141093-09-6	1-226-Osmotin (*N. tabacum* samsun clone pMOG404 reduced)	4273a, 4249
375.	141093-08-5	Osmotin (*N. tabacum* samsun clone pMOG404 reduced)	4273a, 4249
376.	143638-31-7	Osmotin (*N. tabacum* samsun clone pTOL1 precursor reduced) -	3863b, 4249
377.	143638-32-8	Osmotin (*N. tabacum* samsun clone pTOL1 reduced)	3863b, 4249
378.	131553-54-3	Osmotin (*N. tabacum* samsun reduced)	22A36
379.	142583-50-4	Osmotin (tobacco clone pVK5 precursor reduced)	2235a, 4249
380.	142583-51-5	Osmotin (tobacco clone pVK5 reduced)	2235a, 4249
381.	9035-73-8	Oxidase	429b, 2878d, 4249, 4493, 5079, 5123, 5128, 5188, 5189, 5323, 5352, 5382
382.	9029-44-1	Oxidase, ascorbate	429b, 2878d, 2964, 3973, 4249, 4516, 5079, 5137
383.	9028-67-5	Oxidase, choline	4249, 4528
384.	9076-84-0	Oxidase, coproporphyrinogen	429b, 2210b, 2878d, 4249, 4672
385.	9001-16-5	Oxidase, cytochrome c {cytochrome oxidase}	429b, 1127b, 2878d, 3677, 5079, 5123, 5737
386.	9001-53-0	Oxidase, diamine	429b, 1615a, 2878d
387.	9028-71-1	Oxidase, glycolate	429b, 2878d, 4249, 4985

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
388.	9027-85-4	Oxidase, indoleacetate	429b, 2878d, 4249, 4441, 5811b
389.	55326-39-1	Oxidase, isopentenyladenosine	429b, 2878d
390.	37259-79-3	Oxidase, methylputrescine	429b, 2878d, 4249, 4685, 4792, 5811b
391.	9001-96-1	Oxidase, pyruvate	429b, 2878d, 4249,4051a
392.	9032-21-7	Oxidase, reduced nicotinamide adenine dinucleotide	429b, 2878d, 4249, 4834, 5811b
393.	9032-22-8	Oxidase, reduced nicotinamide adenine dinucleotide phosphate	429b, 2878d, 4249, 4834
394.	9014-35-1	Oxidase, succinate	429b, 2878d, 4249, 4839
395.	69671-26-7	Oxidase, ubiquinol	429b, 2878d, 4249
396.	9002-12-4	Oxidase, urate	429b, 2878d, 4249, 4622
397.	9002-17-9	Oxidase, xanthine	429b, 2878d, 4249, 4724
398.	9029-57-6	Oxygenase, 2,5-dihydroxypyridine 5,6-di-	429b, 2878e, 4249, 4918
399.	152060-37-2	Oxygenase, benzoate 2-mono-	429b, 2350, 2878e
400.	9077-75-2	Oxygenase, cinnamate 4-mono- {hydroxylase cinnamate}	429b, 2878e, 4249, 4737
401.	9068-40-0	Oxygenase, *p*-coumarate 3-mono-	429b, 2878e, 4249, 4492
402.	9028-06-2	Oxygenase, protocollagen proline di-	429b, 2878e
403.	39335-11-0	Oxygenase, ribulose diphosphate	429b, 2236a, 2878e, 4249, 4641
404.		*Pantoea*	5369
405.	142193-29-1	Parasiticein	1855a, 3126b, 4249
406.	142193-19-9	Parasiticein (*Phytophthora parasitica* reduced)	1855a, 3126b, 4249
407.	9031-96-3	Peptidase	923, 4249
408.	9055-26-9	Permease, sulfate	4249, 4896
409.	9003-99-0	Peroxidase	543a, 1111, 1127b, 2550, 3103, 3434, 3434a, 3630, 3973, 4221, 4249, 4426, 5079, 5123, 5128, 5137, 5189, 5275, 5301, 5570, 5614, 5615, 5792
410.	72906-87-7	Peroxidase, ascorbate	3973, 4249
411.	9013-66-5 97089-70-8	Peroxidase, glutathione	2954, 4249
412.	9013-05-2	Phosphatase	429b, 1971, 2948a, 4249, 5079, 5188, 5189
413.	122319-88-4	Phosphatase, 2-carboxyarabinitol 1-	429b, 2948a, 4249
414.	9001-77-8	Phosphatase, acid	429b, 2948a, 3973, 4249, 4423, 5811b
415.	9000-83-3	Phosphatase, adenosine tri-	429b, 2948a, 4249
416.	134632-85-2	Phosphatase, adenosine tri- (*Petunia hybrida* strain 3704 mitochondria subunit 9)	429b, 349b, 2948a, 4249
417.	9001-78-9	Phosphatase, alkaline	429b, 2948a, 4249, 4821
418.	9001-52-9	Phosphatase, fructose di-	429b, 2948a, 4249
419.	9001-39-2	Phosphatase, glucose 6-	429b, 2948a, 4249
420.	69669-68-7	Phosphatase, glucose di-	429b, 2948a, 4249, 4827, 4834
421.	9027-69-4	Phosphatase, nucleoside di-	429b, 2948a, 4249, 4693
422.	9075-51-8	Phosphatase, nucleoside tri-	429b, 2948a, 4249, 4726
423.	9055-30-5	Phosphatase, phosphoglycerate	429b, 2948a, 4249, 4705
424.	9025-76-7	Phosphatase, phosphoglycolate	429b, 2948a, 4249, 4546
425.	52227-92-6	Phosphatase, phosphorylcholine	429b, 2948a, 4249, 4912
426.	37341-58-5	Phosphatase, phytate	429b, 2948a, 4249, 4825
427.	9059-33-0	Phosphatase, sucrose	4249, 4489
428.	9025-82-5	Phosphodiesterase	5811
429.	9036-21-9	Phosphodiesterase, adenosine cyclic 3′,5′-phosphate	429b, 4249, 4503, 4970
430.	39434-01-0	Phosphodiesterase, nucleotide	429b, 4249, 4435
431.	12712-31-1	Phosphodoxin	340
432.	9001-81-4	Phosphomutase, glucose	429b, 4249, 4489
433.	9030-26-6	Phosphoribosyltransferase, nicotinate	429b, 922d, 4249, 4764
434.	9035-74-9	Phosphorylase	3973, 4249, 4694
435.	9032-10-4	Phosphorylase a	429b, 4249, 4674
436.	9030-28-8	Phosphorylase, guanosine	429b, 4249

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
437.	9014-12-4	Phosphorylase, polynucleotide {nucleotidyltransferase, polyribonucleotide}	429b, 4249, 4506
438.	37297-20-4	Phytoalexins	2614a
439.		*Planctomycetes, Planctomycetacia*	5369
440.	9032-75-1	Polygalacturonase	429b, 4249, 4446a, 4934
441.	152415-56-0	Polygalacturonase (tobacco clone G27.1/G27.2 gene Npg1 precursor reduced)	3874a, 4249
442.	9002-10-2	Polyphenoloxidase {oxygenase, monophenol mono; tyrosinase}	429b, 543a, 1102, 2550, 2878e, 3630, 3677, 4221, 4249, 4899, 5079, 5123, 5570, 5737, 5739, 5760, 5808, 5811b, 5856
443.		Poly(U)polymerase	4249, 4507
444.	9030-77-7	Polyprenyltransferase, 4-hydroxybenzoate	5085
445.	159965-71-6	Polyubiquitin (*N. tabacum* clone Ubi.U4 gene Ubi.U4)	2969a, 4249
446.	9055-40-7	Porphobilinogenase	429b, 4249
447.	37259-58-8	Protease	543a, 2914, 5079, 5189, 5323
448.		Protease, serine	4287
449.		Protease, sulfhydryl	4249, 4287
450.	144419-45-4	Protein (*A. thaliana* clone G9.1 gene A9 11.6 kDa reduced)	3566a, 4249
451.	132966-19-9	Protein (tobacco 27.4 kDa RNA-binding precursor reduced)	2400b, 4249
452.	132966-16-6	Protein (tobacco 27.4 kDa RNA-binding)	2400b, 4249
453.	137801-72-0	Protein (tobacco chloroplast clone pTB24 gene psbK)	2530b, 4249
454.	139874-83-2	Protein (tobacco clone .lambda.18C gene RB7 reduced)	790d, 4249
455.	139874-82-1	Protein (tobacco clone .lambda.5A gene RB7 reduced)	790c, 4249
456.	162572-20-5	Protein (tobacco clone lambda T-FLO 4 gene NFL2)	2072a, 4249
457.	147445-75-8	Protein (tobacco clone pMG15 extensin-like precursor reduced)	1320a, 4249
458.	146591-93-7	Protein (tobacco clone PRP3g12 gene PRP3 pistil-specific proline-rich precursor)	2169a, 4249
459.	162572-19-2	Protein (tobacco clone pTGF220 gene NFL1)	2072a, 4249
460.	145895-79-0	Protein (tobacco flower-associated reduced)	1841a, 4249
461.	155077-18-2	Protein (tobacco gene MST1 hydrogen ion–monosaccharide cotransporting reduced)	3417a, 4249
462.	160936-45-8	Protein (tobacco leaf curl virus coat)	2911a, 4249
463.	155663-14-2	Protein CPB 20 (tobacco clone cpb20–44 antifungal reduced)	2972a, 4249
464.	155663-12-0	Protein CPB 20 (tobacco clone cpb20–52 antifungal reduced)	2972a, 4249
465.	155663-10-8	Protein CPB 20, prepro-(tobacco clone cpb20–52 antifungal reduced)	2972a, 4249
466.	155663-13-1	Protein CPB 20, pro-(tobacco clone cpb20–44 antifungal reduced)	2972a, 4249
467.	155663-11-9	Protein CPB 20, pro-(tobacco clone cpb20–52 antifungal reduced)	2972a, 4249
468.	144997-83-1	Protein D 2 (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa precursor)	4366a, 4249
469.	144997-84-2	Protein D 2 (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa)	4366a, 4249
470.	146150-25-6	Protein formation initiation factor eIF 4A (*N. plumbaginifolia* clone NeIF-4A2 isoform reduced)	2878b, 4249
471.	146150-27-8	Protein formation initiation factor eIF 4A (*N. plumbaginifolia* clone NeIF-4A3 isoform reduced)	2878b, 4249
472.	162572-22-7	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A9)	2878c, 4249
473.	162572-23-8	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A11)	2878c, 4249
474.	162572-24-9	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A7)	2878c, 4249
475.	162572-25-0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A15)	2878c, 4249
476.	162572-26-1	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A6)	2878c, 4249
477.	162572-27-2	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A13)	2878c, 4249
478.	162572-28-3	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A14)	2878c, 4249
479.	143514-66-3	Protein formation initiation factor eIF 5A (*N. plumbaginifolia* clone NeIF-5A1 isoform C-terminal fragment reduced)	669a, 4249
480.	143514-67-4	Protein formation initiation factor eIF 5A (*N. plumbaginifolia* clone NeIF-5A2 isoform reduced)	669a, 4249
481.	143514-68-5	Protein formation initiation factor eIF 5A (*N. tabacum* samsun clone NeIF-5A3 isoform reduced)	2997b, 4249
482.	152745-97-6	Protein L 17 (tobacco clone TSC81 ribosome reduced)	1274a, 4249

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
483.	142978-88-9	Protein L 27 (tobacco chloroplast clone L27-1 ribosome precursor reduced)	1124b, 4249
484.	142978-89-0	Protein L 27 (tobacco chloroplast clone L27-1 ribosome reduced)	1124b, 4249
485.	160082-04-2	Protein LTP (tobacco)	903a, 4249
486.	143513-70-6	Protein OEE 2 (tobacco strain NK326 precursor reduced)	3625a, 4249
487.	9001-92-7	Proteinase	2997a, 4249, 4452, 5811b
488.	37205-61-1	Proteinase inhibitor	429b, 2997a, 4249
489.	145090-32-0	Proteinase inhibitor, PI-1	174f, 2997a, 4249
490.	150474-41-2	Proteinase inhibitor, prepro-TIMPa (*N. tabacum* samsun reduced)	1615b, 2997a, 4249
491.	150474-40-1	Proteinase inhibitor, prepro-TIMPb (*N. tabacum* samsun reduced)	1615b, 2997a, 4249
492.	150474-44-5	Proteinase inhibitor, pro-TIMPa (*N. tabacum* samsun reduced)	1615b, 2997a, 4249
493.	150474-42-3	Proteinase inhibitor, pro-TIMPb (*N. tabacum* samsun reduced)	1615b, 2997a, 4249
494.	150474-45-6	Proteinase inhibitor, TIMPa (*N. tabacum* samsun reduced)	1615b, 2997a, 4249
495.	150474-43-4	Proteinase inhibitor, TIMPb (*N. tabacum* samsun reduced)	1615b, 2997a, 4249
496.		*Proteobacteria, Alphaproteobacteria*	5369
497.		*Proteobacteria, Betaproteobacteria*	5369
498.		*Proteobacteria, Epsilonproteobacteria*	5369
499.		*Proteobacteria, Gammaproteobacteria*	5369
500.		*Proteobacteria, Alphaproteobacteria*	5369
501.	9013-10-9	*Proteus* {isomerase, glucosamine phosphate}	5369
502.		*Pseudomonas aeruginasa*	5369
503.	9033-44-7	Pyrophosphatase	429b, 4249
504.	9024-82-2	Pyrophosphatase, inorganic	429b, 4249, 4834
505.	37289-33-1	Pyrophosphatase, nicotinamide adenine dinucleotide	429b, 3973, 4249, 4981
506.	9032-64-8	Pyrophosphatase, nucleotide	429b, 4249, 3402a
507.	9038-53-3	Pyrophosphatase, thiamin	429b, 4249, 4462
508.	68858-66-2	Pyrophosphorylase	429b, 4249, 4808
509.	37277-74-0	Pyrophosphorylase, nicotinate mononucleotide (carboxylating) {phosphoribosyltransferase, quinolinate}	429b, 4249, 5090
510.	9037-80-3	Reductase	429b, 1971, 3093c, 4249, 5079, 5188, 5189, 5323
511.	9028-31-3	Reductase, aldose	429b, 3093c, 4249, 4712a
512.	9023-03-4	Reductase, cytochrome c (reduced nicotinamide adenine dinucleotide phosphate)	429b, 3093c, 4249, 4748
513.	37256-44-3	Reductase, ferredoxin–nitrite	429b, 3093c, 4249
514.	9001-48-3	Reductase, glutathione	429b, 2954, 3093c, 4249, 4834, 5811b
515.	9028-32-4	Reductase, glyoxylate	429b, 3093c, 4249, 4834
516.	9032-06-8	Reductase, hydroxylamine	429b, 3093c, 4249, 4519
517.	9028-35-7	Reductase, hydroxymethylglutaryl coenzyme A (reduced nicotinamide adenine dinucleotide phosphate)	429b, 3093c, 4249
518.	9013-03-0	Reductase, nitrate	429b, 2194a, 3093c, 4249, 4656, 5811b
519.	9029-27-0	Reductase, nitrate (reduced nicotinamide adenine dinucleotide (phosphate))	429b, 3093c, 4249
520.	9080-03-9	Reductase, nitrite	429b, 1941, 3093c, 4249
521.	9029-29-2	Reductase, nitrite (reduced nicotinamide adenine dinucleotide (phosphate))	429b, 3093c, 4249
522.	9029-17-8	Reductase, pyrroline-5-carboxylate	429b, 3093c, 4249
523.	51848-43-2	Retine	4249
524.	9001-99-4	Ribonuclease {nuclease, ribo-}	429b, 4249, 4973
525.	63231-63-0	Ribonucleic acid	4249, 4442, 5863
526.	9067-16-7	Ribonucleic acid (*Bombyx mori* fibroin-specifying messenger)	429b, 3126a, 4249
527.	139872-63-2	Ribonucleic acid (tobacco clone .lambda.5A gene RB7 protein-specifying 1524-nucleotide messenger)	790c, 3126a, 4249
528.	139872-64-3	Ribonucleic acid (tobacco clone .lambda.5A gene RB7 protein-specifying 1549-nucleotide messenger)	790c, 3126a, 4249

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
529.	128285-01-8	Ribonucleic acid (tobacco clone lambda CHN17 chitinase basic isoenzyme-specifying messenger)	387a, 4249
530.	9014-25-9	Ribonucleic acids, transferase	429b, 4249, 4604
531.	9027-23-0	Ribulose-1,5-bisphosphate carboxylase {rubisco, F-1 protein, F-1 protein, also known as carboxylase, ribulose diphosphate}	429b, 2236, 2236a, 2394a, 3973, 4249, 4542, 5811b, 22A35
532.		*Staphylococcus saprophyticus*	5369
533.		*Staphylococcus epidermidis*	5369
534.		*Staphylococcus cohnii*	5369
535.		*Staphylococcus sciuri*	5369
536.		*Stenotrophomonas maltophilia*	5369
537.	72506-68-4	Synthase, 1-aminocyclopropanecarboxylate	3844a, 3973, 4249
538.	37211-77-1	Synthase, 5-dehydroquinate	1243a, 3844a, 3973
539.	9068-73-9	Synthase, 5-enolpyruvoylshikimate 3-phosphate	3844a, 3973, 4249
540.	144324-42-5	Synthase, 5-enolpyruvoylshikimate 3-phosphate (petunia clone pMON9531/pMON9556 reduced) 101-*L*-alanine-	3622a, 3844a, 4249, 4483
541.	144324-43-6	Synthase, 5-enolpyruvoylshikimate 3-phosphate (petunia clone pMON9531/pMON9556 reduced) 101-*L*-alanine-192-*L*-threonine-	3622a, 3844a, 4249
542	9027-45-6	Synthase, acetolactate	3844a, 3973, 4249
543.	9031-59-8	Synthase, anthranilate	429b, 3844a, 4249, 4962
544.	37290-89-4	Synthase, cysteine {acetylserine sulfhydrylase}	429b, 3844a, 4249, 4896
545.	9055-59-8	Synthase, dihydrodipicolinate	429b, 3844a, 4249
546.	56803-04-4	Synthase, flavanone	429b, 3844a, 4249
547.	9013-48-3	Synthase, malate	429b, 3844a, 4249, 4978
548.	108281-08-9	Synthase, mannopine	429b, 3844a, 4249
549.	131754-88-6	Synthase, nicotine	429b, 1241a, 3844a, 4249
550.	9036-37-7	Synthase, porphobilinogen	429b, 3844a, 4249, 4473
551.	9023-35-2	Synthase, pseudouridylate	429b, 3844a, 4249, 4773
552.	9077-14-9	Synthase, squalene	429b, 1102, 3844a, 4249, 5581
553.	9014-52-2	Synthase, tryptophan	429b, 3844a, 4249, 4537
554.	9031-56-5	Synthetase	429b, 922d, 3844b, 4249, 4827
555.	37205-63-3	Synthetase, adenosine triphosphate	429b, 922d, 3844b, 4249
556.	9028-02-8	Synthetase, aminoacyl-transfer ribonucleate	922d, 3844b, 4249, 4555
557.	9037-14-3	Synthetase, aminolevulinate {synthase, aminolevulinate}	429b, 3844a, 4249, 4643
558.	37205-35-9	Synthetase, arginyl-transfer ribonucleate	429b, 922d, 3844b, 4249, 4842
559.	37332-51-7	Synthetase, *p*-coumaroyl coenzyme A	429b, 922d, 3844b, 4249
560.	37211-77-1	Synthetase, 5-dehydroquinate	4249, 4483
561.	9023-70-5	Synthetase, glutamine	429b, 922d, 2010, 3844b, 4249, 4691
562.	147626-93-5	Synthetase, glutamine (tobacco clone pcGS2-17 isoenzyme 2 subunit precursor reduced)	429b, 225b, 922d, 3844b, 4249
563.	9068-76-2	Synthetase, glutamyl-transfer ribonucleate	429b, 922d, 3844b, 4249
564.	39341-90-7	Synthetase, indoleacetate	429b, 922d, 3844b, 4249, 4540
565.	9031-15-6	Synthetase, leucyl-transfer ribonucleate	429b, 922d, 3844b, 4249, 4630
566.	37318-64-2	Synthetase, methenyl tetrahydrofolate	4249, 4661
567.	9014-36-2	Synthetase, succinyl coenzyme A (guanosine diphosphate forming)	429b, 922d, 3844b, 4249, 4729
568.	9023-47-6	Synthetase, valyl-transfer ribonucleate	429b, 922d, 3844b, 4249, 4556
569.	149956-84-3	Thioredoxin h2 (tobacco)	1280a, 4249
570.		Transaminase	4249, 4426
571.	50812-37-8	Transferase, glutathione *S*-	429b, 922d, 4249
572.	9014-48-6	Transketolase	429b, 4249, 4551
573.	9029-76-9 9029-75-8 9033-23-2 9012-40-2	Transmethylase	4249, 4456

(*continued*)

TABLE 22.2 (continued)
Enzymes, Genes, Clones, Bacteria in Tobacco

	CAS No.	Name (per CA Collective Index)	Tobacco References
574.	9035-81-8	Trypsin inhibitor	429b, 2811b, 4249
575.	150498-11-6	Trypsin inhibitor, TTI (tobacco isoform 1 reduced)	429b, 2811b, 4249
576.	120904-94-1	Ubiquitin, poly-	4249
577.	9002-13-5	Urease	429b, 4249, 4802a, 5079, 5123
578.	9026-22-6	Uridylyltransferase, glucose 1-phosphate	429b, 922d, 4249, 4489
579	9025-57-4	Xylanase, endo-1,4-β-	429b, 4249
580.	9025-53-0	β-Xylosidase	1837b

23 Hoffmann Analytes

In essence, the terminology "Hoffmann analyte" or "Hoffmann-type analyte" or "Hoffmann list compound" had its beginning over two decades ago in 1985. Early that year, a working group of the International Agency for Research on Cancer (IARC) met to evaluate the carcinogenic risk of chemicals to humans with particular emphasis on tobacco smoking. The next year, the working group's assessment of tobacco smoking was published in an IARC monograph (1870). Among the 28 members of the working group were Ernst L. Wynder and Dietrich Hoffmann from the American Health Foundation whose participation in the discussions on the components of tobacco and particularly tobacco smoke was obviously quite extensive. The number of references cited in the various smoke component figures, tables, and appendixes in the IARC monograph (1870) reveals the extent of the Wynder–Hoffmann contribution to the working group study (see summary in Table 23.1). Nearly 44% of the citations on smoke components considered deleterious represented a Hoffmann-related publication. In all of the 44 references listed in Table 23.1, Hoffmann was a coauthor.

A few months after the *IARC 1985 Working Group Meeting*, Hoffmann and Wynder presented a paper on biologically active tobacco smoke components at a conference, and its contents were published in 1986 (1808). Deriving their assessment of various tobacco smoke components from the conclusions of the IARC 1985 working group, Hoffmann and Wynder listed 40 biologically active components in cigarette mainstream smoke (MSS) and sidestream smoke (SSS). Over the next decade and half, a series of articles were published with Hoffmann as a coauthor of each, and in each article was a listing of tobacco and/or smoke components that were classified as biologically active (1808, 1741), carcinogenic (1808, 1740, 1743, 1744), cocarcinogenic (1808), or tumorigenic (1717, 1773).

Table 23.2 summarizes the chronology of the list-containing articles and the varied classifications of the activity of the components listed. In those publications in which the classification "biologically active" was used, no mention was made of the fact that many biologically active components in tobacco smoke, e.g., α-tocopherol and α- and β-4,8,13-duvane-1,3-diol, have been demonstrated to exert anticarcinogenic or inhibitory effects on the activity of several tobacco smoke components considered potent tumorigens or mutagens [see Table 3 in (3255a), Table 6 in (3265), Table 11 in (3300)]. In contrast to the multiple listings of benz[*a*]anthracene (B[*a*]A) as a biologically active MSS component (1741, 1808) or as a tumorigen (1727, 1773) or as a carcinogen (1740, 1743, 1744), Hoffmann and Wynder (1786) reported in 1959 that, in their mouse-skin-painting study, B[*a*]A coadministered with benzo[a]pyrene (B[*a*]P) reduced the tumorigenicity of the B[*a*]P, i.e., B[*a*]A was anticarcinogenic to B[*a*]P.

Eventually, the number of biologically active smoke components, primarily the tumorigens, was expanded from the 43 listed in 1990 by Hoffmann and Hecht (1727) to 82 listed in 1998 by Hoffmann and Hoffmann (1740). Much of the increase was due to the inclusion of the *N*-heterocyclic amines and several vapor-phase components. Because of the change in its assessment concerning their tumorigenicity, chrysene and di(2-ethylhexyl) phthalate were no longer considered as tumorigens by the IARC. Several other similar lists, not coauthored by Hoffmann, were issued after 1986. They included the 1994 list by the U.S. Occupational Health and Safety Administration (OSHA) (2825) and the 2001 list by Fowles and Bates (1217). Neither of these lists differed significantly from those issued by Hoffmann and his colleagues between 1986 and 2001.

Table 23.3 is a tabulation of the toxicants in tobacco and tobacco smoke from the IARC 1986 publication (1870) plus the seven lengthy publications coauthored from 1986 to 2001 by Hoffmann with his American Health Foundation colleagues. Examination of the various lists reveals several anomalies, none of which detracts from the meaningfulness of the publications. The anomalies include

1. Several instances where the per cigarette yield range unit was listed as μg in one article and ng in another, e.g., the per cigarette yield range for quinoline listed as 1–2 ng in (1743) and 1–2 μg in (1744).
2. Several instances where the per cigarette yield range differs significantly in two different publications, e.g., the per cigarette yield range for *N*-nitrosopyrrolidine is listed as 1.5–110 ng in (1727) and 3–60 ng in (1740).
3. Several instances where the per cigarette yield range differs in different tables in the same article, e.g., the per cigarette yield range for catechol is listed as 25–360 μg in Table 5 in (1808), as 100–350 μg in Table 11 in (1808), and 140–500 μg in Table 13 in (1808).
4. The per cigarette yield range is listed for the wrong component, e.g., the range 1.7–3.2 ng is listed for dibenzo[*a,l*]pyrene in (1741, 1743, 1744), but in each case, that range should be listed for the omitted dibenzo[*a,i*]pyrene, cf. (1727, 1740, 1773).
5. In some instances, particularly with several PAHs, the per cigarette yield ranges include data generated from cigarettes manufactured in the 1950s and 1960s with "tar" and nicotine yields far in excess of more recently manufactured cigarettes.

TABLE 23.1
Hoffmann Contributions on Smoke Components to the 1985 IARC Working Group on Tobacco Smoking

Item	Topic	No. of Specific References Cited	No. of Hoffmann et al. References Cited	Hoffmann et al. References
Figure 5	Some chemical constituents of tobacco smoke	1	1	3491
Table 20	Concentrations of some PAHs and heterocyclic compounds in tobacco smoke	33	13	1560, 1699, 1763, 1765, 1766, 1779, 1780, 1800, 1803, 3088, 4308, 4312, 4317
Table 21	Concentrations of some phenols in tobacco smoke	11	3	497, 1703, 4332
Table 22	Concentrations of free fatty acids in cigarette smoke	1	1	1785
Table 23	Concentrations of aromatic amines in cigarette smoke	1	1	2900
Table 24	Concentrations of major pyridines and pyrazines in mainstream cigarette smoke	2	1	512
Table 25	Concentrations of *N*-nitrosamines in cigarette smoke	1	1	1696
Table 26	Concentrations of *N*-nitrosamines in SSS of commercial cigarettes and cigars	2	2	1685, 1696
Table 30	Physiochemical comparison of MSS and SSS of cigarettes	2	2	1695, 1696
Table 31	Concentrations of selected compounds in nonfilter cigarette MSS and the ratio of their relative distribution in SSS	6	1	1720
Appendix 2	Chemical compounds identified in tobacco smoke that have been evaluated for carcinogenicity in the IARC monograph series	6[a]	3	4332, 4348, 4348a

[a] Three of the cited references were to IARC monographs.

TABLE 23.2
Hoffmann-Related Lists of Toxicants in Tobacco and Tobacco Smoke

Year	Authors	Ref. No.	Table No.	Table Title	No. of Component Listed
1986	International Agency for Research on Cancer (IARC)	1870	19	Concentrations of biologically-active agents in nonfilter cigarette mainstream smoke	60
1986	Hoffmann and Wynder	1808	5	Carcinogens and cocarcinogens in the smoke of a nonfilter cigarette	21
		1808	6	Organ-specific carcinogens in cigarette smoke	14
		1808	13	Biologically-active agents in mainstream smoke (of nonfilter cigarettes)	40
1990	Hoffmann and Hecht	1727	3	Tumorigenic agents in tobacco and tobacco smoke	43
1993	Hoffmann et al.	1773	1	Tumorigenic agents in tobacco and tobacco smoke	41
1997	Hoffmann and Hoffmann	1740	3	Carcinogens in tobacco and cigarette smoke	60
1998	Hoffmann and Hoffmann	1741	1	Biologically-active agents in the mainstream smoke of nonfilter cigarettes	82
2001	Hoffmann and Hoffmann	1743	5-4	Carcinogens in cigarette smoke	68
2001	Hoffmann et al.	1744	4	Carcinogens in cigarette smoke	68

6. The per cigarette yield range is incomplete, e.g., a single value of 4 ng/cig is listed for dibenz[*a,h*]anthracene (DB[*a,h*]A) in (1727, 1773, 1740, 1741, 1743, 1744, 1870), but an incorrect single value of 40 ng is listed in (1808); all DB[*a,h*]A listings in the references cited fail to take into account the reporting of a DB[*a,h*]A yield of 5 ng/cig by Van Duuren in 1958 (4020). The MSS yield of 4 ng/cig of DB[*a,h*]A was obtained by Hoffmann and Wynder in the late 1950s (1787, 1788) from a 1959 cigarette and reported as such in 1963 by Wynder and Hoffmann [see Table 1 in (4317)].
7. A component with no known per cigarette yield is treated the same as a component with literally hundreds of per cigarette yield values, e.g., dibenzo[*a,l*]pyrene *vs.* B[*a*]P.
8. For the identification of dibenzo[*a,l*]pyrene in MSS, IARC [see Footnote 33 in Table 20 in (1870)] cited the footnote in the 1958 publication by Van Duuren (4020). However, like many other investigators

TABLE 23.3
The Basis for the "Hoffmann Analytes": The Lists of Toxicants Issued by Hoffmann et al. from 1986 to 2001

Component	1986 IARC (1870)[a]	1986 Hoffmann and Wynder (1808)	1990 Hoffmann and Hecht (1727)	1993 Hoffmann et al. (1773)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)	2001 Hoffmann and Hoffmann (1743)	2001 Hoffmann et al. (1744)
Polycyclic aromatic hydrocarbons								
Benz[*a*]anthracene	20–70 ng 40–70 ng[b] 4–76 ng[c]	40–70 ng[d] 40–60 ng[e]	20–70 ng	20–70 ng	20–70 ng	20–70 ng	20–70 ng	20–70 ng
Benzo[*b*]fluoranthene	4–22 ng 30 ng[b]	30 ng[d]	4–22 ng	4–22 ng	4–22 ng	4–22 ng	4–22 ng	4–22 ng
Benzo[*j*]fluoranthene	6–21 ng 60 ng[b]	60 ng[d]	6–21 ng	6–21 ng	6–21 ng	6–21 ng	6–21 ng	6–21 ng
Benzo[*k*]fluoranthene	6–12 ng	NL[f]	6–12 ng	612 ng	6–12 ng	6–12 ng	6–12 ng	6–12 ng
Benzo[*a*]pyrene	20–40 ng 10–50 ng[b] 5–78 ng[c]	10–50 ng[d] 10–40 ng[g]	20–40 ng	20–40 ng	20–40 ng	20–40 ng	20–40 ng	20–40 ng
Chrysene	40–60 ng[b]	40–60 ng[d]	40–60 ng	40–60 ng	NL	NL	NL	NL
Chrysene, 5-methyl-	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng
Dibenz[*a,h*]anthracene	4 ng	40 ng	4 ng	4 ng	4 ng	4 ng	4 ng	4 ng
Dibenzo[*a,e*]pyrene	P[h], NYL[f]	NL[f]	NL	NL	NL	P, NYL[i]	P, NYL[i]	P, NYL[i]
Dibenzo[*a,h*]pyrene	P[h], NYL[f]	NL[f]	NL	NL	NL	NL	NL	NL
Dibenzo[*a,i*]pyrene	1.7–3.2 ng 2–3 ng[b] 17–32 ng[c]	NL	1.7–3.2 ng	1.7–3.2 ng	1.7–3.2 ng	NL[i]	NL[i]	NL[i]
Dibenzo[*a,l*]pyrene[d]	P, NYL	P, NYL	P, NYL	P, NYL	P, NYL	1.7–3.2 ng[i]	1.7–3.2 ng[i]	1.7–3.2 ng[i]
Indeno[1,2,3-*cd*]pyrene	4–20 ng	4 ng	4–20 ng	4–20 ng	4–20 ng	4–20 ng	4–20 ng	4–20 ng
Aza-arenes								
Pyridine	16–40 µg	NL	NL	NL	20–200 µg[j]	10–40 µg	20–200 µg[k] 16–40 µg[l]	20–200 µg[m]
Quinoline	NL[f]	NL	1–2 µg	0.2–1.3 µg	1–2 µg	2–180 ng[n]	1–2 ng[n]	1–2 µg[n]
Dibenz[*a,h*]acridine[o]	0.1 ng	0.1 ng[d]	0.1 ng	0.1 ng	0.1 ng	0.1 ng	0.1 ng	0.1 ng
Dibenz[*a,j*]acridine	2.7 ng 3–10 ng[b]	3–10 ng[d]	3–10 ng	3–10 ng	3–10 ng	3–10 ng	3–10 ng	3–10 ng
7*H*-Dibenzo[*c,g*]carbazole	0.7 ng	0.7 ng[d]	0.7 ng	0.7 ng	0.7 ng	0.9 ng	0.7 ng	0.7 ng
N-*Nitrosamines*								
N-Nitrosodimethylamine	2–20 ng 1–200 ng[b]	1–180 ng[o] 2–180 ng[e]	0.1–180 ng	0.1–180 ng	0.1–180 ng	2–180 ng	2–180 ng	2–1000 ng
N-Nitrosoethylmethylamine	0–2.7 ng 0.1–10 ng[b]	1–40 ng[o] 0,1–40 ng[e]	3–13 ng	3–13 ng	3–13 ng	3–13 ng	3–13 ng	3–13 ng

(*continued*)

TABLE 23.3 (continued)
The Basis for the "Hoffmann Analytes": The Lists of Toxicants Issued by Hoffmann et al. from 1986 to 2001

Component	1986 IARC (1870)[a]	1986 Hoffmann and Wynder (1808)	1990 Hoffmann and Hecht (1727)	1993 Hoffmann et al. (1773)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)	2001 Hoffmann and Hoffmann (1743)	2001 Hoffmann et al. (1744)
N-Nitrosodiethylamine	0–2.8 ng 0–10 ng[b]	0.1–28 ng	0–25 ng	0–25 ng	0–2.8 ng	0–2.8 ng	0–2.8 ng	0–2.8 ng
N-Nitrosodi-*n*-propylamine	0–1 ng	0–1 ng	NL	NL	NL	0–1.0 ng	0–1.0 ng	0–1.0 ng
N-Nitrosodi-*n*-butylamine	0–3 ng	0–3 ng	NL	NL	NL	0–30 ng	0–30 ng	0–30 ng
N-Nitrosopyrrolidine	0–110 ng 2–42 ng[b]	2–110 ng[o] 2–42 ng[e]	1.5–110 ng	NL	3–60 ng	3–110 ng	3–110 ng	3–110 ng
N-Nitrosopiperidine	0–9 ng	0–9 ng	NL	NL	NL	0–9 ng	0–9 ng	0–9 ng
N-Nitrosodiethanolamine	0–36 ng 0–90 ng[b]	0–40 ng	0–36 ng	NL	0–68 ng	0–68 ng	0–68 ng	0–68 ng
N-Nitrososarcosine	NL	NL	NL	NL	NYL	ND[f]	NL	NL
N′-Nitrosonornicotine	0.2–3.0 μg 0.13–0.25 μg[b]	0.12–3.7 μg	0.12–3.7 μg	0.12–3.7 μg	0.12–3.7 μg	120–3.700 ng[p]	0.12–3.7 μg[p]	0.12–3.7 μg[p]
4-(*N*-Methylnitrosamino)-1-(3-pyridyl)-1-Butanone	0.08–0.77 μg 0.08–0.7 μg[b]	0.12–0.95 μg	0.08–0.77 μg	0.08–0.77 μg	0.08–0.77 μg	0.08–0.77 μg	0.08–0.77 μg	0.08–0.77 μg
N′-Nitrosoanabasine	0–150 ng 0–200 ng[b]	40–400 ng[o] 120 ng[e]	0.14–4.6 μg	0.14–4.6 μg	0.14–4.6 μg	0–150 ng	NL	NL
N′-Nitrosoanatabine	NL 0–3.7 μg[b]	NL	NL	NL	NL	NL	NL	NL
N-Nitrosomorpholine	NL	NL	ND[q] in MSS	ND in MSS	ND in MSS	ND in MSS	NL	NL
Aromatic amines								
Aniline	NL	360 ng	360 ng	NL	NL	360–655 ng	360–655 ng[l]	NL
2-Toluidine	32–160 ng 30–200 ng[b]	30–160 ng	30–200 ng	30–200 ng	30–200 ng	30–337 ng	30–337 ng	30–337 ng
Aniline, 2,6-dimethyl-	NL	NL	NL	NL	NL	NL	4–50 μg[n]	4–50 ng[n]
1-Naphthylamine	NL 3–4 ng[b]	NL	NL	NL	NL	NL	NL	NL
2-Naphthylamine	1.7–22 ng 1–22 ng[b]	4.3–27 ng	1–22 ng	1–22 ng	1–22 ng	1–334 ng	1–334 ng	1–334 ng
Biphenyl, 3-amino	NL	NL	NL	NL	NL	NL	NL	NL
Biphenyl, 4-amino-	2.4–4.6 ng 2–5 ng[b]	2.4–4.6 ng	2–5 ng	2–5 ng	2–5 ng	2–5.6 ng	2–5.6 ng	2–5.6 ng
N-Heterocyclic amines[q]								
A*a*C	NL	NL	NL	NL	25–260 ng	25–260 ng	25–260 ng	25–260 ng
MeA*a*C	NL	NL	NL	NL	2–37 ng	2–37 ng	NL	2–37 ng
Glu-P-1	NL	NL	NL	NL	0.37–0.89 ng	6.37[n]–0.89 ng	0.37[n]–0.89 ng	0.37[n]–0.89 ng
Glu-P-2	NL	NL	NL	NL	0.25–0.88 ng	0.25–0.88 ng	0.25–0.88 ng	0.25–0.88 ng

PhIP	NL	NL	NL	NL	11–23 ng	11–23 ng	11–23 ng	11–23 ng
IQ	NL	NL	NL	NL	0.26 ng	0.3 ng	0.3 ng	0.3 ng
MeIQ	NL	NL	NL	NL	NL	NL	NL	NL
Trp-P-1	NL	NL	NL	NL	0.29–0.48 ng	0.3–0.5 ng	0.3–0.5 ng	0.3–0.5 ng
Trp-P-2	NL	NL	NL	NL	0.82–1.1 ng	0.8–1.1 ng	0.8–1.1 ng	0.8–1.1 ng
Aldehydes and ketones								
Formaldehyde	70–100 µg 20–88 µg[b]	5–100 µg	70–100 µg	70–100 µg	70–100 µg[r] 20–100 µg[j]	70–100 µg	70–100 µg 20–100 µg[k]	70–100 µg[r] 20–100 µg[m]
Acetaldehyde	500–1200 µg 18–1400 µg[b]	500–1200 µg	18–1400 µg	18–1400 µg	18–1400 µg[r] 400–1400 µg[j]	500-1.400 µg[s]	500–1400 µg[s] 400–1400 µg[k]	500–1400 µg[s] 400–1400 µg[m]
Propionaldehyde	NL	NL	NL	NL	NL	NL	NL	NL
Butyraldehyde	NL	NL	NL	NL	NL	NL	NL	NL
Crotonaldehyde	10–20 µg	NL	10–20 µg	10–20 µg	NL	10–20 µg	NL	NL
Acrolein	60–100 µg 25–140 µg[b]	50–100 µg	NL	NL	60–140 µg[j]	60–140 µg	60–140 µg[k]	60–240 µg[m]
Acetone	100–250 µg	100–250 µg	NL	NL	100–650 µg[j]	NL	100–650 µg[k]	NL
2-Butanone	NL	NL	NL	NL	NL	NL	NL	NL
Volatile hydrocarbons								
1,3-Butadiene	NL	NL	NL	NL	20–75 µg[r] 25–40 µg[j]	20–75 µg	20–75 µg 25–40 µg[k]	20–75 µg 25–40 µg[m]
Isoprene	NL	NL	NL	NL	450–1000 µg[r] 200–400 µg[j]	450–1.00 µg[s]	450–1000 µg[s] 200–400 µg[k]	450–1000 µg[s] 200–400 µg[m]
Benzene	20–50 µg	20–50 µg	12–48 µg	12–48 µg	12–70 µg[r] 6–70 µg[j]	20–70 µg	20–70 µg 12–50 µg[k]	20–70 µg 6–70 µg[m]
Toluene	NL	NL	NL	NL	5–90 µg[j]	NL	20–60 µg[k]	5–90 µg[m]
Styrene	10 µg	NL	NL	NL	10 µg	10 µg	10 µg	10 µg
Miscellaneous organic compounds								
Acetamide	38–56 µg[b]	NL	NL	NL	NL	38–56 µg	38–56 µg	38–56 µg
Acrylonitrile	3.2–15 µg[b]	3.2–15 µg	3.2–15 µg	3.2–15 µg	3.2–15 µg	3–15 µg	3–15 µg	3–15 µg
Acrylamide	NL	NL	NL	NL	P, NYL	P, NYL	P, NYL	P, NYL
Hydrazine, 1,1-Dimethyl-	P, NYL	NL	P, NYL	P, NYL	NYL	P, NYL	P, NYL	P, NYL
Maleic hydrazide	NL	NL	NL	NL	NL	1.16 µg	1.16 µg[l]	
Methanol	NL	NL	NL	NL	80–180 µg[j]	100–250 µg	80–180 µg[k] 100–250 µg[l]	80–180 µg[m]
Methyl isocyanate	NL	NL	NL	NL	NL	1.5–5 µg	NL	NL
Nitromethane	NL	NL	NL	NL	NL	NL	0.3–0.6 µg	0.5–0.6 µg
2-Nitropropane	0.2–2.2 µg 0.73–1.21 µg[b]	0.2–2.2 µg	0.73–1.21 µg	0.73–1.21 µg	0.73–1.21 µg	0.2–2.2 µg	0.7–1.2 µg	0.7–1.2 µg
Nitrobenzene	NL	NL	NL	NL	NL	25 µg	25 µg	25 µg

(*continued*)

TABLE 23.3 (continued)
The Basis for the "Hoffmann Analytes": The Lists of Toxicants Issued by Hoffmann et al. from 1986 to 2001

Component	1986 IARC (1870)[a]	1986 Hoffmann and Wynder (1808)	1990 Hoffmann and Hecht (1727)	1993 Hoffmann et al. (1773)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)	2001 Hoffmann and Hoffmann (1743)	2001 Hoffmann et al. (1744)
Vinyl chloride	1.3–16 ng 1–16 ng[b]	1.3–16 ng	1–16 ng	1–16 ng	1–16 ng	11–15 ng	11–15 ng	11–15 ng
Ethyl carbamate	20–38 ng	20–38 ng	20–38 ng	20–38 ng	20–38 ng	20–38 ng	20–38 µg	20–38 µg
Ethylene oxide	NL	NL	NL	NL	7 µg	7 µg	7 µg	7 µg
Propylene oxide	NL	NL	NL	NL	NL	NL	12–100 ng	0–100 ng
Di(2-ethylhexyl) phthalate	NL	NL	NL	NL	20 µg	20 µg	NL	NL
Furan	NL	NL	NL	NL	18–30 µg[r] 20–40 µg[j]	18–30 ng[s]	18–37 ng[s]	18–37 µg[s]
Benzo[*b*]furan	NL	NL	NL	NL	P, NYL	P, NYL	P, NYL	P, NYL
Phenols								
Phenol	60–140 µg	60–140 µg	80–60	NL	NL	80–160 µg	80–160 µg[l]	60–180 µg[t]
o-Cresol	14–30 µg	NL	NL	NL	NL	NL	NL	NL
m-Cresol	NL	NL	NL	NL	NL	NL	NL	NL
p-Cresol	NL	NL	NL	NL	NL	NL	NL	NL
Catechol	40–350 µg	25–360 µg[d] 100–350 µg[g] 140–500 µg[e]	200–400 µg	NL	NL	200–400 µg	100–360 µg 200–400 µg[l]	90–2000 µg 100–200 µg[t]
Resorcinol	8–80 µg[b]	NL	NL	NL	NL	NL	NL	NL
Hydroquinone	88–155 µg[b]	110–300 µg	NL	NL	NL	NL	NL	NL
Methyleugenol	NL	NL	NL	NL	NL	20 ng	20 ng	20 ng
Caffeic acid	NL	NL	NL	NL	NL	NL	<3 µg	<3 µg
Chloroaromatic compounds								
DDT	NL 0.7–1.2 µg[b]	NL	NL	NL	800–1200 ng	800–1.200 ng[s]	800–1200 µg	800–1200 µg
DDE	NL	NL	NL	NL	200–370 ng	200–370 ng	200–370 µg	200–370 µg
Polychlorodibenzo-*p*-dioxins	NL	NL	NL	NL	NL	NL	NL	NL
Polychlorodibenzofurans	NL	NL	NL	NL	NL	NL	NL	NL
Inorganic components								
Hydrazine	24–43 ng	24–43 ng	24–43 ng	24–43 ng	24–43 ng	24–34 µg[n]	24–43 ng[n]	24–43 ng[n]
Hydrogen sulfide	NL	NL	NL	NL	20–90 µg[j]	10–90 µg	20–90 µg[k]	20–90 µg[m]
Arsenic	1–25 µg	NL	40–120 ng	40–120 ng	40–120 ng	40–120 ng	40–120 µg	40–120 µg
Beryllium	NL	NL	NL	NL	NL	0.3 µg	0.5 ng	0.5 ng
Cadmium	9–70 ng	NL	41–62 ng	41–62 ng	41–62 ng	NL	7–350 ng	7–350 ng

Chromium vi	4–70 ng	NL	4–70 ng	4–70 ng	4–70 ng	4–70 ng	4–70 ng	4–70 ng
Cobalt	0.2 ng	NL	NL	NL	NL	0.13–0.2 ng	0.13–0.2 ng	0.13–0.2 ng
Nickel	0–600 ng[b]	20–3000 ng	0–600 ng	0–600 ng	0–600 ng	0–600 ng	0–600 ng	0–600 ng
Mercury	NL	NL	NL	NL	NL	4 ng	NL	
Lead	P[c]	NL	35–85 ng	35–85 ng	35–85 ng	34–85 ng	34–85 ng	34–85 ng
Polonium-210	0.03 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi
Selenium	P[c]	NL	NL	NL	NL	NL	NL	NL
Additional components								
Nicotine	1.0–2.3 mg	1–2.5 mg	1.0–3.0 mg	NL	0.1–3.0 mg[u]	1.0–3.0 mg	1.0–3.0 mg[v]	0.1–3.0 mg[t]
Carbon monoxide	10–23 mg	10–23 mg	NL	NL	14–23 mg[j]	10–23 mg	14–23 mg[k]	14–23 mg[m]
Ammonia	50–130 µg	50–170 µg[g] 50–130 µg[e]	NL	NL	10–130 µg[j]	10–130 µg	10–130 µg[k]	10–130 µg[m]
Nitrogen oxides	100–600 µg	50–600 µg	NL	NL	100–600 µg[j]	100–600 µg	100–600 µg[k]	100–600 µg[m]
Hydrogen cyanide	400–500 µg	400–500 µg	NL	NL	400–500 µg[j]	400–500 µg	400–500 µg[k]	400–500 µg[m]

[a] See Table 19 in (1870).
[b] See Appendix 2 in (1870).
[c] See Table 20 in (1870).
[d] See Table 5 in (1808).
[e] See Table 13 in (1808).
[f] NL, not listed; NYL, no per cigarette MSS yield listed; ND, not detected
[g] See Table 11 in (1808).
[h] P, present, as listed in Appendix 2 in (1870).
[i] The yield range listed for dibenz[*a,l*]pyrene is incorrect. It is the range usually listed for dibenzo[*a,i*]pyrene. The P, NYL designation should also apply to dibenzo[*a,l*]pyrene.
[j] See Table 1 in (1740).
[k] See Table 5-1 in (1743).
[l] See Table 5-3 in (1743).
[m] See Table 2 in (1744).
[n] Compare yields listed in Tables in (1741, 1743, 1744).
[o] See Table 6 in (1808).
[p] Compare yield listed in Table 1 in (1741) with those listed in (1727, 1740, 1743, 1744).
[q] A*a*C, 2-amino-9*H*-pyrido[2,3-*b*]indole; MeA*a*C, 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole; Glu-P-1, 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole; Glu-P-2, 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole; PhIP, 2-amino-1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridine; IQ, 2-amino-3-methyl-3*H*-imidazo[4,5-*f*]quinoline; MeIQ, 2-amino-3,4-dimethyl-3*H*-imidazo[4,5-*f*]quinoline; Trp-P-1, 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole; Trp-P-2, 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole.
[r] See Table 3 in (1740).
[s] Compare yield listed in Table 1 in (1741), Table 5-4 in (1743), and Table 4 in (1744).
[t] See Table 3 in (1744).
[u] See Table 2 in (1740).
[v] See Table 5-2 in (1743).

[Lyons and Johnston (2430), Rodgman and Cook (3273), Wynder and Wright (4354), Wynder et al. (4355)], Van Duuren had reported the identification of dibenzo[*a*,*l*]pyrene in MSS. However, in 1966, Lavit-Lamy and Buu-Hoï (2314) reported that the compound previously thought to be dibenzo[*a,l*] pyrene was actually its isomer dibenz[*a,e*]aceanthrylene (dibenz[*a,e*]fluoranthene) [see also Lacassagne et al. (2250)]. In 1983, IARC had commented that all pre-1966 studies involved with dibenzo[*a,l*]pyrene were actually dealing with dibenz[*a,e*]fluoranthene not dibenzo[*a,l*]pyrene (1868a). Dibenzo[*a,l*]pyrene was eventually identified in MSS by Snook et al. (3756), but no quantitative data were given.

9. The repetitious inclusion in the lists published by Hoffmann and his colleagues (1727, 1773, 1740, 1741, 1743, 1744, 1808) of the aza-arenes dibenz[*a,h*] acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*] carbazole reported by Van Duuren et al. despite the failure of numerous investigators in several countries between 1970 and 2000 to confirm their presence in MSS [(3260), also see Table 12-7 in Baker (172) and Table 4 in Rodgman (3265)].

These and other anomalies were described in detail by Rodgman (3265).

A more recent publication by Hoffmann and Hoffmann on the "changing cigarette" presents an interesting situation. In a chapter in a book published in 2010, Hoffmann and Hoffmann once again present their list of carcinogens in cigarette smoke [see Table 6.4 in (5512)]. Examination of the data presented for the amount of each listed carcinogen in the MSS of a non-filter cigarette reveals that the presented data are identical with the data presented for each carcinogen in the 2001 article by Hoffmann, Hoffmann, and El-Bayoumy (1744). Does the similarity between the two identical listings of cigarette smoke data indicate that, despite the title of their 2010 article "The changing cigarette" (5512), the authors consider that the MSS delivery of the cigarette has not changed between 2001 and 2010, particularly in regard to the listed carcinogens?

Although one or more of the earlier problems and/or anomalies were described in publications by Rodgman in 1998 and 2003 (3260, 3265), Baker in 1999 (1972), Rodgman and Green in 2002 and 2003 (3300), and Rodgman and Perfetti in 2008 (5078) in response to the numerous lists on tobacco and/or tobacco smoke toxicants (1217, 1727, 1773, 1740, 1741, 1743, 1744, 1808, 1870, 2825), no toxicant list author or agency—whether Wynder, Dietrich Hoffmann, Ilse Hoffmann, Hecht, El-Bayoumy, Fowles, Bates, IARC or OSHA—has ever published a single contradiction to any item in the previous list of problems and anomalies.

The many publications coauthored by Hoffmann (1727, 1773, 1740, 1741, 1743, 1744, 1808), each of which contained a list of biologically active components identified in tobacco smoke, led to two interesting episodes as a result of his efforts. Because of those numerous coauthored publications and the listing of toxicants in tobacco and tobacco smoke, Dr. Dietrich Hoffmann was dubbed "The Author of the List" in 2002 (23A05). This recognition was subsequently extrapolated in numerous scientific conference presentations and journal publications in which Dr. Hoffmann's list contributions were acknowledged by the authors in the title of many scientific conference presentations and journal publications by inclusion of the term "Hoffmann analytes" or "Hoffmann-type analytes" or "Hoffmann list compounds." In some published articles, the term "Hoffmann analytes" does not appear in the title but does appear in the headings of tables in the articles, e.g., in several publications by Baker and his colleagues at British American Tobacco (BAT), the term "Hoffmann analytes" appears in the title of several tables (174a, 174c). Table 23.4 catalogs some of the presentations and/or publications in which the term "Hoffmann analyte" or its equivalent was used in tobacco-related scientific literature from the year 2000 to 2006.

Table 23.5 catalogs the components in the various Hoffmann coauthored lists. In an attempt at simplification, the sequence of components in Table 23.5 approximates the sequence in many of the Hoffmann coauthored list articles. Also in Table 23.5, the various components listed by Hoffmann and his colleagues in their various articles (1727, 1740, 1741, 1743, 1744, 1773, 1808) are listed in the most recently accepted nomenclature, e.g., benzo[*b*]fluoranthene is listed as benz[*e*]acephenanthrylene, dibenzo[*a,l*]pyrene is listed as dibenzo[*def,p*] chrysene, catechol is listed as 1,2-benzenediol. In each case, the nomenclature used in the Hoffmann coauthored articles accompanies the most recent nomenclature listing.

Also included in Table 23.5 are several components which do not appear in any of the Hoffmann coauthored lists but recently have been included with analyses of Hoffmann-listed components, e.g., 1-naphthalenamine (1-aminonaphthalene; α-naphthylamine), 3-aminobiphenyl ([1,1′-biphenyl]-3-amine), propionaldehyde (propanal), butyraldehyde (butanal), and acetone (2-propanone). Table 23.5 includes several tobacco smoke components which the IARC has reclassified with regard to their tumorigenicity, e.g., chrysene and di(2-ethylhexyl) phthalate. Thus, chrysene no longer appears on the more recent Hoffmann lists (1740, 1741, 1743, 1744) and di(2-ethylhexyl) phthalate was omitted from other lists (1743, 1744).

One point of interest in the Table 23.5 catalog is the tremendous number of references which deal with some aspect of the various Hoffmann-listed components.

Over the years, numerous reports have been issued in which analytical data were presented on the per cigarette yields of numerous components in the MSS of the 1R4F Kentucky Reference Cigarette. Many of the analytes were defined as "Hoffmann analytes." Table 23.6 summarizes several such analyses on the 1R4F MSS reported by Baker et al. [see Table 11 in (174b)], Rustemeir et al. (3370), and R.J. Reynolds Tobacco (RJRT) (3190)]. Also included in Table 23.6 are the "Hoffmann analyte" yields reported by Chen and Moldoveanu (688) for the MSS of the 2R4F Kentucky Reference Cigarette. Similar examples of "Hoffmann analyte" data are available in Baker et al. [see Table 12 in (174b)] and Rodgman and Green (3300). Table 23.6 lists the MSS analytes proposed by the

TABLE 23.4
Abbreviated Chronology of the Use of the Term "Hoffmann Analyte" or Its Equivalent in Tobacco Smoke-Related Scientific Literature

Year	Author(s) and Title of Article
2000	While it did not use the term "Hoffmann analyte" in its report, the Department of Health (Canada) proposed that analytical data on the following smoke components from tobacco smoke should be a requirement (23A06): " 'tar,' nicotine, formaldehyde, acetaldehyde, propionaldehyde, butyraldehyde, acrolein, crotonaldehyde, acetone, benzo[*a*]pyrene, NNN, NNK, NAB, NAT, 1-aminonaphthalene, 2-aminonaphthalene, 3-aminobiphenyl, 4-aminobiphenyl, pyridine, quinoline, styrene, catechol, resorcinol, hydroquinone, phenol, *o*-cresol, *m*-cresol, *p*-cresol, eugenol, 1,3-butadiene, isoprene, benzene, toluene, acrylonitrile, NH_3, CO, HCN, NO, NO_x, As, Cd Cr, Pb, Hg, Ni, Se." Examination of the Department of Health (Canada) list reveals that most of its listed components appear in the biologically-active component lists in the publications coauthored by Hoffmann (1727, 1773, 1808, 1740, 1741, 1743, 1744)
2001	In a memorandum to the Department of Health (Canada), Levine (23A10) described the results of an interlaboratory comparison on "Hoffmann analytes" in the MSSs from three different cigarette brands
2001	At the *55th Tobacco Science Research Conference* (TSRC), Purkis et al. (3007) in their description of the reliability of measurements of smoke analytes discussed the measurement of 44 "Hoffmann analytes." Their TSRC presentation was published in 2003
2002	At the *56th TSRC*, Baker and Willoughby (later Bishop) (172a) described the compounds generated by the pyrolysis of relatively volatile tobacco ingredients. Subsequently, the presentation was published in 2004 and linked to the "Hoffmann analyte" concept
2002	At the *56th TSRC*, Cashmore (631) presented a paper entitled: Alternative smoking regimes: *Hoffmann analyte* formation and prediction as a consequence of changing smoking regimes and filter vent blocking
2003	At the *57th TSRC*, Chang et al. (23A04) presented a paper entitled: Influence of tip ventilation on *Hoffmann analyte* deliveries
2003	In their study of a new Kentucky Reference Cigarette 2R4F, Chen and Moldoveanu (688) described the quantitation of more than 44 analytes in smoke, including most compounds considered as biologically active and described elsewhere as "Hoffmann analytes." They referred to the biologically-active components listed in 1998 by Hoffmann and Hoffmann (1741)
2003	At the *57th TSRC*, Dimandia et al. (23A07) described the analysis of *Hoffmann list compounds* by comprehensive 2D gas chromatography/ time-of-flight mass spectrometry
2003	Also at the *57th TSRC*, Ellisor et al. (23A08) described the variation in the level of *Hoffmann analytes* for cigarette MSS when a large volume of air passes through the collection device and Volgger et al. (23A14) described the influence of different cigarette paper properties on the formation of *Hoffmann-type analytes* in smoke
2003	Warren presented two papers at the *57th TSRC*; both of which dealt with "Hoffmann analytes." They were entitled: The *Hoffmann analyte* to "tar" ratio paradox (4136) and Prediction of mainstream cigarette smoke *Hoffmann analyte* yields by statistical modeling (4137)
2004	Baker and Bishop (172a) in their report on the pyrolysis of tobacco ingredients noted the following: "Of the approximately 4800 substances in tobacco smoke (1373), 44 are believed … to be relevant to tobacco-related diseases (23A06). These include … some volatile carbonyl compounds, tobacco-specific *N*-nitrosamines, aromatic amines, phenols, volatile alkenes, benzo[*a*]pyrene and metals. These substances are sometimes called colloquially 'Hoffmann analytes' since similar lists of toxicological substances have been proposed by Dietrich Hoffmann et al. of the American Health Foundation in New York since the mid 1980s. The latest compilation by Hoffmann et al. lists 82 substances (1741, 1743, 1744)." From their experimental findings, Baker and Bishop concluded "Particular attention has been paid to assessing the generation of 'Hoffmann analytes,' i.e., biologically-active analytes in smoke, from the pyrolysis f the ingredients. In general, the number of 'Hoffmann analytes' detected among the pyrolytic products of the ingredients, and their levels, are low."
2004	In a series of three papers on the effect of tobacco ingredients on smoke chemistry, Baker et al. (174a, 174b, 174c) did not include the term "Hoffmann analyte" or its equivalent in the three titles. However, the term "Hoffmann analyte" was used throughout each of the publications, e.g., in the abstract of Baker et al. (174a), it is stated: "The studies are: pyrolysis of the ingredients; influence of the ingredients on smoke constituents believed by regulatory authorities to be relevant to smoking-related diseases ("Hoffmann analytes") … " The term "Hoffmann analytes" also appeared in the title of Table 3 in (174a). In the abstract of Baker et al. (174b), the following was stated: "The effects of 450 tobacco ingredients added to tobacco on the 44 'Hoffmann analytes' in mainstream cigarette smoke have been determined … They are based on lists published by D. Hoffmann and coworkers of the American Health Foundation …" In their summary of the effect of casing ingredients on smoke composition, Baker et al. (174c) stated "The effects of 29 casing flavour ingredients and three humectants on the yields of 44 'Hoffmann analytes' in cigarette smoke have been assessed." The term "Hoffmann analytes" also appeared in the title of Table 10 in (174c)
2004	Case and Warren (23A03) were issued a European patent on a multivariate regression system for predicting "Hoffmann analytes" in tobacco smoke. While the term "Hoffmann analyte" did not appear in the title of the patent, in its text, the term was used as follows: "The concentration of yields of a first set of components in a particular tobacco smoke, such as the *Hoffmann analytes*, are predicted on the basis of a statistical model"

(*continued*)

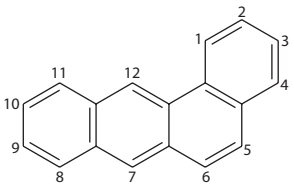
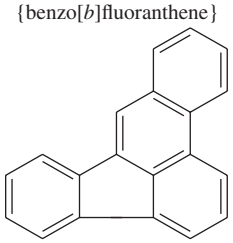
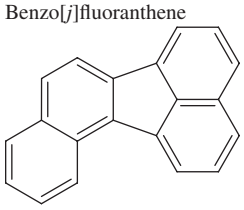
TABLE 23.4 (continued)
Abbreviated Chronology of the Use of the Term "Hoffmann Analyte" or Its Equivalent in Tobacco Smoke-Related Scientific Literature

Year	Author(s) and Title of Article
2004	Imperial Tobacco Co. (23A09) discussed "Hoffmann analytes" as follows: "Additional information may be requested by governmental agencies. This may include measurements of large numbers of smoke constituents of regulatory interest such as the 'Hoffmann analytes' (usually a list of 44 smoke constituents). We have participated in studies requested by Australian and U.K. agencies and have provided information to Health Canada. Our interpretation of these studies, other studies in the literature, and our own internally-produced data is that these smoke constituents are generally proportional to tar measurements for a given blend style"
2004	At the *58th TSRC*, Loureau et al. (2400d) described the influence of cigarette paper and filter ventilation on the yields of "Hoffmann analytes"
2004	At the *CORESTA Congress* in Japan, Röper et al. (23A11) presented a paper entitled: "Hoffmann" analytes and cigarette smoke *in vitro* toxicity revisited—How do the data compare?
2005	Baker and Bishop (172b) did not mention the term "Hoffmann analyte" in the title of their publication on the pyrolysis of nonvolatile tobacco ingredients but did note the following: "The study has concentrated on the biologically active substances produced by pyrolysis, in particular the 'Hoffmann analytes.' These analytes are believed by regulatory authorities in Canada and U.S.A. to be relevant to smoking-related diseases. They are based on lists published by Hoffmann and co-workers of the American Health Foundation in New York. For the pyrolysis of many of the non-volatile ingredients, no 'Hoffmann analytes' were detected amongst the products. When they were occasionally formed, they included phenols, benzene, toluene, styrene and furfural (furfural is biologically active but it does not appear on any of the Hoffmann or regulatory authority lists)"
2005	At the *CORESTA Joint Study Group Meeting* in Stratford-on-Avon, United Kingdom, in 2005, BAT personnel presented the following three papers under the general heading "The effect of cigarette design variables on assays of interest to the Tobacco Industry": Case et al. (23A01) presented the first paper subtitled: (1) Experimental design and some initial findings on Hoffmann analyte yields. Sheppard et al. (23A12) presented the second paper subtitled: (2) Prediction of smoke and *Hoffmann analytes* using two different modeling methods. Winter et al. (23A15) presented the third paper subtitled: (3) Tobacco blend types. Although the latter paper did not include the term "Hoffmann analytes" in its title, its abstract indicated it involved the examination of the potential relationships between various tobacco blend components and "Hoffmann analyte" yields across three distinct lamina tobacco blend styles, Virginia, burley, and Oriental plus a 1:1 Virginia–burley mixture
2005	At the *59th TSRC*, Zemann et al. (4406a) presented a paper entitled: On-line puff-by-puff analysis of gaseous and *Hoffmann analytes* in cigarette smoke
2006	At the *60th TSRC*, Case et al. (23A02) presented a paper entitled: The role of cigarette paper and other factors that influence *Hoffmann analyte* yields in sidestream smoke
2006	Also at the *60th TSRC*, Streibel et al. (23A13) presented a paper entitled: Real-time on-line characterization of selected *Hoffmann analytes* in inhaled and exhaled cigarette smoke (mouthspace) by photo ionisation time-of-flight mass spectrometry
2007	At presentations at the *61st TSRC*, much emphasis was placed on the determination of Hoffmann analytes. Gerardi et al. (4623) described an improved analytic procedure to determine Hoffmann analytes in cigarette smoke with particular emphasis on selected carbonyls and phenols. Guan et al. (4636) reported the relationship of cigarette tobacco composition and the MSS yield of various Hoffmann analytes such as PAHs, TSNAs, aza-arenes, NO, carbonyl compounds, and phenols. Lauterbach (4732) recommended the determination of several cytotoxic components in smoke other than a variety of Hoffmann analytes. He mentioned several compounds not on the Hoffmann analyte list. They included cyanohydrins and dicarbonyl compounds such as diacetyl and malondialdehyde.
2009	Intorp et al. (5049) described their findings on "Hoffmann analytes" in cigarette MSS in a study conducted on behalf of CORESTA
2010	At the *2010 CORESTRA Congress*, the results of several studies on "Hoffmann analytes" were presented. Le Moigne et al. (5529) described the effect of additive-treated filters and their fibers on the MSS deliveries of specific "Hoffmann analytes." Nie et al. (5546) reported the effect of cigarette paper and filters on "Hoffmann analytes."; *2010 CORESTA Congress Abstracts*, Paper SSPT 12, p. 112. Otte and Intorp (5547) described a GC–MS method for the determination of selected volatile "Hoffmann analytes" in cigarette MSS

Department of Health (Canada) (23A06). Assessment of all the lists in Table 23.6 reveals that the number of analytes in each case is in the mid-1940s, and most of them may be considered, based on the various listings by Hoffmann and his colleagues, as "Hoffmann analytes." The sequence of components in Table 23.6 parallels the component class sequence usually used in the tables in the various articles by Hoffmann and his colleagues (1727, 1740, 1741, 1743, 1744, 1773, 1808).

Table 23.6 also indicates the many components in the Hoffmann lists that are not usually analyzed or included in the "Hoffmann analyte" list of 44 or 45 biologically active components.

TABLE 23.5
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
		Polycyclic aromatic hydrocarbons			
1.	56-55-3	Benz[*a*]anthracene {B*a*A or B[*a*]A} 	39, 104, 126, 126a, 126b, 128, 139, 141–143, 147, 151, 203, 216, 237, 239, 290, 291, 329, 394, 397–399, 603, 624, 646a, 726, 746a, 797, 869, 1025, 1136, 1139, 1148, 1211, 1217, 1287–1289, 1329, 1330, 1332, 1333, 1373, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1471, 1492, 1674, 1709, 1727, 1740, 1741, 1743, 1744, 1760, 1767a, 1773, 1781, 1787, 1788, 1792, 1798, 1800, 1802, 1803, 1808, 1842, 1870, 1871, 1873, 1933b, 1971, 2013, 2037a, 2078, 2079, 2099, 2113, 2116, 2121, 2126, 2127, 2130, 2133, 2134, 2142, 2195, 2199, 2215, 2238, 2256, 2313a, 2352, 2366, 2367, 2425, 2426, 2430, 2438, 2524a, 2537, 2596a, 2710, 2799a, 2825, 2893, 2939, 2960–2962, 2964, 3003, 3007, 3024, 3030, 3032, 3033, 3047, 3049, 3081, 3082, 3087, 3088, 3131, 3158, 3162, 3176, 3190, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3264, 3265, 3272–3275, 3286, 3292, 3300, 3302, 3307, 3308, 3370, 3437, 3470, 3472, 3493, 3616, 3618–3620, 3713, 3741, 3756–3759, 3878, 3788, 3797, 3814, 3847, 3952, 3973, 3975, 3984, 3992, 4001, 4005–4007, 4009–4011, 4248, 4249, 4282, 4300, 4307, 4308, 4311, 4315, 4316, 4319, 4322, 4324, 4332, 4355, 5010, 5077, 5512, 5531, 5539, 5732, 5811b, 5869a	903, 3205, 4249, 4332, 5567, 5811b	1330, 1332, 1375a, 1377, 1378
2.	205-99-2	Benz[*e*]acephenanthrylene {benzo[*b*]fluoranthene} 	50, 117, 126a, 128, 141–143, 147, 151, 216, 239, 290, 291, 603, 726, 804, 1019, 1139, 1148, 1217, 1237, 1373, 1375a, 1377, 1378, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1786–1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2013, 2079, 2099, 2116, 2428, 2438, 2473, 2474, 2501, 2524a, 2825, 2939, 3259, 3149, 3176, 3191, 3255, 3257, 3262, 3265, 3286, 3292, 3300, 3302, 3308, 3370, 3437, 3616, 3618–3620, 3714, 3756, 3758, 3759, 3787, 3788, 3797, 4005–4007, 4009–4011, 4037, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 4323, 4324, 4332, 4353, 4354, 5010, 5077, 5512, 5539, 5811b	1127a, 4037, 4249, 5567, 5811b	50, 1375a, 1377, 1378
3.	205-82-3	Benzo[*j*]fluoranthene 	128, 141–144, 147, 151, 216, 239, 290, 291, 603, 1139, 1148, 1217, 1373, 1397, 1405, 1406, 1408, 1409, 1471, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1787, 1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2037a, 2134, 2438, 2524a, 2939, 3251, 3255, 3257, 3262, 3265, 3273, 3292, 3300, 3302, 3308, 3370, 3437, 3714, 3756, 3758, 3759, 3787, 3797, 3999, 4005, 4009–4011, 4031, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 4323, 4324, 4332, 5077, 5512, 5811b, 5869a	5567	

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

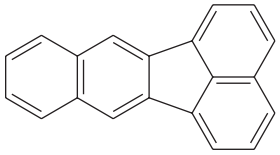
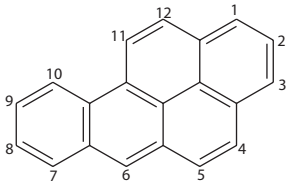
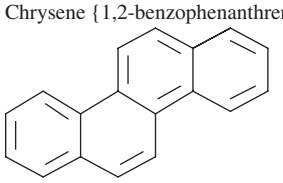
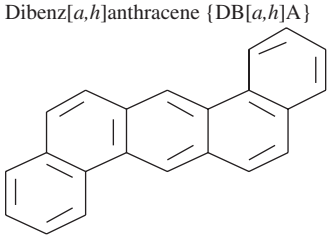
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
4.	207-08-9	Benzo[*k*]fluoranthene 	49, 141–144, 147, 151, 216, 239, 290, 291, 432, 603, 646a, 726, 746a, 1139, 1148, 1217, 1375a, 1377, 1378, 1397, 1405, 1406, 1408, 1409, 1445, 1471, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1787, 1788, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2013, 2037a, 2099, 2116, 2134, 2238, 2327, 2427, 2430, 2438, 2524a, 2825, 2939, 3176, 3251, 3255, 3257, 3262, 3265, 3273, 3286, 3292, 3300, 3302, 3308, 3370, 3437, 3514, 3616, 3618–3620, 3714, 3756, 3758, 3759, 3787, 3788, 3797, 4018, 4019, 4031, 4110, 4248, 4249, 4300, 4307, 4308, 4315, 4316, 4319, 5010, 5077, 5512, 5539, 5732, 5811b	5567, 5811b	1375a, 1377, 1378
5.	50-32-8	Benzo[*a*]pyrene {B[*a*]P} 	28, 30, 31, 39, 40, 48–50, 55–57, 83, 83a, 104, 116, 117, 126, 126a, 126b, 128, 132, 139–144, 147, 151, 158a, 167, 172, 174b, 174c, 174e, 179, 180, 183, 194, 203, 215, 216, 237, 239, 239a, 274, 276, 278, 284–286, 290, 291, 329, 351–354, 392–394, 397–399, 402, 433, 488, 489, 520, 521, 527, 532, 583, 584, 588, 589, 592–594, 603, 606a, 624, 636, 646, 646a 658, 688, 694, 695, 704, 710, 722, 726, 765–767, 784, 785, 796a, 797, 804–808, 814, 817, 819–821, 825A, 830, 869, 875–878, 882, 885, 913, 916, 933, 934, 949, 953, 964, 966, 977–981, 988a, 1001, 1006a, 1007, 1015, 1016, 1016a, 1019, 1025, 1051, 1056, 1060, 1060a, 1061, 1076, 1091, 1098–1100, 1136, 1139, 1148, 1172, 1181, 1182, 1211, 1217, 1236, 1237, 1246, 1272, 1286–1289, 1329, 1330, 1332, 1333, 1348–1350, 1354, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1396, 1397, 1403–1406, 1406a, 1406b, 1407–1409, 1410a, 1435, 1435a, 1437, 1442, 1443, 1445, 1462, 1471, 1473, 1475, 1492, 1502, 1537, 1538, 1551, 1557, 1572, 1573, 1589, 1592–1594, 1674, 1709, 1727, 1740, 1741, 1743, 1744, 1754, 1755, 1760, 1764, 1766, 1767a, 1773, 1781, 1786–1788, 1792, 1793, 1797, 1798, 1800, 1802, 1803, 1807a, 1808, 1826, 1842–1846, 1870, 1871, 1873, 1933a, 1937, 1962b, 1966, 2011, 2013, 2037a, 2060, 2071, 2072, 2079, 2099, 2114–2116, 2119, 2121, 2126, 2127, 2130, 2133, 2134, 2134a, 2142, 2156, 2170, 2184–2192, 2194–2197, 2199, 2200, 2210, 2237, 2238, 2254–2258, 2260, 2268, 2270, 2313a, 2313e, 2319, 2320, 2327, 2335, 2352–2354, 2365–2368, 2370, 2374, 2426, 2430, 2438, 2457b, 2465, 2473, 2474, 2479, 2480, 2484a, 2518, 2524a, 2537, 2543, 2545, 2557, 2570, 2589, 2596a, 2614, 2648–2650, 2651, 2654, 2683, 2707, 2710, 2713–2715, 2717, 2719, 2737, 2738, 2744, 2761, 2762, 2767, 2775, 2777, 2799a, 2817a, 2817b, 2819, 2820a, 2825, 2856, 2865, 2881, 2893, 2894, 2899, 2906, 2911, 2918, 2927, 2939, 2935, 2960–2962, 2964, 3003, 3007, 3024, 3030, 3032, 3033, 3046, 3047, 3049, 3059, 3076, 3077, 3081, 3082, 3084, 3085, 3087, 3088, 3116, 3131, 3135–3137, 3141, 3148a, 3158, 3162, 3176, 3190, 3191, 3224, 3232, 3235, 3239–3243, 3245, 3246, 3249–3251, 3254, 3255, 3257, 3259, 3262, 3264, 3265, 3269, 3273–3275, 3286, 3291, 3292, 3299a, 3300–3304, 3307, 3308, 3310, 3311, 3316, 3323–3327, 3340a, 3365, 3370,	903, 1077b, 1722, 2079, 2484a, 2939, 3974b, 4098a, 4249, 4332, 4623, 5001, 5018, 5053, 5533, 5567, 5811b	50, 1330, 1332, 1354, 1375a, 1377, 1378, 2210, 3192

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Benzo[*a*]pyrene {B[*a*]P} (cont.)	3377, 3378, 3415, 3419, 3421–3424, 3437, 3440, 3441a, 3452, 3465–3467, 3469, 3470, 3472, 3482, 3493, 3497, 3503, 3505, 3514, 3557, 3572, 3578, 3579a, 3610, 3615–3620, 3625, 3638, 3644, 3685, 3686, 3713, 3741, 3756, 3758, 3759, 3787–3789, 3797, 3811a, 3830, 3831, 3840, 3844, 3847, 3863, 3876, 3877, 3878, 3889, 3924, 3952, 3973, 3975, 3976, 3984, 3992, 3999–4001, 4005–4007, 4009–4011, 4018, 4019, 4020, 4031, 4037, 4106, 4110, 4114, 4117, 4232, 4241, 4248, 4249, 4281, 4282–4284, 4293–4296, 4300, 4301, 4303, 4307, 4309–4311, 4315, 4317–4319, 4322–4326, 4328, 4330, 4338, 4339–4341, 4342, 4351–4356, 4365, 4404, 4410, 4581, 5010, 5049, 5067, 5077, 5079, 5080, 5088, 5092, 5359, 5512, 5531, 5532, 5539, 5546, 5556, 5558, 5602, 5630, 5679, 5692, 5707, 5732, 5811b, 5836, 5869a	903, 1077b, 1722, 2079, 2484a, 2939, 3974b, 4098a, 4249, 4332, 4623, 5001, 5018, 5053, 5533, 5567, 5811b	50, 1330, 1332, 1354, 1375a, 1377, 1378, 2210, 3192
6.	218-01-9	Chrysene {1,2-benzophenanthrene} 	39, 104, 126a, 128, 141–143, 147, 151, 216, 290, 291, 329, 432, 603, 646a, 710, 726, 746a, 966, 1136, 1139, 1148, 1172, 1148, 1211, 1217, 1373, 1397, 1405, 1406, 1408, 1409, 1445, 1462, 1471, 1475, 1560, 1573, 1649, 1712, 1727, 1740, 1743, 1773, 1781, 1787, 1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 1933b, 2013, 2037a, 2079, 2099, 2113, 2121, 2130, 2195, 2134, 2238, 2256, 2313a, 2430, 2438, 2524a, 2537, 2557, 2799a, 2825, 2893, 2939, 2961, 2962, 2964, 3003, 3033, 3162, 3176, 3191, 3240–3243, 3246, 3249, 3251, 3255, 3257, 3262, 3263, 3265, 3269, 3273–3275, 3286, 3291, 3292, 3300, 3302, 3308, 3370, 3377, 3437, 3452, 3470, 3472, 3493, 3514, 3610, 3616, 3618–3620, 3741, 3756, 3758, 3759, 3787, 3788, 3797, 3814, 3876, 3924, 3927, 3952, 4005–4007, 4009–4011, 4031, 4037, 4110, 4248, 4249, 4282, 4284, 4300, 4307, 4308, 4315, 4317, 4319, 4323, 4324, 4354, 4355, 5010, 5077, 5539, 5732, 5811b, 5869a	903, 3205, 5567, 5811b	
7.	3697-24-3	Chrysene, 5-methyl-	126a, 237, 290, 291, 603, 1148, 1217, 1373, 1557, 1560, 1573, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1800, 1808, 1842, 1870, 1871, 1873, 2527e, 2825, 3255, 3257, 3260, 3265, 3300, 3370, 3618–3620, 3714, 4005–4007, 4009–4011, 4249, 4319, 4332. 5512, 5869a	5567	
8.	53-70-3	Dibenz[*a,h*]anthracene {DB[*a,h*]A} 	126a, 126b, 139–143, 174e, 239, 291, 329, 351, 726, 760, 869, 1021, 1136, 1139, 1148, 1184, 1211, 1217, 1373, 1397, 1405, 1406, 1406a, 1408, 1409, 1425, 1445, 1462, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1787, 1788, 1798, 1800, 1802, 1808, 1842, 1870, 1871, 1873, 2013, 2079, 2134, 2191, 2313a, 2438, 2465, 2518, 2601b, 2825, 2939, 2961, 2962, 2964, 3003, 3024, 3176, 3191, 3251, 3255, 3257, 3260, 3262, 3263, 3265, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3365, 3685, 3713, 3714, 3741, 3756, 3787, 3788, 3797, 3814, 3847, 3952, 3999, 4005, 4009–4011, 4024, 4031, 4110, 4232, 4249, 4296, 4300, 4307, 4308, 4311, 4315, 4317, 4319, 4323, 4324, 4332, 4355, 5010, 5077, 5512, 5539, 5811b, 5869a	5567, 5811b	

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

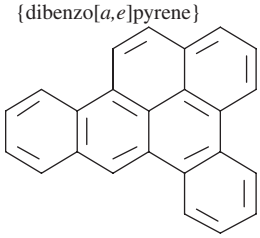
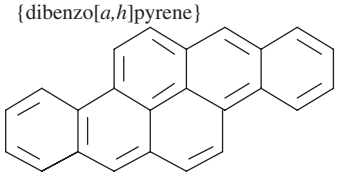
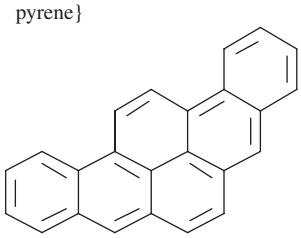
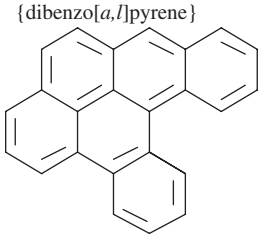
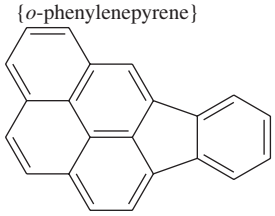
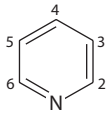
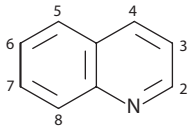
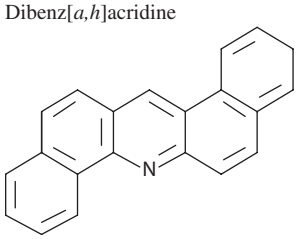
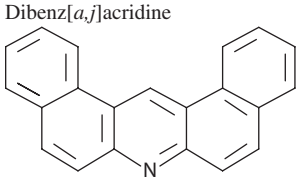
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
9.	192-65-4	Naphtho[1,2,3,4-*def*]chrysene {dibenzo[*a,e*]pyrene} 	142, 151, 290, 291, 1741, 1743, 1744, 1870, 1871, 1873, 2037a, 2825, 3257, 3262, 3265, 3300, 3308, 3714, 3756, 3787, 3788, 4249, 5512, 5869a		
10.	189-64-0	Dibenzo[*b,def*]chrysene {dibenzo[*a,h*]pyrene} 	139, 142, 143, 290, 291, 432, 1025, 1139, 1781, 1870, 1871, 1873, 2037a, 2114, 2430, 2438, 2825, 2939, 3003, 3033, 3243, 3244, 3251, 3257, 3262, 3265, 3273, 3292, 3300, 3302, 3308, 3520, 3714, 3741, 3756, 3787, 3788, 3797, 3973, 4005–4007, 4009–4011, 4249, 4282, 4296, 4319, 4332, 4354, 4355, 5077, 5732, 5811b, 5869a		
11.	189-55-9	Benzo[*rst*]pentaphene {dibenzo[*a,i*]pyrene} 	126a, 141–143, 151, 239, 392, 394, 397–399, 726, 793, 794, 1139, 1148, 1157b, 1217, 1286, 1373, 1557, 1727, 1740, 1773, 1798, 1824, 1842, 1870, 1871, 1873, 2037a, 2079, 2438, 2708–2711, 2825, 3033, 3251, 3255, 3257, 3260, 3262, 3265, 3273, 3286, 3292, 3300, 3302, 3308, 3365, 3377, 3520, 3714, 3756, 3787, 3788, 3797, 3999, 4005, 4009–4011, 4249, 4296, 4319, 4332, 4355, 5077, 5811b, 5869a		
12.	191-30-0	Dibenzo[*def,p*]chrysene {dibenzo[*a,l*]pyrene} 	126a, 141, 143, 151, 399, 726, 1139, 1148, 1211, 1217, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1798, 1808, 1842, 1870, 1871, 1873, 2079, 2134, 2250, 2427, 2430, 2825, 2939, 3003, 3251, 3255, 3257, 3260, 3262, 3265, 3273, 3286, 3300, 3307, 3714, 3756, 3787, 3788, 3999, 4249, 4317, 4319, 4324, 4332, 4353, 4354, 4355, 5077, 5512, 5811b, 5869a	5811b	
13.	193-39-5	Indeno [1,2,3-*cd*]pyrene {*o*-phenylenepyrene} 	104, 126a, 128, 141, 142, 151, 239, 290, 291, 603, 1099, 1139, 1217, 1397, 1405, 1406, 1408, 1409, 1445, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1788, 1798, 1800, 1802, 1808, 1870, 1871, 2013, 2134, 2438, 2479, 2524a, 2601b, 2799a, 2825, 3176, 3255, 3257, 3262, 3265, 3300, 3302, 3308, 3370, 3616, 3714, 3756, 3758–3759, 3797, 4005, 4010, 4011, 4249, 4311, 4315, 4317, 4319, 4324, 4325, 4332, 5010, 5077, 5512, 5539, 5811b, 5869a	5567	

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
14.	*Aza-arenes* 110-86-1	Pyridine 	38, 107, 126b, 156, 167, 172, 173a, 174b, 195, 237, 239, 299, 376, 395, 424, 462, 480, 512, 568b, 688, 775, 920, 985–988, 1063–1075, 1078, 1084, 1099, 1100, 1137, 1140, 1225, 1263, 1314, 1338, 1348, 1349, 1360, 1364, 1365, 1369, 1371, 1375a, 1386, 1426, 1427, 1437, 1445, 1580, 1587a, 1590, 1634, 1644, 1645, 1647–1649, 1659, 1673, 1674, 1699, 1741, 1803, 1812, 1842, 1857, 1884, 1890, 1891, 1903, 1911, 1966, 2001, 2006, 2088, 2133, 2142, 2170, 2191, 2224, 2226, 2228, 2230, 2233, 2234, 2267, 2270, 2313a, 2313c, 2326, 2337, 2342, 2342a, 2343, 2349, 2382, 2470, 2493, 2506, 2507, 2524, 2543, 2545, 2628, 2629, 2634, 2636, 2710, 2724, 2734, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 2857, 2858, 2869, 2912, 2936–2938, 2939, 2973, 2986–2988, 3007, 3008, 3022, 3025, 3029, 3044, 3059, 3204, 3140, 3255, 3257, 3261, 3266, 3300, 3302, 3308, 3324, 3386, 3397, 3398, 3410, 3444, 3463, 3482, 3499, 3505, 3692, 3761, 3797, 3803, 3909, 3910, 3912, 3924, 3934, 3967, 3976, 3992, 3999, 4005–4007, 4064, 4065, 4120–4122, 4127, 4132, 4202, 4228, 4249, 4407, 5034, 5079, 5124, 5138, 5140, 5189, 5263, 5359, 5770, 5811b, 5836, 5869a	120, 568b, 984, 1020, 1053, 1263, 1580, 1590, 1852, 2001, 2079, 2337, 2339a, 2359, 2389, 2544, 2724, 2917a, 2939, 2987, 3022, 3044, 3204, 3266, 3444, 3499, 3797, 3973, 3974a, 4064, 4249, 5079 5390a, 5173, 5382, 5720, 5811b, 17B56	1360, 1375a, 2506 (0), 2507 (0), 3393
15.	91-22-5	Quinoline {1-azanaphthalene} 	27, 35, 126a, 126b, 167, 172, 174b, 174c, 237, 402, 568b, 688, 722, 1077a, 1099, 1148, 1217, 1263, 1360, 1371, 1375, 1375a, 1375b, 1386, 1426, 1427, 1437, 1445, 1586, 1647, 1649, 1656, 1674, 1727, 1740, 1741, 1743, 1744, 1773, 1839, 1842, 1853b, 1880, 1881, 2006, 2132, 2133, 2134a, 2142, 2228, 2270, 2543, 2545, 2724–2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2939, 3007, 3140, 3190, 3255, 3257, 3265, 3300, 3302, 3308, 3386, 3397, 3398, 3410, 3463, 3491, 3499, 3557, 3559, 3729, 3733–3735, 3750, 3752, 3992, 4010, 4011, 4249, 4319, 4407, 4570a, 4830, 4921, 5034, 5079, 5512, 5811b, 5836, 25A84	172, 568b, 937, 2339a, 2359, 2389, 2544, 2917a, 3491, 3547, 3973, 3974a, 3974b, 4249, 5811b	1360, 1375a
16.	226-36-8	Dibenz[*a,h*]acridine 	126a, 139, 172, 239, 587, 1148, 1217, 1373, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1802, 1808, 1842, 1870, 1871, 2228, 2724, 2825, 2939, 3059, 3255, 3257, 3260, 3265, 3279, 3300, 3302, 3308, 3414, 3491, 3512, 3714, 3733–3735, 3741, 3750, 3752, 3797, 3999, 4005, 4009–4011, 4027, 4249, 4319, 4327, 4332, 5512, 5811b, 5869a		
17.	224-42-0	Dibenz[*a,j*]acridine 	126a, 172, 239, 587, 603, 1148, 1217, 1373, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1802, 1808, 1842, 1870, 1871, 2229, 2724, 2825, 2939, 3059, 3255, 3257, 3260, 3265, 3279, 3300, 3302, 3308, 3370, 3414, 3491, 3512, 3714, 3733–3735, 3750, 3752, 3797, 3999, 4005–4007, 4009–4011, 4027, 4249, 4317, 4319, 4327, 4332, 5512, 5811b, 5869a		

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

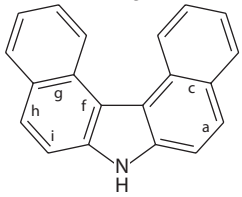
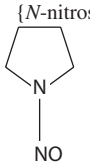
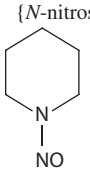
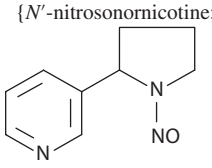
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
18.	194-59-2	7*H*-Dibenzo[*c,g*]carbazole 	126a, 172, 239, 587, 1148, 1217, 1373, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1802, 808, 1842, 1870, 1871, 2724, 2825, 2939, 3255, 3257, 3059, 3255, 3257, 3260, 3265, 3279, 3300, 3302, 3414, 3491, 3512, 3714, 3733–3735, 3750, 3752, 3797, 3999, 4005, 4009–4011, 4027, 4249, 4319, 4327, 4332, 5512, 5811b, 5869a		
N-Nitrosamines					
19.	62-75-9	Methanamine, *N*-methyl-*N*-nitroso- {*N*-nitrosodimethylamine; NDMA} $(H_3C)_2$═N-NO$(H_3C)_2$═NH	28, 30, 31, 50, 59, 126, 126a, 126b, 158a, 167, 172, 185, 191, 192, 203, 226, 237, 239, 241, 379, 380, 463, 466, 467, 471, 478, 480, 488, 489, 499, 514, 572, 573, 603, 649, 677b, 746c, 1057–1059, 1099, 1217, 1236, 1428, 1437, 1442, 1443, 1580, 1445, 1674, 1685, 1692, 1693, 1725, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1781, 1784, 1808, 1842, 1870, 1871, 1885, 1952, 1953, 2008, 2057a, 2118, 2129, 2133, 2135, 2134a, 2142, 2205, 2206, 2404, 2405, 2440–2443, 2472, 2516, 2537, 2561, 2635, 2686, 2724, 2750, 2751, 2825, 2884, 2990, 2991, 3123, 3124, 3190, 3255–3257, 3265, 3300, 3308, 3343, 3366, 3370, 3378, 3441a, 3491, 3493, 3595–3598, 3713, 3777, 3812, 3943a, 3944–3946, 3951, 3952, 3985, 3992, 3994, 4010, 4011, 4249, 5508, 5512, 5811b, 5869a	468, 478, 498, 499, 677b, 1685, 1712, 1727, 1870, 1871, 2313a, 2686, 2990, 3811a, 3943a, 3944–3948, 3973, 3974b, 4010, 4011, 4249, 5001, 5029, 5053. 5496, 5811b	45
20.	10595-95-6	Ethanamine, *N*-methyl-*N*-nitroso- {*N*-nitrosoethylmethylamine; NEMA} H_3C-CH_2-N(NO)-CH_3	31, 126a, 239, 457, 467, 470, 480, 486, 572, 573, 746c, 1058, 1148, 1217, 1236, 1428, 1445, 1580, 1725, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1784, 1808, 1842, 1870–1872, 1953, 2142, 2158, 2516, 2537, 2726, 2884, 2990, 2991, 3190, 3256, 3265, 3300, 2993, 3491, 3493, 3714, 3943a, 3944–3946, 3951, 3952, 3992, 3994, 4010, 4010, 4011, 4249, 5512, 5811b	486, 498, 1712, 1727, 1870–1872, 2516, 2655, 3943a, 3944–3948, 4249, 5496, 5811b	
21.	55-18-5	Ethanamine, *N*-ethyl-*N*-nitroso- {*N*-nitrosodiethylamine; NDEA} $(H_3C$-$CH_2)_2$═N-NO	31, 126, 126a, 126b, 172, 203, 239, 379, 457, 470, 480, 486, 510, 568b, 572, 573, 649, 746c, 1058, 1148, 1217, 1236, 1428, 1445, 1557, 1580, 1674, 1727, 1736, 1740, 1741, 1743, 1744, 1761, 1773, 1808, 1842, 1870–1872, 1952, 2118, 2129, 2142, 2440–2443, 2516, 2635, 2686, 2722, 2724, 2825, 2884, 2990, 2991, 3123, 3255–3257, 3265, 3300, 3308, 3343, 3378, 3491, 3595–3598, 3713, 3994, 4010, 4011, 4249, 4332, 5512, 5811b, 5869a	465, 468, 486, 568b, 1712, 1727, 1870–1872, 2516, 2655, 3973, 4010, 4010, 4011, 4249, 5496	
22.	621-64-7	1-Propanamine, *N*-nitroso-*N*-propyl- {*N*-nitrosodi-*n*-propylamine; NDPA} $(CH_3CH_2CH_2)_2$═N-NO	203, 239, 379, 457, 486, 572, 573, 746c, 1058, 1428, 1740, 1741, 1743, 1744, 1870–1872, 2442, 2443, 2516, 2825, 2884, 3255–3257, 3265, 3300, 3491, 3711, 3713, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	486, 498, 1870–1872	
23.	924-16-3	1-Butanamine, *N*-butyl-*N*-nitroso- {NDBA} $[CH_3$-$(CH_2)_3]_2$═N-NO	203, 239, 486, 572, 573, 746c, 1058, 1217, 1740, 1741, 1743, 1744, 1781, 1870, 1871, 1952, 2442, 2443, 2516, 2561, 2724, 2751, 2825, 2884, 3219, 3257, 3265, 3300, 3308, 3491, 3711, 3713, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	5811b	

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

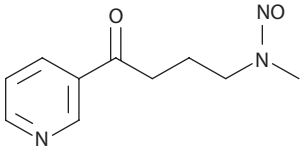
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
24.	930-55-2	Pyrrolidine, 1-nitroso- {*N*-nitrosopyrrolidine; NPYR} 	28, 30, 31, 50, 64, 126, 126a, 126b, 172, 203, 237, 239, 467, 478, 480, 486, 514, 572, 573, 576, 603, 649, 746c, 1058, 1099, 1148, 1217, 1373, 1428, 1445, 1567a, 1580, 1674, 1685, 1691–1693, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 1885, 2118, 2133, 2134a, 2142, 2325, 2404, 2405, 2516, 2561, 2686, 2724, 2750, 2825, 2879, 2884, 2990, 2991, 3190, 3255–3257, 3260, 3265, 3300, 3308, 3343, 3370, 3378, 3491, 3714, 3943a, 3944–3946, 3951, 3952, 3976, 3992, 3994, 4010, 4011, 4249, 4332, 5508, 5512, 5811b, 5869a	172, 463, 468, 466, 478, 486, 498, 514, 993, 1567a, 1685, 1712, 1727, 1740, 1741, 1743, 1744, 1870, 1871, 2139, 2686, 2990, 3943a, 3944–3948, 4010, 4249, 5001, 5496, 5811b	50 (0)
25.	100-75-4	Piperidine, 1-nitroso- {*N*-nitrosopiperidine; NPIP} 	30, 31, 203–206, 239, 457, 568b, 572, 573, 746c, 1058, 1428, 1740, 1741, 1743, 1744, 1781, 1784, 1808, 1870–1872, 1952, 2118, 2205, 2442, 2443, 2516, 2724, 2825, 2884, 3255–3257, 3265, 3300, 3302, 3308, 3491, 3595–3598, 3714, 3994, 4010, 4011, 4249, 5512, 5811b, 5869a	498, 568b, 1870–1872, 2139, 2205, 2516, 3947, 3948, 3994, 4249, 5001, 5496, 5811b	
26.	1116-54-7	Ethanol, 2,2′-(nitrosoimino) bis- {*N*-nitrosodiethanolamine; NDELA} $(HO\text{-}CH_2CH_2)_2{=}N\text{-}NO$	126, 126a, 126b, 172, 237, 239, 458, 471, 477–479, 481, 482, 485, 486, 510, 603, 1058, 1148, 1159, 1217, 1445, 1674, 1704, 1705, 1725, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1867, 1870–1872, 2516, 2825, 2655, 3190, 3255–3257, 3265, 3300, 3370, 3480, 3714, 3973, 3992, 4010, 4011, 5512, 5869a	458, 468, 471, 477–479, 481, 482, 485, 486, 490, 498, 1704, 1705, 1727, 1867, 1870–1872, 2990, 3265, 3300, 3480, 3481, 3491, 3947, 3948, 3973, 4010, 4011, 4249, 5001, 5811b	
27.	13256-22-9	Glycine, *N*-methyl-*N*-nitroso- {*N*-nitrososarcosine; NSAR} $H_3C\text{-}N(NO)\text{-}CH_2\text{-}COOH$	1058, 2442, 3256, 3300	464, 466, 485, 486, 498, 2442, 3947, 3948, 5001, 5811b	
28.	16543-55-8	Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-, (S)- {*N*′-nitrosonornicotine; NNN} 	24–26, 28–31, 59, 76, 97–99, 126, 126a, 126b, 167, 172, 174b, 174c, 203, 226, 237, 239, 313, 368, 402, 422, 423, 458–460, 463, 471, 478, 483, 484, 486, 488, 489, 499, 501, 568b, 572, 573, 575, 576, 595, 603, 632, 651, 684, 688, 772, 895, 1011, 1015, 1016, 1051, 1057, 1058, 1099, 1148, 1191–1200, 1216, 1217, 1304, 1373, 1386, 1437, 1442, 1445, 1559, 1564, 1567a, 1568–1571, 1580, 1569, 1574, 1578, 1584, 1585, 1653, 1672, 1674, 1692, 1696, 1702, 1710, 1712, 1717, 1725, 1727, 1722, 1730–1732, 1734, 1736, 1740, 1741, 1743, 1744, 1746, 1750, 1751, 1753, 1761, 1769, 1773, 1781, 1808, 1842, 1870–1872, 1987, 1988, 2128, 2133, 2134a, 2136, 2138, 2142, 2168,	29, 33, 64, 97–99, 174c, 201, 313, 322, 324, 326, 368, 458, 468, 478, 483, 484, 486, 498, 501, 503, 505, 507, 548–550, 557, 568b, 595, 650, 653–657, 660, 667, 677b, 685, 720, 772, 895,	

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke**	**Tobacco**	**Tobacco Substitute Smoke**
	Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-, (S)- {*N*′-nitrosonornicotine; NNN} (cont.)	2169, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2730, 2799a, 2825, 2879, 2949, 2991, 3007, 3050, 3080, 3094, 3190, 3255–3257, 3265, 3300, 3302, 3308, 3313, 3342, 3343, 3364, 3370, 3491, 3493, 3654, 3714, 3844, 3943a, 3944–3946, 3952, 3976, 3992, 4009–4011, 4059, 4078, 4128, 4249, 4547, 4570a, 4683, 4885, 5008, 5049, 5071, 5494, 5508, 5512, 5518, 5531, 5569, 5679, 5692, 5811b, 5836. 5859a	951, 988a, 994, 995, 997, 1003, 1010, 1015, 1051, 1175a, 1191–1200, 1206a, 1216, 1385, 1564, 1567a, 1568–1571, 1576, 1577, 1579, 1569, 1575, 1577, 1579, 1580, 1584, 1585, 1679, 1696, 1702, 1704, 1712, 1725, 1727, 1731, 1733, 1734, 1742–1734, 1750, 1753, 1771, 1870–1872, 1916a, 1988, 2050–2052, 2138, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2637, 2638, 2660, 2674, 2700, 2914–2917, 2949, 2996, 2997, 3144a, 3176a, 3177, 3491, 3654, 3670a, 3773, 3774, 3816, 3943a, 3943b, 3944–3948, 3973, 3974b, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4247, 4249, 4410b, 4413, 4547, 4683, 4885, 5001, 5005, 5007, 5008, 5018, 5023, 5033, 5038, 5053, 5063, 5531, 5561, 5579, 5584, 5811b	

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
29.	64091-91-4 110053-55-9 121268-99-3 126165-82-0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}  {1-Butanone, 4-[(nitrosomethyl) amino]-1-(3-pyridinyl)-}	7, 23–26, 28–31, 34, 59, 70, 75, 97–99, 126, 126a, 126b, 172, 174b, 174c, 237, 239, 402, 458–460, 463, 478, 483, 484, 486, 501, 502, 508, 514, 568b, 572, 573, 595, 603, 688, 728, 772, 895, 998, 1001, 1002, 1004, 1006a, 1011, 1013–1016, 1016a, 1051, 1058, 1099, 1148, 1191–1200, 1373, 1386, 1445, 1557, 1564, 1566, 1567, 1567a, 1569–1571, 1571a, 1572, 1573a, 1580, 1584, 1674, 1679, 1685, 1692, 1696, 1702, 1710, 1725, 1727, 1728, 1730, 1731, 1736, 1741, 1746, 1750, 1751, 1768, 1769, 1781, 1842, 1870–1872, 1987, 1988, 2133, 2134a, 2142, 2168, 2235, 2354, 2404, 2405, 2407, 2441, 2561, 2588, 2599, 2617, 2618, 2674, 2879, 2949, 2991, 2992, 2993, 3007, 3094, 3178, 3179, 3180, 3181, 3182, 3184, 3190, 3255–3257, 3265, 3300, 3342, 3343, 3365, 3370, 3376, 3378, 3844, 3952, 3973, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5070, 5087, 5494, 5531, 5546, 5556, 5569, 5679, 5692, 5811, 5811a, 5811b, 5836	29, 33, 34, 64, 70, 97–99, 174c, 201, 324–326, 458, 463, 465, 468, 478, 483, 484, 486, 498, 501, 505, 508, 510, 548–550, 553, 554, 557, 568b, 595, 655, 720, 772, 895, 998, 1002, 1004, 1010, 1014, 1015, 1051, 1156, 1191–1200, 1385, 1564, 1566, 1567, 1567a, 1569–1571, 1573a, 1576, 1577, 1584, 1679, 1685, 1696, 1702, 1712, 1722, 1725, 1728, 1730, 1731, 1746, 1750, 1768, 1771, 1870–1872, 1988, 2050–2052, 2169, 2235, 2326c, 2362, 2363, 2406, 2407, 2436, 2437, 2441, 2637, 2638, 2674, 2700, 2914–2917, 2949, 2992, 2996, 2997, 3144a, 3176a, 3177, 3183, 3441a, 3491, 3773, 3774, 3816, 3943b, 3947, 3948, 3973, 3974b, 4010, 4011, 4059, 4077,	

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

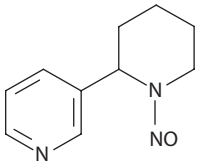
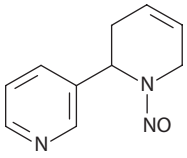
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK} (cont.)		4090, 4128, 4161, 4236, 4247, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5531, 5579, 5584, 5589, 5811, 5811a, 5811b	
30.	1133-64-8 37620-20-5	Pyridine, 3-(1-nitroso-2-piperidinyl)-, (*S*)- {*N*′-nitrosoanabasine; NAB} 	28–31, 174b, 174c, 239, 422, 423, 460, 478, 483, 484, 486, 568b, 572, 573, 576, 603, 688, 890, 895, 1148, 1193–1196, 1199–1200, 1216, 1217, 1304, 1373, 1386, 1445, 1559, 1566, 1567, 1567a, 1569–1571, 1576, 1578, 1584, 1653, 1672, 1696, 1702, 1725, 1727, 1732, 1736, 1740, 1741, 1751, 1753, 1773, 1808, 1842, 1870–1872, 1987, 1988, 2235, 2354, 2407, 2442, 2443, 2516, 2588, 2617, 2618, 2730, 2879, 3007, 3080, 3094, 3190, 3255–3257, 3265, 3300, 3302, 3308, 3313, 3342, 3343, 3370, 3943a, 3944–3946, 3992, 4010, 4011, 4059, 4078, 4128, 4249, 4319, 4547, 5008, 5049, 5494, 5531, 5569, 5679, 5692, 5811b, 5836	29, 33, 174c, 201, 324, 468, 478, 483, 484, 486, 505, 510, 557, 568b, 655, 720, 890, 895, 922, 995, 998, 1002, 1192, 1206a, 1216, 1566, 1567, 1567a, 1569–1571, 1575, 1578, 1579, 1584, 1679, 1696, 1702, 1725, 1727, 1732, 1870–1872, 1988, 2050–2052, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2637, 2638, 2700, 2724, 2822a, 2914, 3144a, 3176a, 3661, 3773, 3774, 3816, 3943a, 3943b, 3944–3948, 3973, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5063, 5531, 5584, 5811b	

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
31.	71267-22-6 71608-13-4	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-nitroso-, (S)-{*N*′-nitrosoanatabine; NAT} 	24, 28–31, 34, 59, 174b, 174c, 239, 402, 459, 463, 478, 483, 484, 486, 501, 502, 514, 568b, 572, 573, 603, 688, 895, 1002, 1015, 1051, 1192–1196, 1198, 1199, 1217, 1304, 1386, 1437, 1445, 1569–1571, 1584, 1672, 1685, 1692, 1694, 1696, 1702, 1725, 1736, 1751, 1769, 1870, 1871, 1987, 1988, 2142, 2235, 2354, 2407, 2516, 2588, 2617, 2618, 2879, 2949, 2991, 3007, 3080, 3094, 3190, 3255, 3265, 3300, 3342, 3343, 3370, 3844, 3943a, 3944–3946, 3952, 3976, 3992, 4005–4007, 4010, 4011, 4059, 4078, 4128, 4249, 4547, 5008, 5049, 5494, 5531, 5569, 5679, 5692, 5811b, 5836	29, 33, 34, 64, 174c, 201, 324, 404, 468, 478, 483, 484, 486, 501, 502, 505, 514, 548–550, 557, 568b, 655, 720, 895, 951, 995, 998, 1002, 1010, 1015, 1175a, 1192–1196, 1198, 1199, 1206a, 1385, 1569–1571, 1576, 1679, 1685, 1694, 1696, 1702, 1712, 1725, 1733, 1916a, 1988, 2050–2052, 2139, 2235, 2362, 2363, 2406, 2407, 2436, 2437, 2637, 2638, 2674, 2700, 2914, 2949, 3144a, 3176a, 3177, 3661, 3773, 3774, 3816, 3943a, 3944–3948, 3973, 4010, 4011, 4059, 4077, 4128, 4161, 4236, 4249, 4410b, 4547, 5001, 5007, 5008, 5053, 5063, 5518, 5531, 5579, 5584, 5811b	

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

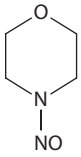
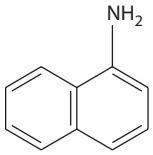
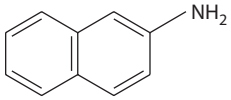
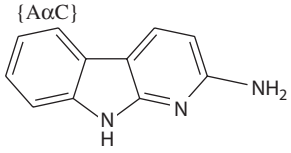
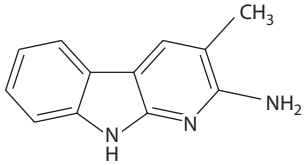
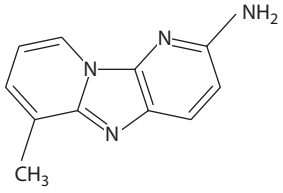
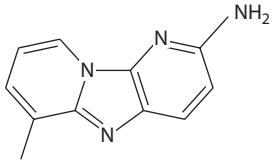
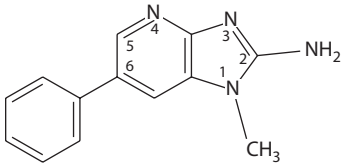
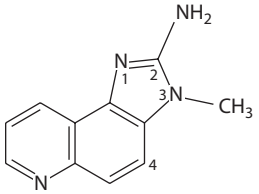
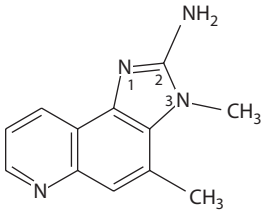
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
32.	59-89-2	Morpholine, 4-nitroso- {*N*-nitrosomorpholine; NMOR} 	31, 126a, 203, 471, 478, 485, 510, 746c, 1058, 1059, 1727, 1842, 2442, 2443, 3255, 3257, 4010, 4011, 5811b	468, 478, 498, 510, 1217, 1727, 1740, 1741, 1773, 3256, 3265, 3300, 3973, 3974b, 4010, 4011, 4249, 5001, 5496, 5811b	
Aromatic amines					
33.	95-53-4	Benzenamine, 2-methyl- {*o*-toluidine; 2-toluidine}	126, 126a, 126b, 237, 239, 568b, 722, 1123, 1148, 1217, 1360, 1375a, 1410, 1445, 1674, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 2142, 2313a, 2724, 2761, 2762, 2765, 2766, 2773, 2777, 2825, 2889, 3255, 3257, 3260, 3265, 3300, 3491, 3714, 3729, 3781, 3797, 4010, 4011, 4249, 4763, 5512, 5811b, 5869a	568b, 1877, 3491, 4249, 5811b	1360, 1375a
34.	87-62-7	Benzenamine, 2,6-dimethyl- {2,6-dimethylaniline-; 2,6-xylidine}	1743, 1744, 2142, 2313a, 2724, 2883, 2889, 3255, 3265, 3300, 3491, 3714, 3797, 4010, 4011, 4249, 5512, 5811b	1877, 3491, 4249, 5811b	
35.	134-32-7	1-Naphthalenamine {naphthalene, 1-amino-; α-naphthylamine} 	174b, 174c, 239, 329, 568b, 688, 1217, 1373, 1386, 1410, 1437, 1735, 1747, 1870, 1871, 2142, 2485, 2587, 2724, 2883, 2900, 3007, 3255, 3265, 3300, 3491, 3797, 4137, 4249, 4816, 5049, 5071, 5516, 5811b, 5836		
36.	91-59-8	2-Naphthalenamine {naphthalene, 2-amino-; β-naphthylamine} 	126, 126a, 126b, 139, 174b, 174c, 239, 402, 688, 988a, 1026, 1099, 1217, 1373, 1386, 1410, 1437, 1442, 1445, 1674, 1727, 1740, 1741, 1743, 1744, 1747, 1773, 1781, 1808, 1842, 1870, 1871, 2489, 2553, 2587, 2724, 2825, 2900, 3007, 3255, 3257, 3260, 3265, 3300, 3441a, 3493, 3711, 3781, 4009, 4249, 4407, 4816, 5022, 5512, 5516, 5811b, 5836, 5869a		
37.	2243-47-2	[1,1′-Biphenyl]-3-amine {3-aminobiphenyl}	174b, 174c, 688, 1386, 1735, 2142, 2313a, 2587, 3007, 3148a, 3255, 3300, 4010, 4011, 4249, 5022, 5049, 5516, 5811b, 5836		
38.	92-67-1	[1,1′-Biphenyl]-4-amine {4-aminobiphenyl}	126, 126a, 126b, 174b, 174c, 237, 239, 402, 688, 988a, 1099, 1148, 1212, 1217, 1373, 1386, 1410, 1445, 1674, 1727, 1735, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1870, 1871, 2142, 2313a, 2587, 2825, 3007, 3148a, 3255, 3257, 3265, 3300, 3441a, 3711, 3781, 4010, 4011, 4249, 4407, 4687, 4763, 4816, 5049, 5065, 5512, 5516, 5811b, 5836, 5869a		
N-*Heterocyclic amines*					
39.	26148-68-5	1*H*-Pyrido[2,3-*b*]indol-2-amine {AαC} 	179a, 179b, 751, 755, 756, 933, 1740, 1741, 1743, 1744, 2354a, 2449, 2450, 2484a, 2492, 3265, 3300, 3714, 4367, 4368, 4388, 4389, 4390, 5002, 5512, 5869a		

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
40.	68006-83-7	1*H*-Pyrido[2,3-*b*]indol-2-amine, 3-methyl- {MeAαC} 	179a, 179b, 751, 755, 756, 933, 1740, 1741, 1743, 1744, 2354a, 2449, 2450, 2484a, 2492, 3265, 3300, 3714, 4367,4368, 4388, 4389, 4390, 5002, 5512, 5811b, 5869a, 17F01		
41.	67730-11-4	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 6-methyl- {Glu-P-1} 	751, 755, 756, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 5002, 5512, 5811b, 5869a		
42.	67730-10-3	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine {Glu-P-2} 	751, 755, 756, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 5002, 5512, 5811b, 5869a		
43.	105650-23-5	1*H*-Imidazo[4,5-*b*]pyridin-2-amine, 1-methyl-6-phenyl- {PhIP} 	1740, 1741, 1743, 1744, 2095a, 2448, 2484a, 2601, 3265, 3300, 3714, 5002, 5512, 5811b		
44.	76180-96-6	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3-methyl- {IQ} 	158a, 179a, 751, 755, 756, 1740, 1741, 1743, 1744, 2095a, 2327c, 2354a, 2484a, 2601, 3255, 3257, 3265, 3300, 3714, 3865c, 4367, 4368, 5002, 5512, 5811b, 5869a		
45.	77094-11-2	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3,4-dimethyl- {MeIQ} 	179a, 2095a, 2327c, 2354a, 2484a, 3255, 3257, 3265, 3300, 3714, 5002		

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

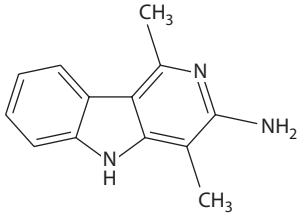
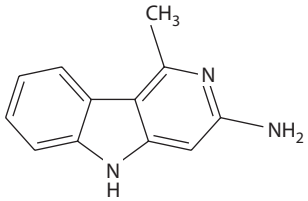
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
46.	62450-06-0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1,4-dimethyl- {Trp-P-1} 	751, 755, 756, 1373, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4367, 4368, 5002, 5512, 5869a		
47.	62450-07-1	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1-methyl- {Trp-P-2} 	751, 755, 756, 1373, 1740, 1741, 1743, 1744, 2327c, 2449, 2484a, 3255, 3257, 3265, 3300, 3714, 4367, 4368, 5002, 5512, 5869a		
Aldehydes and ketones					
48.	50-00-0	Formaldehyde H-CH═O	69, 73, 126, 126a, 126b, 126d, 172, 172c, 174a, 174b, 174c, 174e, 213, 237, 239, 243, 270, 376, 402, 405, 407, 408, 486, 544–546, 564, 591, 603, 688, 722, 748, 764a, 778, 872, 929, 1023, 1039, 1049, 1051, 1063–1074, 1099, 1140, 1148, 1217, 1218, 1238, 1283, 1284, 1292, 1329, 1330, 1332–1334, 1336, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1437, 1442, 1443, 1445, 1487, 1492, 1589, 1668–1670, 1673, 1674, 1695, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1835c, 1840, 1842, 1870, 1871, 2022, 2079, 2083–2085, 2086b, 2089, 2133, 2134a, 2170, 2180, 2195, 2200, 2252, 2270, 2293, 2310, 2313a, 2343, 2354, 2452, 2456, 2524, 2529, 2537, 2543, 2545, 2558, 2570, 2591, 2601b, 2683, 2690–2695, 2702, 2702a, 2706, 2761, 2762, 2775, 2777, 2782, 2799a, 2804, 2822, 2825, 2887, 2927, 2939, 3007, 3059, 3116, 3133, 3135, 3136, 3149, 3169, 3187, 3190, 3251, 3254, 3255, 3257, 3260, 3264, 3265, 3300, 3302, 3308, 3335, 3370, 3396, 3427, 3431, 3436, 3438, 3493, 3557, 3713, 3776, 3789b, 3791, 3844, 3871, 3872, 3880, 3882, 3897, 3912, 3924, 3952, 3963, 3992, 4010, 4011, 4078, 4159, 4249, 4259, 4288, 4301, 4304, 4305, 4319, 4342, 4360, 4689, 4743, 4816, 5006, 5065, 5069, 5079, 5124, 5423, 5508, 5512, 5529, 5531, 5679, 5692, 5811b, 5835, 5836, 5869a, 3A01, 3A02, 3A03, 3A05, 3A06, 3A07, 3A10, 3A11, 3A12, 3A16, 3A20, 3A21, 3A23, 3A24, 3A25	2703, 2939, 3335, 3626, 3797, 3973, 3974a, 3974b, 4249, 5053, 5079, 5811b	1228, 1330, 1332, 1354, 1375a, 1377, 1378

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
49.	75-07-0	Acetaldehyde CH_3-CH═O	37, 38, 69, 73, 83, 85, 126a, 126b, 156, 167, 172, 173a, 174a, 174b, 174c, 174e, 199, 213, 239, 270, 299, 314, 329, 337, 348, 376, 402, 405, 407, 408, 480, 491, 500, 544–546, 564, 568b, 603, 605, 639, 643, 645, 688, 722, 762, 764a, 778, 804, 830a, 892, 893, 916, 929, 966, 988a, 1023, 1039, 1050, 1051, 1063–1075, 1140, 1148, 1153, 1154, 1167, 1168, 1217, 1237–1239, 1283, 1284, 1329, 1330, 1332–1334, 1348–1352, 1354, 1360, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1418, 1422, 1426, 1427, 1437, 1445, 1449, 1487, 1489, 1492, 1495–1497, 1586, 1589, 1590, 1634, 1637, 1668, 1673, 1674, 1693, 1709, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1803, 1808, 1822, 1829, 1835c, 1840, 1842, 1870, 1871, 1875, 1884, 1963, 1971, 2002, 2003, 2063, 2070, 2079, 2081–2086, 2089, 2091, 2131, 2134a, 2144, 2159, 2170, 2252, 2270, 2293, 2296, 2298, 2301, 2302, 2304, 2305, 2313a, 2337, 2411, 2444, 2452, 2483, 2506, 2507, 2519, 2520, 2525, 2537, 2543, 2545, 2558, 2570, 2573–2575, 2582, 2591, 2601b, 2634, 2644, 2683, 2690–2695, 2702, 2761, 2762, 2765, 2767, 2775, 2777, 2781, 2782, 2799a, 2800, 2804, 2822, 2825, 2857, 2858, 2866, 2868, 2887, 2927, 2936, 2939, 2942, 2948, 3007, 3059, 3088, 3105, 3116, 3131, 3132, 3135, 3136, 3140, 3169, 3187, 3190, 3251, 3254, 3255, 3257, 3260, 3264, 3265, 3289, 3300, 3302, 3306, 3308, 3370, 3373, 3396, 3418, 3431, 3436, 3438, 3479, 3482, 3493, 3508, 3530, 3551, 3557, 3559, 3577, 3579, 3581–3584, 3692, 3713, 3714, 3794, 3797, 3817, 3844, 3871, 3876, 3880, 3882, 3883, 3897, 3901, 3904, 3935, 3939, 3952, 3973, 3976, 3984, 3992, 4005–4007, 4009–4011, 4052, 4056, 4062, 4078, 4104, 4109, 4155, 4159, 4162, 4249, 4254–4258, 4288, 4290, 4301, 4304, 4319, 4330, 4332, 4342, 4365, 4394, 4418, 5006, 5034, 5049, 5065, 5069, 5079, 5135, 5136, 5512, 5531, 5547, 5554, 5679, 5692, 5770, 5811b, 5835, 5836, 5869a, 3A12, 4A02	120, 212, 568b, 984, 1550, 1590, 1893b, 2079, 2270, 2293, 2337, 2702, 2702a, 2860a, 2914, 2939, 3194, 3350, 3626, 3797, 3973, 3974a, 3974b, 4223, 4225, 5053, 5079, 5165, 5811b, 5896	1228, 1330, 1332, 1354, 1360, 1375a, 1377, 1378, 2244, 2506, 2507, 3401, 4052, 4056
50.	123-38-6	Propanal {propionaldehyde} H_3C-CH_2-CH═O	172, 174a, 174b, 174c, 174e, 299, 314, 405, 407, 408, 480, 564, 568b, 591, 605, 639, 688, 722, 764a, 778, 830a, 929, 1050, 1063–1074, 1140, 1167, 1168, 1238, 1239, 1284, 1348–1351, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1415, 1418, 1419, 1445, 1449, 1495, 1586, 1589, 1668, 1853b, 1875, 1966, 2003, 2079, 2089, 2091, 2134a, 2144, 2270, 2310, 2313a, 2337, 2506, 2507, 2519, 2520, 2525, 2543, 2545, 2570, 2573–2575, 2591, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2887, 2927, 2939, 3007, 3105, 3132, 3135, 3136, 3190, 3254, 3257, 3300, 3302, 3308, 3396, 3431, 3436, 3438, 3482, 3530, 3557, 3583, 3584, 3817, 3901, 3940, 3992, 4052, 4056, 4078, 4104, 4135, 4162, 4249, 4290, 4304, 4319, 4570a, 5006, 5028, 5065, 5069, 5811b, 5835, 5836, 5869a	568b, 1550, 1893b, 2337, 2914, 2939, 3350, 3626, 3797, 3829e, 3973, 3974a, 4223, 4249, 5811b, 5896	1228, 1354, 1375a, 1377, 1378, 2244, 2506, 2507, 4052, 4056

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
51.	123-72-8	Butanal {butyraldehyde} $H_3C\text{-}(CH_2)_2\text{-}CH{=}O$	174a, 174b, 174c, 174e, 299, 314, 564, 568b, 605, 688, 764a, 1038, 1039, 1140, 1238, 1365, 1374, 1375, 1375b, 1386, 1412–1414, 1416, 1419, 1634, 1853b, 2079, 2089, 2170, 2270, 2310, 2313a, 2337, 2519, 2520, 2545, 2591, 2702, 2767, 2782, 2804, 2822, 2887, 2939, 3007, 3059, 3105, 3135, 3136, 3254, 3300, 3302, 3308, 3396, 3436, 3557, 3794, 3901, 3935, 4078, 4249, 4304, 4319, 4570a, 5034, 5049, 5079, 5135, 5136, 5770, 5811b, 5835, 5836	568b, 1550, 1893b, 2337, 2914, 3350, 3626, 3797, 3973, 3974a, 5811b	2244
52.	123-73-9 4170-30-3	2-Butenal {crotonaldehyde} $H_3C\text{-}CH{=}CH\text{-}CH{=}O$	112, 126a, 174b, 174c, 239, 270, 299, 329, 405, 407, 408, 480, 564, 568b, 591, 605, 689, 764a, 830a, 1063–1074, 1140, 1148, 1153, 1217, 1348–1351, 1354, 1375a, 1378, 1386, 1412–1414, 1416, 1418, 1419, 1586, 1589, 1634, 1727, 1741, 1773, 1842, 2002, 2079, 2088, 2089, 2313a, 2337, 2387, 2506, 2507, 2520, 2543, 2545, 2570, 2591, 2761, 2762, 2765, 2767, 2777, 2782, 2804, 2857, 2887, 2927, 2939, 3007, 3029, 3133, 3135, 3136, 3140, 3187, 3255, 3257, 3265, 3300, 3302, 3308, 3441a, 3482, 3530, 3557, 4005–4007, 4052, 4056, 4078, 4079, 4162, 4249, 4257, 4290, 4304, 4319, 5006, 5022, 5034, 5049, 5065, 5069, 5070, 5546, 5770, 5811b, 5836	120, 568b, 984, 2337, 2862a, 2917a, 2939, 3797, 3974a, 3974b, 4249, 5053, 5065, 5811b	1354, 1375a, 1378, 2244, 2387, 2506, 2507, 3401, 3402, 3404, 4052, 4056
53.	107-02-8	2-Propenal {acrolein} $H_2C{=}CH\text{-}CH{=}O$	83, 111, 112, 126a, 126b, 126d, 172, 173a, 174a, 174b, 174c, 174e, 203, 213, 237, 239, 270, 280, 314, 299, 329, 337, 376, 402, 405, 407, 408, 480, 491, 494, 495, 568b, 591, 603, 639, 645, 688, 722, 748, 764a, 778, 830a, 860, 915, 929, 1023, 1039, 1048, 1050, 1051, 1063–1074, 1099, 1140, 1148, 1153, 1167, 1168, 1217, 1238, 1283, 1284, 1329–1334, 1336, 1338, 1348–1351, 1354, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412, 1413, 1416, 1418, 1419, 1437, 1442, 1449, 1487, 1489, 1492, 1495–1497, 1586, 1589, 1634, 1637, 1638, 1673, 1674, 1709, 1727, 1741, 1760, 1773, 1781, 1803, 1807a, 1829, 1840, 1842, 1870, 1871, 1875, 1947, 1956, 2063, 2070, 2079, 2083–2085, 2091, 2131, 2133, 2134a, 2170, 2252, 2270, 2296, 2301, 2302, 2304, 2305, 2313a, 2337, 2411, 2452, 2506, 2507, 2520, 2524, 2537, 2543, 2545, 2558, 2570, 2591, 2601b, 2634, 2644, 2683, 2761, 2762, 2765, 2767, 2775, 2777, 2781, 2782, 2800, 2804, 2822, 2857, 2927, 2939, 3007, 3087, 3088, 3116, 3126, 3131, 3132, 3135, 3136, 3145, 3169, 3187, 3190, 3251, 3254, 3255, 3257, 3264, 3265, 3300, 3302, 3308, 3370, 3396, 3441a, 3482, 3493, 3530, 3551, 3557, 3577, 3692,	568b, 2337, 3974a, 4249, 5053, 5811b	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 2244, 2506, 2507, 3401, 4052, 4056
54.			3844, 3871, 3880, 3882, 3883, 3885, 3897, 3901, 3976, 3984, 3992, 4005–4007, 4010, 4011, 4052, 4056, 4078, 4104, 4159, 4162, 4249, 4257, 4259, 4288, 4290, 4301, 4319, 4330, 4360, 4418, 5006, 5022, 5028, 5034, 5065, 5070, 5079, 5490, 5512, 5531, 5547, 5554, 5556, 5583, 5811b, 5836, 5869a, 3A08, 3A17, 3A25		

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
55.	67-64-1	2-Propanone {acetone} H_3C-CO-CH_3-	38, 111, 112, 126a, 126b, 172, 173a, 174b, 174c, 199, 237, 239, 298, 299, 314, 329, 402, 405, 407, 408, 480, 544–546, 564, 568b, 639, 643, 645, 688, 722, 764a, 778, 830a, 892, 893, 929, 966, 1023, 1039, 1051, 1063–1074, 1099, 1140, 1153, 1154, 1167, 1168, 1238, 1239, 1283, 1284, 1329, 1338, 1348–1352, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412, 1413, 1416, 1418, 1419, 1437, 1449, 1489, 1495–1497, 1586, 1589, 1590, 1634, 1637, 1638, 1668, 1674, 1842, 1875, 1947, 1963, 2002, 2003, 2063, 2079, 2083–2085, 2091, 2133, 2170, 2171, 2252, 2270, 2296, 2301, 2302, 2304, 2305, 2313a, 2337, 2452, 2483, 2519, 2520, 2525, 2543, 2570, 2573–2575, 2591, 2634, 2644, 2702, 2765, 2767, 2777, 2781, 2782, 2800, 2801, 2822, 2857, 2868, 2927, 2939, 2942, 3007, 3059, 3132, 3135, 3136, 3169, 3190, 3251, 3254, 3255, 3257, 3300, 3302, 3306, 3308, 3373, 3396, 3418, 3431, 3436, 3438, 3482, 3493, 3530, 3551, 3553, 3557, 3581–3584, 3692, 3797, 3817, 3844, 3871, 3876, 3880, 3882, 3883, 3897, 3901, 3973, 3992, 4005–4007, 4052, 4056, 4078, 4159, 4162, 4194, 4202, 4249, 4254, 4256, 4257, 4290, 4319, 4360, 5028, 5034, 5079, 5512, 5547, 5554, 5583, 5770, 5811b, 5836, 5869a, 4A02	120, 568b, 647, 984, 1550, 1590, 1668, 2293, 2337, 2339a, 2863, 2866, 2914, 2939, 3626, 3797, 3974a, 4064, 4223, 4225, 4249, 5079, 5811b, 5896	1228, 1354, 1375a, 1377, 1378, 2244, 3401, 4052, 4056
56.	78-93-3	2-Butanone {methyl ethyl ketone} H_3C-CO-CH_2-CH_3	37, 38, 111, 112, 172, 173a, 174b, 174c, 299, 314, 480, 544–546, 564, 568b, 605, 643, 645, 688, 764a, 778, 966, 1038, 1050, 1063–1074, 1140, 1153, 1154, 1215, 1238, 1284, 1348–1352, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1416, 1418, 1419, 1427, 1495, 1586, 1589, 1590, 1637, 1668, 1875, 1947, 1966, 2002, 2003, 2063, 2079, 2089, 2091, 2270, 2293, 2310, 2337, 2387, 2483, 2506, 2507, 2520, 2543, 2545, 2559, 2559a, 2570, 2591, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2858, 2866, 2939, 2942, 3007, 3059, 3105, 3132, 3135, 3136, 3254, 3255, 3266, 3300, 3308, 3396, 3413, 3431, 3436, 3438, 3482, 3493, 3530, 3551, 3555, 3557, 3692, 3794, 3797, 3817, 3876, 3897, 3901, 3939, 4005–4007, 4052, 4056, 4078, 4104, 4162, 4249, 4257, 4290, 4319, 4360, 4570a, 5034, 5049, 5770, 5811b, 5836	404, 568b, 647, 984, 1053, 1590, 2337, 2339a, 2914, 2939, 3266, 3555, 3626, 3797, 3974a, 4223, 4225, 4249, 5811b	1354, 1375a, 1377, 1378, 2244, 2387, 2506, 2507, 3401, 4052, 4056
Volatile hydrocarbons					
57.	106-99-0	1,3-Butadiene H_2C=CH–CH=CH_2	73, 126a, 143, 154, 174b, 174c, 199, 216, 329, 402, 493–495, 603–605, 621, 688, 710, 722, 966, 1037a, 1037b, 1099, 1100, 1140, 1153, 1154, 1243, 1262a, 1386, 1472, 1557, 1571a, 1632, 1740, 1741, 1743, 1744, 1842, 1971, 2060, 2270, 2293, 2310, 2313a, 2634, 2644, 2645, 2782, 2804, 2857, 2866, 2942, 2946, 3007, 3260, 3265, 3300, 3302, 3308, 3370, 3441a, 3583, 3584, 3713, 3797, 3876, 3882, 3897, 3901, 4052, 4056, 4078, 4135, 4150, 4153, 4162, 4166, 4249, 4319, 4360, 4998, 5034, 5049, 5070, 5512, 5554, 5679, 5692, 5692a, 5770, 5811b, 5836, 5869a		4052, 4056

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

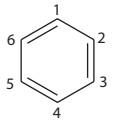
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
58.	78-79-5	1,3-Butadiene, 2-methyl- {isoprene} $H_2C{=}C(CH_3){-}CH{=}CH_2$	73, 112, 142, 143, 172, 173a, 174b, 174c, 199, 216, 239, 298, 299, 314, 323, 329, 402, 494, 495, 544–546, 568b, 603–605, 628, 639, 643, 645, 688, 722, 892, 893, 966, 1050, 1099, 1100, 1063–1066, 1068–1074, 1140, 1153, 1154, 1217, 1243, 1262a, 1284, 1286, 1329, 1330, 1332–1334, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1418–1420, 1437, 1445, 1449, 1492, 1497, 1586, 1589, 1634, 1637–1639, 1642, 1643, 1693, 1699, 1709, 1740, 1741, 1743, 1744, 1760, 1842, 1875, 1956, 1974, 2002, 2003, 2060, 2062, 2063, 2073, 2079, 2091, 2131, 2171, 2270, 2293, 2301, 2310, 2313a, 2520, 2543, 2570, 2582, 2589, 2634, 2644, 2645, 2683, 2761, 2762, 2767, 2775, 2777, 2782, 2799a, 2800, 2804, 2822, 2857, 2864b, 2866, 2874, 2939, 2942, 2946, 3007, 3059, 3105, 3106, 3132, 3254, 3255, 3257, 3260, 3265, 3300, 3302, 3306, 3308, 3370, 3373, 3418, 3482, 3493, 3551, 3557, 3583, 3584, 3692, 3714, 3797, 3862, 3876, 3882, 3897, 3901, 3939, 3973, 3976, 3999, 4005–4007, 4052, 4056, 4057, 4078, 4104, 4135, 4150, 4166, 4249, 4254–4256, 4258, 4290, 4319, 4360, 4636, 4731, 4830, 4998, 5034, 5049, 5512, 5531, 5554, 5679, 5692, 5692a, 5770, 5811b, 5836, 4A02	568b, 4249, 4731, 5811b	1330, 1332, 1354, 1375a, 1377, 1378, 4052, 4056
59.	71-43-2	Benzene 	73, 111, 112, 126, 126a, 126b, 141–143, 147, 151, 156, 157, 167, 172, 173a, 174a, 174b, 174c, 174e, 199, 203, 222–224, 237, 239, 299, 314, 315, 402, 414, 462, 493- 495, 544–546, 566, 568, 568b, 603, 605, 643, 645, 688, 705, 902, 966, 1026, 1050, 1063–1074, 1139, 1140, 1148, 1153, 1154, 1168, 1217, 1243, 1262a, 1313, 1348–1351, 1354, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1412–1414, 1416, 1418, 1423, 1443, 1445, 1472, 1485, 1571a, 1586, 1589, 1634, 1637, 1639, 1643, 1649, 1673, 1674, 1701, 1727, 1740, 1741, 1743, 1744, 1751, 1760, 1773, 1842, 1849–1852, 1868, 1870, 1871, 1873, 1947, 1966, 1975, 2002, 2063, 2079, 2088, 2090, 2096, 2114, 2133, 2142, 2256, 2270, 2293, 2310, 2313a, 2354, 2520, 2543, 2545, 2570, 2589, 2601b, 2634, 2644, 2645, 2765, 2767, 2777, 2782, 2799a, 2800, 2804, 2822, 2825, 2857, 2870, 2939, 2942, 3003, 3007, 3059, 3106, 3135–3137, 3190, 3251, 3254, 3255, 3257, 3260, 3265, 3300, 3302, 3308, 3370, 3368, 3441a, 3410, 3418, 3464–3470, 3482, 3493, 3498, 3500, 3530, 3557, 3692, 3711, 3729, 3794, 3797, 3876, 3897, 3901, 3992, 4005–4007, 4052, 4056, 4078, 4104, 4111, 4135, 4151, 4162, 4166, 4249, 4257, 4259, 4319, 4360, 5034, 5049, 5070, 5512, 5531, 5547, 5554, 5692a, 5770, 5811b, 5869a	568b, 984, 4249, 5811b	1228, 1354, 1375a, 1377, 1378, 2244, 3401, 4052, 4056

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
60.	108-88-3	Benzene, methyl- {toluene} C_6H_5–CH_3	37, 38, 73, 104, 111, 112, 126a, 126b, 141–143, 151, 152, 156, 157, 167, 173a, 174a, 174b, 174c, 174e, 199, 222–224, 237, 239, 299, 314, 315, 402, 462, 480, 493–495, 544–546, 566, 568, 568b, 603, 605, 643, 645, 688, 892, 893, 966, 1050, 1063–1074, 1110, 1139, 1140, 1153, 1154, 1168, 1243, 1262a, 1313, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1412–1414, 1416, 1418, 1419, 1423, 1437, 1445, 1472, 1485, 1586, 1589, 1634, 1637, 1639, 1643, 1649, 1674, 1842, 1849–1852, 1947, 1966, 1975, 1981, 2002, 2003, 2060, 2063, 2079, 2088, 2091, 2133, 2134a, 2142, 2270, 2310, 2313a, 2520, 2543, 2545, 2570, 2589, 2634, 2644, 2645, 2731, 2735, 2765, 2767, 2777, 2782, 2799a, 2800, 2804, 2822, 2857, 2870, 2939, 2942, 3007, 3059, 3105, 3106, 3190, 3254, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3373, 3418, 3464–3470, 3482, 3493, 3498, 3500, 3508, 3530, 3557, 3692, 3794, 3797, 3876, 3897, 3939, 3992, 4005–4007, 4052, 4056, 4078, 4104, 4135, 4162, 4166, 4249, 4257, 4259, 4290, 4319, 4360, 4570a, 5012, 5025, 5034, 5049, 5512, 5547, 5554, 5692a, 5770, 5811b, 5836, 5869a, 4A02	568b, 984, 1590a, 2339a, 2917a, 3186, 3188, 4249, 5811b	1354, 1375a, 1377, 1378, 2244, 3401, 3402, 4052, 4056
61.	100-42-5	Benzene, ethenyl- {styrene} C_6H_5–CH═CH_2	73, 104, 111, 112, 141–143, 151, 156, 157, 174a, 174b, 174c, 174e, 299, 314, 315, 566, 568, 568b, 688, 798, 1063–1066, 1068–1074, 1139, 1140, 1153, 1154, 1168, 1217, 1262a, 1313, 1339, 1348–1350, 1354, 1365, 1374, 1375a, 1386, 1414, 1416, 1418, 1419, 1443, 1445, 1472, 1586, 1589, 1634, 1637, 1649, 1740, 1741, 1743, 1744, 1842, 1870, 1871, 1873, 1947, 1975, 1981, 2142, 2313a, 2543, 2570, 2765, 2767, 2777, 2799a, 2825, 2870, 3007, 3190, 3255, 3257, 3265, 3300, 3308, 3464, 3468, 3470, 3498, 3508, 3530, 3557, 3711, 3713, 3714, 3729, 3797, 3992, 4078, 4166, 4249, 4570a, 4998, 5012, 5034, 5049, 5512, 5554, 5770, 5811b, 5835, 5836, 5869a	568b, 984, 1983, 2260, 2339a, 2389, 2544, 2917a, 4249, 5811b	1354, 1375a, 3401
Miscellaneous organic compounds					
62.	60-35-5	Acetamide CH_3-CO-NH_2	167, 172, 568b, 1099, 1350, 1354, 1360, 1371, 1375, 1375a, 1375b, 1586, 1590, 1741, 1743, 1744, 1870, 1871, 1965, 1968, 2387, 2543, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 3190, 3255, 3265, 3300, 3386, 3397, 3410, 3491, 3553, 3557, 3559, 3714, 3992, 4228, 4249, 5512, 5811b, 5869a	568b, 2471, 4249	1354, 1360, 1375a, 2387
63.	107-13-1	2-Propenenitrile {acrylonitrile} H_2C═CH–CN	73, 126a, 174b, 299, 314, 402, 566–568, 603, 688, 1140, 1148, 1217, 1262a, 1365, 1373, 1374, 1375a, 1377, 1386, 1413, 1416, 1422, 1445, 1634, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 2270, 2313a, 2520, 2545, 2634, 2645, 2724, 2767, 2781, 2782, 2804, 2825, 2857, 3007, 3190, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3491, 3530, 3557, 3692, 3714, 3882, 3897, 3992, 4005–4007, 4078, 4166, 4249, 4319, 4332, 4360, 4998, 5049, 5512, 5547, 5554, 5692a, 5770, 5811b, 5836, 5869a		1375a, 1377, 4249

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

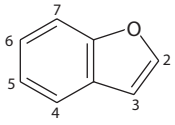
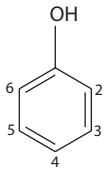
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
64.	79-06-1	2-Propenamide {acrylamide} $H_2C{=}CH\text{-}CONH_2$	568b, 1360, 1371, 1375, 1375a, 1375b, 1586, 1740, 1741, 1743, 1744, 2570, 2767, 3051, 3190, 3265, 3300, 3410, 3441a, 3553, 3557, 3713, 3992, 4228, 4249, 5032, 5070, 5512, 5811b, 5869a	568b, 4249, 5032, 5493	1360, 1375a
65.	57-14-7	Hydrazine, 1,1-dimethyl-	126a, 568b, 967, 1148, 1217, 1373, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 2825, 3255, 3257, 3265, 3300, 4249, 5512, 5869a	568b, 3480, 3481, 3491, 3974b, 4249	
66.	75-52-5	Methane, nitro- {nitromethane} $H_3C\text{-}NO_2$	112, 172, 480, 1663a, 1667, 1743, 1744, 1755, 1756, 1884, 2724, 3081, 3082, 3086, 3265, 3300, 3491, 3493, 4249, 4342, 5512		
67.	79-46-9	Propane, 2-nitro- {2-nitropropane} $(H_3C)_2{=}CH\text{-}NO_2$	126a, 239, 566, 567, 568b, 1148, 1217, 1373, 1727, 1740, 1741, 1743, 1744, 1755, 1773, 1781, 1808, 1842, 1870, 1871, 1884, 2329, 2724, 2799a, 2825, 2977, 3086, 3265, 3300, 3491, 3714, 4009–4011, 4249, 5512, 5811b, 5869a		
68.	98-95-3	Benzene, nitro- {nitrobenzene}	480, 1428, 1580, 1741, 1743, 1744, 1758, 1884, 2329, 3081, 3082, 3265, 3300, 3493, 3714, 4010, 4011, 4249, 5512		
69.	75-01-4	Ethene, chloro- {vinyl chloride} $H_2C{=}CH\text{-}Cl$	203, 239, 603, 1037b, 1148, 1217, 1325, 1373, 1437, 1673, 1706, 1727, 1740, 1741, 1743, 1744, 1752, 1773, 1781, 1808, 1842, 1870, 1871, 2825, 3255, 3257, 3260, 3265, 3300, 3370, 3711, 4010, 4011, 4227, 4249, 4998, 5512, 5811b, 5869a		
70.	51-79-6	Carbamic acid, ethyl ester {ethyl carbamate; urethane} $H_2N\text{-}COO\text{-}C_2H_5$	126a, 239, 757, 1148, 1217, 1557, 1727, 1740, 1741, 1743, 1744, 1773, 1808, 1842, 1870, 1871, 2825, 3255, 3257, 3265, 3300, 3483, 3714, 4005–4007, 4010, 4011, 4249, 5512, 5811b, 5869a	757, 3483, 3973, 3974b, 4249, 5524	
71.	75-21-8	Oxirane {ethylene oxide}	126a, 333, 1037b, 1325, 1740, 1741, 1743, 1744, 3265, 3300, 3714, 3882, 4249, 4612, 4998, 5508, 5512, 5836, 5811b, 5869a		
72.	75-56-9	Oxirane, methyl- {propylene oxide}	126a, 968, 1037b, 1325, 1743, 1744, 2009, 2825, 3265, 3300, 4998, 5512, 5869a		
73.	117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester i(2-ethylhexyl) {phthalate}	1375, 1375b, 1586, 1741, 2761, 2762, 2765–2767, 2777, 2807, 3300, 3302, 3553, 3557, 4249, 4570a, 5809a, 5811b, 5869a	2339a, 2389, 2544, 2917a, 3547, 3973, 3974a, 4249, 5811b	
74.	110-00-9	Furan 	112, 199, 199, 299, 480, 568b, 605, 639, 722, 1063–1074, 1140, 1284, 1348–1352, 1374, 1375a, 1377, 1378, 1412–1414, 1416, 1418, 1419, 1449, 1586, 1589, 1634, 1740, 1741, 1743, 1744, 1842, 1875, 2002, 2003, 2063, 2079, 2270, 2293, 2310, 2313a, 2337, 2508, 2520, 2543, 2570, 2634, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2939, 2940, 2942, 2946, 3059, 3105, 3132, 3193, 3251, 3260, 3265, 3300, 3302, 3308, 3557, 3583, 3584, 3714, 3797, 3901, 4052, 4056, 4162, 4249, 4257, 4290, 4319, 5034, 5508, 5512, 5770, 5811b	5811b	1228, 1375a, 1377, 1378, 2244, 3401, 4052, 4056
75.	271-89-6	Benzofuran {benzo[*b*]furan; coumarone} 	174e, 299, 568b, 1313, 1427, 1444, 1649, 1740, 1741, 1743, 1744, 1842, 2570, 2731, 2735, 2742, 2799a, 3193, 3255, 3265, 3300, 3410, 3714, 4249, 5034, 5512, 5811b	5811b	3401

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

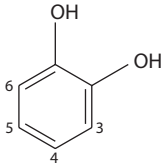
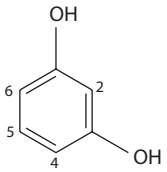
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Phenols					
76.	108-95-2	Phenol 	37, 38, 50, 83, 100, 126a, 126b, 155, 157, 167, 172, 173a, 174a, 174b, 174c, 174e, 213, 237, 239, 248, 269, 270, 274–277, 293, 295, 337, 351, 359, 392, 396, 397, 402, 414, 520, 521, 532, 539, 568b, 603, 615, 616, 636, 640, 663, 664, 688, 722, 723, 765, 789, 789a, 804, 828, 830a, 851, 859, 884, 891a, 912, 922c, 1051, 1063–1074, 1091, 1099, 1115, 1129, 1132, 1138, 1140, 1153, 1158, 1213, 1215, 1232, 1236, 1283, 1284, 1292, 1303, 1329, 1330, 1332, 1333, 1336, 1339, 1348–1350, 1354, 1360, 1361,1364, 1365, 1369, 1371, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1423, 1426, 1427, 1437, 1442, 1445, 1449, 1450, 1492, 1494, 1502, 1589, 1647, 1648, 1649, 1673, 1674, 1699, 1709, 1741, 1751, 1760, 1764, 1766, 1789, 1791, 1797, 1803, 1807a, 1827, 1842, 1857, 1879, 1881, 1882 1884, 1906, 1928, 1966, 1981, 1995, 1999, 2042–2045, 2062, 2079, 2082–2086, 2088, 2089, 2114, 2125, 2133, 2142, 2170, 2190, 2191, 2195, 2230, 2245, 2253, 2254, 2261, 2262a, 2270, 2274, 2295, 2306, 2307, 2311, 2312, 2313a, 2327c, 2351, 2374, 2376–2378, 2379a, 2387, 2397, 2399, 2400d, 2408, 2476, 2480, 2493, 2506, 2507, 2508, 2526, 2543, 2545, 2570, 2577, 2578, 2582, 2583, 2598, 2601a, 2605, 2681, 2683, 2691–2695, 2719, 2731, 2735, 2737, 2739, 2740, 2747, 2761, 2762, 2775, 2777, 2799a, 2800, 2820, 2857, 2858, 2876, 2899, 2927, 2939, 2983, 3007, 3043, 3059, 3–65, 3087, 3088, 3090, 3093, 3095, 3105, 3111, 3121a, 3131, 3132, 3165, 3166, 3171–3175, 3187, 3190, 3228, 3251, 3255, 3257, 3263–3265, 3277, 3286, 3291, 3300, 3302, 3305, 3306, 3308, 3314, 3370, 3373, 3394, 3397, 3410, 3447, 3451–3453, 3454, 3457, 3462, 3468, 3470, 3476, 3482, 3486, 3488, 3493, 3497, 3500, 3551, 3553, 3555, 3557, 3559, 3572, 3576, 3577, 3616, 3625, 3650, 3671, 3712, 3716–3720, 3746, 3747, 3764, 3765, 3767, 3795, 3797, 3800, 3826, 3844, 3884, 3892, 3912a,3939, 3952, 3984, 3990a, 3992, 4005–4007, 4009, 4036, 4064, 4065, 4067, 4113, 4118, 4121, 4122, 4159, 4228, 4232, 4248, 4249, 4259, 4268, 4269a, 4290, 4301, 4304, 4311, 4314, 4317, 4319, 4322, 4328–4330, 4338, 4349, 4350, 4407, 4418, 4636, 4796, 4965, 5011, 5031, 5034, 5079, 5093, 5140, 5207, 5500, 5512, 5531, 5532, 5546, 5555, 5564, 5576, 5588, 5643a, 5811b, 5835, 5836, 5869a	100, 120, 404, 568b, 937, 984, 1085, 1590a, 1825, 1876, 1877a, 1980, 2014, 2338, 2339a, 2379a, 2386, 2389, 2544, 2607, 2862, 2917a, 2939, 3090, 3194, 3350, 3430, 3547, 3549, 3973, 3974a, 4064, 4202, 4249, 5079, 5093, 5811b	50, 1330, 1332, 1354, 1360, 1375a, 1377, 1378, 2387, 2506, 2507, 3395, 3401, 3402, 3405

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
77.	95-48-7	Phenol, 2-methyl- {*o*-cresol}	50, 155, 172, 174a, 174b, 174c, 174e, 239, 274, 276, 277, 402, 414, 521, 532, 539, 568b, 603, 615, 616, 688, 722, 723, 765, 786, 787, 789, 789a, 830a, 851, 966, 1063–1066, 1068–1075, 1099, 1132, 1158, 1215, 1329, 1330, 1332, 1333, 1339, 1360, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1427, 1437, 1445, 1450, 1586, 1626, 1647, 1648, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1906, 1928, 1981, 1995, 2043, 2044, 2079, 2191, 2210, 2245, 2270, 2307, 2313a, 2387, 2526, 2543, 2545, 2557a, 2570, 2577, 2598, 2601a, 2628, 2629, 2636, 2681, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2820, 2857, 2876, 2939, 3007, 3059, 3088, 3090, 3095, 3105, 3131, 3171–3175, 3190, 3251, 3255, 3263, 3264, 3277, 3300, 3302, 3370, 3394, 3397, 3410, 3447, 3452, 3453, 3476, 3486, 3488, 3493, 3553, 3557, 3559, 3616, 3671, 3712, 3716–3719, 3741, 3746, 3747, 3764, 3797, 3800, 3826, 3844, 3876, 3952, 3984, 3992, 4005–4007, 4228, 4249, 4259, 4268, 4313, 4317, 4319, 4350, 4354, 4407, 4414, 4796, 5011, 5034, 5079, 5093, 5500, 5532, 5564, 5576, 5588, 5643a, 5811b, 5836, 5869a	568b, 937, 1825, 1876, 1877a, 2338, 2389, 2544, 3547, 4249, 5093, 5811b	50, 1330, 1332, 1360, 1375a, 1377, 1378, 2210, 2387, 3395, 3401, 3402
78.	108-39-4	Phenol, 3-methyl- {*m*-cresol}	50, 155, 172, 174a, 174b, 174c, 174e, 239, 274, 276, 277, 293, 402, 414, 521, 532, 539, 568b, 603, 615, 616, 688, 723, 765, 786, 787, 789, 789a, 830a, 851, 966, 1051, 1063–1066, 1068–1075, 1099, 1132, 1158, 1329, 1330, 1332, 1333, 1339, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1427, 1437, 1445, 1450, 1586, 1626, 1647, 1648, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1906, 1928, 1981, 1995, 2043, 2079, 2191, 2203, 2245, 2270, 2307, 2313a, 2327c, 2387, 2493, 2526, 2543, 2545, 2557a, 2570, 2577, 2598, 2628, 2681, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2857, 2858, 2876, 2939, 3007, 3059, 3088, 3090, 3095, 3131, 3165, 3166, 3171–3175, 3190, 3255, 3263, 3264, 3300, 3302, 3370, 3394, 3397, 3410, 3447, 3452, 3453, 3476, 3486, 3488, 3493, 3557, 3559, 3616, 3671, 3712, 3716–3719, 3741, 3746, 3747, 3764, 3765, 3800, 3826, 3844, 3876, 3952, 3984, 3990a, 3992, 4005–4007, 4228, 4249, 4268, 4313, 4317, 4319, 4350, 4351, 4407, 4414, 4796, 5011, 5014, 5034, 5079, 5093, 5500, 5532, 5564, 5576, 5588, 5643a, 5811b, 5836, 5869a	120, 568b, 1825, 1876, 1877a, 2283, 2338, 2389, 2544, 2862, 2939, 3059, 3194, 3547, 3797, 3973, 3974a, 4249, 5079, 5093, 5811b	50, 1330, 1332, 1360, 1375a, 1377, 1378, 2387, 3395, 3401, 3402, 3405

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
79.	106-44-5	Phenol, 4-methyl- {*p*-cresol}	37, 38, 50, 155, 156, 157, 172, 174a, 174b, 174c, 174e, 239, 274, 276, 277, 293, 402, 414, 521, 532, 539, 568b, 603, 615, 616, 688, 723, 765, 786, 787, 789, 789a, 830a, 851, 966, 1051, 1063–1066, 1068–1075, 1099, 1158, 1231, 1232, 1329, 1330, 1332, 1333, 1339, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1386, 1388–1390, 1427, 1437, 1445, 1450, 1586, 1626, 1647, 1648, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1906, 1928, 1981, 1995, 2043, 2079, 2133, 2191, 2210, 2245, 2270, 2311, 2313a, 2327c, 2387, 2493, 2526, 2543, 2545, 2557a, 2570, 2577, 2601a, 2628, 2681, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2820, 2857, 2876, 2939, 3007, 3059, 3088, 3095, 3131, 3165, 3166, 3171–3175, 3190, 3251, 3255, 3263, 3264, 3277, 3286, 3300, 3302, 3305, 3370, 3394, 3397, 3410, 3447, 3452, 3453, 3476, 3486, 3488, 3493, 3553, 3557, 3559, 3616, 3671, 3712, 3716–3718, 3741, 3746, 3747, 3764, 3765, 3797, 3800, 3826, 3844, 3876, 3952, 3984, 3990a, 3992, 4005–4007, 4159, 4228, 4249, 4268, 4313, 4317, 4319, 4350, 4354, 4407, 4414, 4796, 5011, 5014, 5034, 5079, 5093, 5500, 5532, 5564, 5576, 5588, 5643a, 5811b, 5836, 5869a	404, 568b, 1085, 1825, 1876, 1877a, 2014, 2338, 2389, 2544, 2611, 2917a, 3430, 3547, 4249, 5093	50, 1330, 1332, 1360, 1375a, 2210, 2387, 3395, 3401, 3402, 3405
80.	120-80-9	1,2-Benzenediol {catechol; pyrocatechol} 	28, 30, 31, 100, 102, 126a, 126b, 172, 174b, 174c, 190, 237, 239, 396, 402, 414, 496, 497, 568b, 596, 598–603, 636, 688, 722, 723, 789, 789a, 830a, 859, 988a, 1051, 1089a, 1099, 1132, 1158, 1217, 1284, 1285, 1332, 1333, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1427, 1437, 1442, 1445, 1448a, 1450, 1562, 1582, 1586, 1626, 1673, 1674, 1741, 1743, 1744, 1749, 1751, 1781, 1798, 1808, 1810, 1842, 1870, 1871, 1879, 1882, 1883, 1884, 1887a, 1898, 1981, 2016, 2017, 2060, 2079, 2133, 2195, 2203, 2210, 2313a, 2379a, 2387, 2493, 2524a, 2527c, 2527d, 2527f, 2527g, 2545, 2570, 2594, 2598, 2601a, 2605, 2607, 2615, 2631, 2683, 2767, 2775, 2799a, 2892, 2939, 3007, 3131, 3165, 3166, 3171–3175, 3190, 3255, 3265, 3300, 3302, 3308, 3365, 3370, 3394, 3447, 3453, 3454, 3457, 3462, 3476, 3493, 3551, 3553, 3557, 3602, 3712, 3715–3719, 3737, 3741, 3743, 3746, 3747, 3753, 3754, 3797, 3844, 3879, 3891, 3952, 3992, 4005–4007, 4009–4011, 4113, 4120, 4121, 4123, 4159, 4248, 4249, 4268, 4277, 4319, 4386, 4407, 4414, 4702, 4796, 4965, 5011, 5034, 5049, 5079, 5243, 5500, 5512, 5532, 5564, 5571, 5576, 5643a, 5811b, 5835, 5836	100, 568b, 970, 1077b, 1102, 1825, 1877a, 2079, 2154, 2379a, 2939, 3430, 3705, 3797, 3973, 3974a, 3976, 4249, 5079, 5811b, 5856	1375a, 1377, 1378, 2210, 2387, 3395, 3402, 4249
81.	108-46-3	1,3-Benzenediol {resorcinol} 	100, 102, 174b, 174c, 174e, 396, 414, 497, 568b, 603, 688, 723, 789, 789a, 859, 1371, 1375, 1375b, 1386, 1626, 1853b, 1879, 1882, 1883, 2060, 2079, 2195, 2313a, 2379a, 2387, 2570, 2598, 2681, 2939, 3007, 3131, 3171–3175, 3190, 3300, 3302, 3308, 3370, 3394, 3457, 3474, 3557, 3712, 3716, 3717, 3753, 3797, 3992, 3999, 4005–4007, 4113, 4249, 4319, 4332, 4407, 4414, 4796, 5011, 5034, 5049, 5532, 5576, 5588, 5643a, 5811b, 5835, 5836	100, 568b, 2379a, 4249, 5811b	2387, 3395, 3402

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

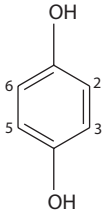
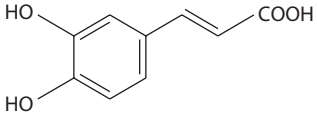
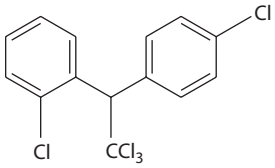
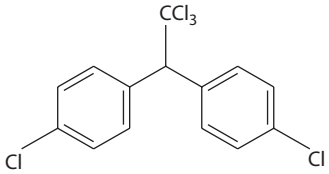
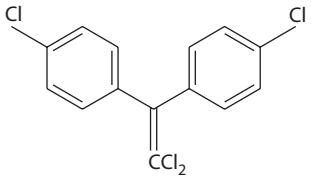
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
82.	123-31-9	1,4-Benzenediol {hydroquinone} 	100–102, 126a, 126b, 172, 173a, 174b, 174c, 190, 237, 239, 329, 392, 396, 402, 414, 497, 568b, 603, 663, 688, 723, 777, 778, 787, 788, 830a, 859, 1051, 1063–1066, 1068–1074, 1089a, 1099, 1158, 1235, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1386, 1437, 1445, 1582, 1586, 1626, 1674, 1751, 1879, 1882, 1884, 1887a, 1898, 2060, 2079, 2133, 2313a, 2327c, 2379a, 2387, 2493, 2524a, 2545, 2570, 2598, 2601a, 2615, 2681, 2691–2695, 2761, 2762, 2765–2767, 2775, 2777, 2799a, 2857, 2939, 3007, 3059, 3131, 3171–3175, 3190, 3255, 3300, 3302, 3308, 3370, 3394, 3453, 3454, 3457, 3474, 3553, 3557, 3602, 3712, 3716, 3717, 3737, 3741, 3743, 3753, 3797, 3844, 3891, 3992, 3999, 4005–4007, 4113, 4137, 4159, 4249, 4277, 4319, 4332, 4407, 4414, 4796, 5011, 5034, 5049, 5079, 5532, 5555, 5571, 5576, 5811b, 5643a, 5835, 5836	100, 120, 568b, 739, 1077b, 1877a, 2379a, 3430, 3973, 4249, 4566, 4910, 5079, 5440, 5811b	1360, 1375a, 1377, 1378, 2387, 3395, 3402
83.	93-15-2	Phenol, 2-methoxy-methyl-4-(2-propenyl)- {methyleugenol}	568b, 1741, 1743, 1744, 3265, 3300, 5512, 5537	5515	
84.	331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid} 	1626, 1743, 1744, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3300, 3308, 3712, 3714, 3797, 4036, 4113, 4163, 4249, 4376, 5079, 5389, 5512, 5811b, 4A01	72, 120, 722, 835, 890, 1102, 1626, 1981, 2154, 2216, 2270, 2514, 2939, 2954, 3029, 3103, 3161, 3462, 3476, 3655b, 3660, 3700, 3748, 3749, 3751, 3973, 3974a, 4249, 4999, 5079, 5126, 5385, 5389, 5591, 5652, 5672. 5673, 5705, 5713, 5722, 5809, 5810, 5811b, 5830, 5831, 5900, 5908, 4A01	

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
Chloroaromatic compounds					
85.	789-02-6	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl) ethyl]- {*o,p′*-DDT} 	517, 518, 758, 759, 1000, 1006, 1333, 1373, 1756, 1767, 1767a, 1781, 2697, 3257, 3493, 3685, 4005–4007, 4249, 4342, 5811b, 5869a, 21A19	517, 518, 644, 722, 758, 759, 1000, 1006, 1029, 1030, 1219, 1219a, 1219b, 1333, 1460, 1740, 1767, 2697, 3138, 3633, 3637, 3767a, 3770, 3915, 3977, 3973, 3977, 3984, 4249, 4271a, 5079, 5439, 5811b, 21A19	
86.	50-29-3	Benzene, 1,1′-(2,2,2-trichloroethylidene) bis[4-chloro-] {*p,p′*-DDT} 	517, 518, 707–709, 711, 712, 714, 758, 759, 1333, 1373, 1740, 1741, 1743, 1744, 1756, 1767, 1767a, 1781, 1884, 2697, 2825, 3257, 3265, 3300, 3493, 3634, 3685, 4249, 4342, 5512, 5811b, 5869a	517, 518, 644, 707–709, 711–714, 758, 759, 1028–1030, 1219, 1219a, 1333, 1460, 1756, 1767, 2318, 2697, 3138, 3188a, 3633, 3634, 3637, 3681, 3767a, 3770, 3915, 3973, 3974b, 3977, 4249, 4271a, 5079, 5439, 5811b	
87.	72-55-9	Benzene, 1,1′-(dichloroethenylidene) bis[4-chloro-] {*p,p′*-DDE} 	518, 707, 708, 713, 714, 758, 759, 1000, 1006, 1375, 1375b, 1740, 1741, 1743, 1744, 1767, 1781, 2697, 2767, 3265, 3300, 3557, 4005–4007, 4249, 5512, 5811b	518, 644, 708, 722, 758, 759, 1000, 1006, 1029, 1030, 1219, 1219a, 1460, 1740, 2389, 2544, 2697, 3188a, 3633, 3637, 3770, 3915, 3974b, 4249, 4271a, 5811b	72-55-9
88.		Dibenzo[*b,e*][1,4]dioxin, polychloro- {polychlorodibenzo-*p*-dioxins}	854, 4249		
89.		Dibenzofuran, polychloro- {polychlorodibenzofurans; dioxins}	177, 854, 1217, 2490, 2491,3265, 3300, 3715, 4249		

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
Inorganic components					
90.	302-01-2	Hydrazine	126, 126a, 126b, 172, 237, 239, 427, 1148, 1217, 1373, 1437, 1445, 1507, 1557, 1571a, 1580, 1674, 1706, 1727, 1740, 1741, 1743, 1744, 1761, 1773, 1781, 1808, 1870, 1871, 2133, 2384, 2385, 2825, 3255, 3257, 3260, 3265, 3300, 3491, 3493, 3714, 3811a, 4010, 4011, 4249, 5512, 5811b, 5869a	1571a, 1580, 1581, 2385, 3481, 3491, 3493, 3811a, 3973, 3974b, 4249	
91.	7440-38-2	Arsenic	47, 50, 126a, 159, 174b, 174c, 273, 373, 516, 603, 688, 769, 889, 889a, 933, 1026, 1148, 1163, 1217, 889, 1273, 1373, 1386, 1395, 1430, 1439, 1445, 1557, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1815–1817, 1842, 1845,1870, 1871, 2060, 2079, 2170, 2172, 2313a, 2468, 2524, 2609, 2667, 2799a, 2825, 2911, 2918, 2939, 2980, 3007, 3059, 3104, 3234, 3238, 3252, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3377, 3378, 3417, 3711, 3775, 3830, 3899, 3927, 3934, 4005–4007, 4009–4011, 4229, 4230, 4242, 4249, 4319, 4331, 4354, 5061, 5079, 5124, 5160, 5201, 5264, 5512, 5541, 5811b, 5869a	46, 47, 159, 174c, 373, 516, 769, 889, 889a, 1163, 1391, 1395, 1445, 1459, 1460, 1534, 1535 1815–1817, 2079, 2172, 2338, 2468, 2609, 2667, 2939, 2978–2980, 3059, 3104, 3138, 3234, 3238, 3377, 3416, 3417, 3699, 3775, 3797, 3834, 3973, 3974a, 3974b, 4070, 4071, 4249, 4273, 4357, 4381, 5018, 5053, 5061, 5079, 5119, 5120, 5139, 5142, 5160, 5189, 5264, 5281, 5283, 5284, 5322, 5338, 5438, 5541, 5600, 5648, 5684, 5729, 5811b, 5849	50
92.	7440-41-7	Beryllium	50, 641, 1217, 1445, 1741, 1743, 1744, 3265, 3300, 3711, 4229, 4230, 4243, 4249, 5512, 5811b, 5869a	3059, 3797, 3973, 3974a, 4243, 4249, 5001, 5811b	50

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
93.	7440-43-9	Cadmium	50, 126, 126a, 126b, 134–136, 172, 174b, 174c, 174e, 237, 239, 344, 461, 603, 623, 641, 688, 988a, 1125, 1126, 1148, 1185, 1217, 1227, 1273, 1329, 1373, 1386, 1437, 1445, 1454, 1557, 1673, 1674, 1727, 1740, 1743, 1744, 1773, 1781, 1842, 1870, 1871, 1896, 2012, 2133, 2134a, 2142, 2214, 2357, 2530, 2792, 2799a, 2825, 2929, 2933, 2953, 3007, 3135, 3136, 3255, 3257, 3265, 3300, 3370, 3376, 3378, 3441a, 3519, 3711, 3846, 3927, 4005–4007, 4009–4011, 4220, 4229, 4230, 4249, 4384, 4410a, 5512, 5541, 5811b, 5869a	54, 134, 174c, 250, 764, 1185, 1219, 1219a, 1219b, 1219c, 1227, 1329, 1330, 1445, 1454, 1896, 2313a, 2530, 2680, 2792, 2929, 2933, 3519, 3846, 3973, 3974b, 4074, 4220, 4249, 4357, 4384, 4721, 4816, 5018, 5051, 5053, 5079, 5094, 5514, 5531, 5541, 5811b, 20A26	50
94.	7440-47-3	Chromium vi	50, 126a, 174b, 174c, 273, 603, 688, 746b, 769, 966, 1148, 1217, 1273, 1329, 1373, 1386, 1445, 1557, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 2214, 2270, 2667, 2799a, 2825, 2939, 3007, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3377, 3378, 3711, 3876, 4005–4007, 4230, 4242, 4249, 4331, 5512, 5541, 5811b, 5869a	174c, 769, 1219, 1219a, 1219b, 1329, 1330, 1445, 1951, 2079, 2270, 2313a, 2338, 2667, 2939, 3377, 3797, 3973, 3974a, 3974b, 4249, 4381, 4816, 5018, 5053, 5079, 5094, 5514, 5541, 5811b, 20A26	50
95.	7440-48-4	Cobalt	50, 273, 1445, 1673, 1741, 1743, 1744, 1870, 1871, 1933, 1934, 2667, 2792, 2799a, 3265, 3300, 3302, 3377, 3714, 3785, 3786, 4005–4007, 4229, 4230, 4249, 5512, 5541, 5811b, 5869a	1933, 1934, 2667, 2792, 3377, 3785, 3786, 3797, 3973, 3974a, 3974b, 4249, 4357, 4381, 5079, 5308, 5309, 5541, 5811b, 20A26	50

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
96.	7439-92-1	Lead	50, 160, 174b, 174c, 174e, 273, 603, 623, 688, 769, 1217, 1227, 1273, 1329, 1386, 1445, 1673, 1727, 1740, 1741, 1743, 1744, 1773, 1842, 1870, 1871, 1896, 2079, 2214, 2270, 2354, 2460, 2466, 2792, 2799a, 2825, 2901, 2929, 2939, 3007, 3255, 3257, 3265, 3300, 3302, 3308, 3370, 3376, 3442, 3714, 3846, 4005–4007, 4134, 4220, 4229, 4230, 4242, 4249, 4319, 4410a, 5079, 5512, 5541, 5811b, 5869a	174c, 250, 769, 1219, 1227, 1445, 1896, 2079, 2270, 2313a, 2338, 2460, 2792, 2929, 3138, 3442, 3797, 3846, 3973, 3974a, 3974b, 4046, 4220, 4249, 4357, 4816, 5018, 5053, 5079, 5094, 5514, 5541, 5811b, 5883	50, 641, 4249
97.	7439-97-6	Mercury	50, 174b, 174c, 344, 623, 641, 672, 688, 1329, 1386, 1741, 2214, 2517b, 2799a, 3005, 3006, 3007, 3300, 4005–4007, 4249, 5054, 5811b, 5869a	174c, 1219, 2667, 3797, 3973, 3974a, 3974b, 4249, 4357, 4381, 5018, 5079, 5094, 5241, 5811b, 20A26	50, 641, 4249
98.	7440-02-0	Nickel	50, 126, 126a, 126b, 160, 172, 174b, 174c, 237, 239, 273, 344, 603, 623, 641, 688, 769, 918, 966, 1125, 1217, 1262, 1273, 1329, 1386, 1437, 1445, 1454, 1515, 1557, 1673, 1674, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1842, 1870, 1871, 2133, 2134a, 2142, 2214, 2270, 2460, 2468, 2530, 2792, 2799a, 2825, 2886, 2929, 2939, 3007, 3255, 3257, 3265, 3300, 3308, 3370, 3378, 3711, 3714, 3775, 3785, 3786, 3837, 3838, 3846, 4005–4007, 4009–4011, 4220, 4229, 4230, 4246, 4249, 4319, 5079, 5512, 5541, 5629, 5811b, 5869a	174c, 250, 769, 918, 1125, 1219, 1445, 2270, 2313a, 2338, 2460, 2468, 2530, 2792, 2929, 2939, 3775, 3785, 3786, 3797, 3846, 3973, 3974a, 3974b, 4220, 4249, 5018, 5053, 5079, 5094, 5232, 5308, 5379, 5514, 5541, 5811b, 5883, 20A26	50, 641, 4249

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
99.	13981-52-7	Polonium, isotope of mass 210 ^{210}Po	126, 126a, 126b, 237, 264, 374, 1130, 1148, 1160, 1177, 1179, 1180, 1445, 1509, 1557, 1571a, 1674, 1722, 1727, 1740, 1741, 1743, 1744, 1773, 1781, 1808, 1823, 1842, 1864, 1870, 1871, 2069, 2158, 2396, 2468, 2536, 2663b, 2799a, 2813–2815, 2998, 3002, 3066–3070, 3255, 3257, 3265, 3300, 3302, 3308, 3408, 3442, 3680, 3981–3983, 4002, 4005, 4044, 4010, 4011, 4249, 4319, 4332, 4342, 5512, 5811b, 5869a	264, 265, 374, 1130, 1160, 1179, 1180, 1387, 1509, 2158, 2468, 2536, 2663b, 2815, 3002, 3005, 3066–3070, 3442, 3797, 3969, 3973, 3974a, 3974b, 3981–3983, 4044, 4249, 4383, 5053, 5066, 5617, 5683, 5733, 5811b, 20A115	
100.	7782-49-2	Selenium	50, 174b, 174c, 273, 641, 688,724, 1273, 1386, 1445, 1455, 1456, 1842, 2468, 2667, 2799a, 3007, 3257, 3265, 3300, 3685, 3775, 4005–4007, 4230, 4249, 5541, 5811b, 5869a	174c, 374, 721, 724, 1445, 1455, 1456, 2468, 2667, 3707, 3775, 3797, 3895, 3973, 3974a, 4249, 5018, 5053, 5079, 5094, 5274, 5541, 5811b	50, 641, 4249
Additional components					
101.	630-08-0	Carbon monoxide	28, 30, 31, 82, 83, 90, 123a, 126, 126a, 126b, 130, 162–170, 172, 173, 173a, 174, 174a, 174b, 174c, 199, 217, 220, 221, 238, 239, 251, 288, 335, 337, 354, 357a, 375, 376, 383, 386, 401, 403, 421, 445, 447, 469a, 474, 480, 488, 489, 491, 492, 499, 534, 544–546, 603, 621, 636, 686, 688, 722, 781, 855, 886, 893, 916, 918a, 920, 929a, 957, 966, 988a, 1007, 1048a, 1051, 1063–1074, 1089, 1099, 1119, 1140, 1166, 1167, 1202, 1205, 1208, 1243, 1263, 1276, 1292, 1284, 1306, 1329, 1330, 1332–1334, 1331, 1343, 1344, 1348–1350, 1354, 1361, 1373–1375, 1375a, 1377, 1378, 1352, 1386, 1388–1390, 1419, 1420, 1435, 1437, 1442, 1443, 1445, 1466–1468, 1476–1478, 1492, 1493a, 1503, 1504, 1506, 1541, 1586, 1589, 1605, 1629, 1639, 1664, 1668, 1673, 1674, 1692, 1693, 1695, 1699, 1709, 1719, 1741, 1760, 1803, 1807a, 1830, 1842, 1847, 1855, 1920, 1921, 1924, 1931, 1932, 1935–1937, 1956, 1963, 1966, 1976, 1977, 1986a, 1989, 2012, 2029, 2030, 2055, 2059, 2060, 2062, 2066, 2068, 2079, 2117, 2123, 2124, 2133, 2134a, 2142, 2159, 2170, 2183, 2196, 2203, 2213, 2252, 2265, 2270, 2293, 2310, 2323, 2326, 2330, 2326, 2342a, 2343, 2344, 2347, 2348, 2358, 2359, 2400c, 2400d, 2419, 2445a, 2457, 2518,	4249, 4796, 5811b	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 4052, 4056

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Carbon monoxide (cont.)	2524, 2537, 2540, 2543, 2545, 2548, 2549, 2555, 2570, 2571,2582, 2624, 2626, 2634, 2659, 2662, 2683, 2690, 2761, 2762, 2777, 2780, 2782, 2785, 2798, 2799a, 2800, 2804, 2866, 2867, 2878, 2878a, 2913, 2928, 2929, 2920–2922, 2927, 2928, 2939, 2942, 2965, 2970, 2973, 3007, 3059, 3087, 3088, 3102, 3110, 3112–3120, 3132, 3135–3137, 3139, 3140, 3142, 3143, 3148a, 3190, 3254, 3255, 3257, 3300, 3302, 3308, 3317, 3324, 3336, 3370, 3378, 3407, 3412, 3441a, 3482, 3493, 3516, 3522, 3548, 3557, 3564, 3640, 3722, 3729, 3795, 3844, 3845, 3860, 3870, 3876, 3880–3883, 3898, 3907, 3909, 3910, 3917a, 3929, 3939, 3952, 3973, 3987, 3992, 4009–4011, 4052, 4055, 4056, 4064, 4065, 4067, 4078a, 4079, 4105, 4120, 4121, 4137, 4143, 4145, 4162, 4212, 4215, 4249, 4251, 4285, 4319, 4330, 4332, 4342, 4364–4366, 4391, 4398, 4406, 4418, 4581, 4745, 4980, 5006, 5030, 5042, 5045, 5047, 5065, 5071, 5079, 5124, 5140, 5154, 5189, 5207, 5219, 5263, 5313, 5359, 5411, 5483, 5484, 5512, 5532, 5546, 5558, 5575, 5643a, 5679, 5811b, 5835, 5836, 5869a, 19A02, 19A05		
102.	7664-41-7	Ammonia NH_3	30, 31, 50, 126b, 129, 167, 172, 173a, 174a, 174b, 174c, 195, 197, 198, 213, 237, 239, 364, 365, 375, 376, 402, 407, 408, 424, 472, 473, 475, 480, 491, 688, 827, 916, 985–987, 989, 1051, 1063–1066, 1068–1075, 1091, 1099, 1100, 1128b, 1137, 1140, 1222, 1245, 1263, 1277, 1293, 1335, 1348–1351, 1354, 1369, 1375a, 1386, 1388–1390, 1437, 1442, 1445, 1469, 1489, 1492, 1522, 1524, 1531, 1532, 1539, 1580, 1589, 1673, 1674, 1709, 1741, 1808, 1841, 1842, 1853b, 1884, 1902, 1911, 1966, 2079, 2083–2085, 2133, 2134a, 2142, 2161, 2170, 2217, 2224, 2263, 2267, 2270, 2326, 2330, 2338, 2342, 2342a, 2343, 2368, 2480, 2524, 2529, 2541, 2543, 2545, 2607, 2627, 2688, 2691–2695, 2724, 2761, 2762, 2775, 2777, 2781, 2782, 2804, 2858, 2919, 2927, 2928, 2934, 2936, 2937, 2939, 2973, 2986–2988, 3007, 3022, 3029, 3059, 3140, 3187, 3190, 3213, 3214, 3251, 3254, 3255, 3257, 3266, 3300, 3302, 3306, 3308, 3324, 3369, 3385, 3482, 3491, 3493, 3583, 3584, 3623, 3659, 3693, 3695, 3797, 3844, 3909, 3910, 3934, 3955, 3956, 3973, 3992, 4005–4007, 4009–4011, 4041, 4052, 4056, 4060–4062, 4064, 4065, 4136, 4226, 4245, 4249, 4301, 4319, 4332, 4406, 4636, 4686, 4743, 5042, 5049, 5082, 5079, 5099, 5100, 5129, 5189, 5263, 5359, 5382, 5389,, 5512, 5546, 5811b, 5836, 5869a, 19A02	129, 174b, 212, 385, 555, 622, 677b, 826a, 856, 927, 989, 1053, 1063–1066, 1068–1074, 1128b, 1189, 1222, 1244, 1263, 1329, 1330, 1332, 1333, 1335, 1351, 1369, 1493, 1527, 1835b, 1941, 2079, 2313a, 2330, 2337, 2338, 2339b, 2356, 2381, 2394a, 2453, 2529, 2543, 2545, 2607, 2746, 2761, 2762, 2765, 2766, 2787, 2914, 2919, 2939, 2987, 3022, 3214, 3254, 3261, 3266, 3385, 3420, 3491, 3499, 3693,	50, 1354, 1375a, 4052, 4056

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Ammonia (cont.)		3707, 3780, 3797, 3974a, 3974b, 4244, 4249, 4837a, 5018, 5079, 5126, 5165, 5186, 5189, 5194, 5298, 5382, 5389, 5396, 5669, 5712, 5803, 5811b, 5872, 5907, 17B40	
103.	10102-43-9	Nitrogen oxide (NO) {nitric oxide}	21, 28, 199, 172, 173a, 189, 239, 386, 387, 401, 480, 499, 574, 603, 688, 753, 815, 816, 845, 855, 887, 960b, 988a, 1051, 1063–1074, 1089, 1140, 1331, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1465, 1602, 1634, 1693, 1741, 1833, 1834, 1859, 1929, 1930, 1952, 1955, 1956, 1963, 2062, 2079, 2083–2085, 2122, 2133, 2134a, 2142, 2159, 2270, 2293, 2297, 2310, 2360, 2545, 2557a, 2634, 2690, 2724, 2738, 2782, 2800, 2801, 2803, 2804, 2806, 2878a, 2919, 2927, 2939, 3007, 3116, 3132, 3135–3137, 3139, 3149, 3255, 3300, 3302, 3308, 3370, 3441, 3491, 3557, 3587, 3655, 3671, 3691, 3694, 3720, 3818, 3862, 3907, 3952, 3973, 3993, 3997, 4005–4007, 4052, 4056, 4162, 4219, 4249, 4250, 4252, 4319, 4332, 4365, 5008, 5034, 5042, 5590, 5811b, 5836	1175a, 4249	642, 1375a, 1377, 1378, 3192, 4052, 4056, 4249
104.		Nitrogen oxides (N_2O + NO + NO_2) {NO_x}	82, 83, 126a, 126b, 174a, 174b, 237, 379, 386, 402, 499, 688, 804, 815, 816, 887, 960b, 1067, 1099, 1100, 1292, 1329, 1330, 1332–1334, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1388–1390, 1420, 1442, 1445, 1465, 1492, 1497, 1528, 1580, 1589, 1673, 1674, 1741, 1807a, 1842, 1955, 2036, 2051, 2293, 2313a, 2373, 2537, 2543, 2570, 2625, 2627, 2691–2695, 2733, 2736, 2761, 2762, 2775, 2777, 2782, 2803, 2804, 3190, 3251, 3254, 3255, 3308, 3388, 3441, 3587, 3694, 3844, 3848, 3880, 3939, 3952, 3992, 4010, 4011, 4232, 4249, 4301, 4319, 4332, 4342, 4581, 4980, 5512, 5569, 5590, 5836, 19A02, 19A07	2700, 4249, 5053	1330, 1332, 1354, 1375a, 1377
105.	74-90-8	Hydrocyanic acid {hydrogen cyanide} HCN	80–83, 110, 112, 126b, 167, 172, 174a, 174b, 174c, 174e, 213, 237–239, 267, 269, 270, 314, 337, 402, 429a, 480, 491, 513, 577, 603, 631, 688, 722, 747, 748, 765, 779, 780, 804, 861, 916, 918a, 920, 966, 1051, 1063–1074, 1077a, 1091, 1092, 1099, 1119, 1140, 1202, 1235, 1276, 1283, 1284, 1292, 1329, 1330, 1332–1336, 1348–1350, 1354, 1374, 1375, 1375a, 1375b, 1377, 1331, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1442, 1445, 1466, 1467, 1469, 1492, 1497, 1498, 1589, 1668, 1673, 1674, 1693, 1695, 1719, 1741, 1746, 1751, 1760, 1781, 1803, 1807a, 1842, 1932, 1956, 1966, 1967, 2059, 2062, 2067, 2068,	2607, 3290, 3633, 4064, 4271a, 5079, 5189, 5811b	1330 (0), 1332 (0) 1354, 1375a, 1377, 1378, 2506, 2507, 4052, 4056, 4249

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

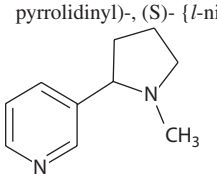
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Hydrocyanic acid {hydrogen cyanide} (cont.)	2079, 2083–2086, 2133, 2134a, 2142, 2157, 2159, 2170, 2252, 2270, 2293, 2310, 2313a, 2313c, 2313d, 2326, 2342, 2342a, 2343, 2344, 2502, 2506, 2507, 2537, 2543, 2545, 2570, 2607, 2608, 2628, 2634, 2679, 2683, 2724, 2761, 2762, 2775, 2777, 2780, 2782, 2799a, 2801, 2804, 2805, 2866, 2939, 2942, 2956, 2971, 2973, 3007, 3029, 3059, 3087, 3088, 3101, 3116, 3120, 3121, 3121a, 3132, 3135–3137, 3139, 3140, 3145, 3148, 3149, 3190, 3251, 3254, 3255, 3257, 3290, 3300–3302, 3306, 3308, 3370, 3482, 3491, 3493, 3524, 3525, 3530, 3557, 3690, 3724, 3729, 3844, 3872, 3876, 3880–3882, 3897, 3909–3911, 3917a, 3939, 3952, 3973, 3976, 3984, 3992, 3996, 4005–4007, 4010, 4011, 4052, 4053, 4056, 4063, 4064, 4109, 4143, 4162, 4202, 4249, 4259, 4260, 4301, 4319, 4342, 4360, 4365, 4398, 4418, 4502, 4743, 4745, 4816, 5042, 5079, 5140, 5189, 5208, 5219, 5263, 5512, 5531, 5546, 5547, 5554, 5587, 5811b, 5835, 5836, 5869a		
106.	54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} 	14, 29–31, 41–43, 50, 83, 85a, 86–89, 95, 96, 106, 107, 117, 119, 123, 126, 126a, 126b, 126c, 160, 171, 172, 173a, 174b, 174c, 175, 178, 187, 188, 196–198, 207, 209, 211, 218, 222–224, 237, 239, 270, 274–276, 282, 288, 292b, 293, 294, 302, 306, 308, 337–339, 352, 353, 355, 357a, 357b, 362–365, 375, 376, 378, 382, 388, 395, 409, 410, 413, 424, 427–429, 429e, 437, 438, 441, 442, 445, 446, 456, 462, 469a, 473, 480, 488, 489, 491, 492, 499, 521, 527, 559, 568b, 575, 576, 578, 590, 603, 636, 638, 677b, 678, 679, 681, 686, 688, 723, 761, 765, 767, 768, 804, 824, 830a, 849, 850, 852, 866, 887, 888, 916, 918a, 919, 921, 953, 959, 962, 966, 973, 975, 988a, 989, 998, 999, 1006a, 1007, 1011, 1016, 1022, 1031, 1051, 1063–1075, 1078, 1083, 1084, 1088, 1089a, 1097, 1099, 1100, 1107, 1112, 1118, 1128b, 1129, 1134, 1137, 1138, 1162, 1166–1170, 1177b, 1187, 1188, 1199, 1203, 1215, 1225, 1232, 1263, 1271, 1275, 1283, 1284, 1293, 1301, 1314, 1317–1319, 1320, 1323, 1329–1334, 1334a, 1336, 1338, 1339, 1341, 1348–1350, 1354, 1360–1363, 1366, 1368, 1371–1375, 1375a, 1375b, 1376, 1377, 1378, 1380, 1384–1386, 1388–1390, 1423, 1427, 1437, 1442–1445, 1449, 1450, 1464, 1466, 1469, 1483, 1484, 1491, 1492, 1497, 1502, 1519, 1523, 1536, 1542, 1546, 1567a, 1568, 1580, 1584, 1586, 1589, 1606, 1607, 1614, 1615, 1637, 1639, 1642, 1673, 1674, 1686, 1687, 1692, 1695, 1696, 1700, 1702, 1709, 1719, 1725, 1730, 1736, 1738, 1741, 1743, 1749, 1760, 1761, 1764, 1766, 1797, 1807a, 1810–1812, 1814, 1818, 1827, 1836, 1837, 1842, 1848, 1860a, 1878, 1882, 1887a, 1890, 1891, 1901, 1908, 1909, 1912, 1913, 1921, 1928, 1933, 1942, 1950, 1966, 1984–1996, 1989, 1990, 2006, 2007, 2012, 2055, 2061,2062, 2079, 2088, 2097, 2100, 2103, 2110, 2111, 2133, 2134a, 2142, 2144, 2146–2153, 2164, 2166, 2167, 2170, 2171, 2181, 2191, 2211, 2212, 2223, 2225–2229, 2231, 2247, 2254, 2261, 2263, 2267, 2269, 2270–2272, 2294, 2303, 2313, 2313b, 2324, 2327c, 2337, 2338, 2349,	29, 64, 69, 120, 174c, 207, 212, 256, 261, 262, 306, 308, 324, 337, 339, 374, 404, 410, 427–429, 429e, 468, 480, 499, 504, 506- 508, 515, 548–550, 555, 555a, 557, 559, 568b, 647, 654, 660, 667, 677b, 678, 679, 685, 687, 689, 722, 792, 830a, 856, 866, 867, 888, 910, 914, 915a, 915b, 959, 963, 984–986, 989, 995, 997, 998, 1003, 1004, 1007, 1015, 1020, 1033, 1035, 1036, 1063–1066, 1068–1074, 1086, 1088, 1090, 1101, 1107, 1113, 1114, 1118, 1176, 1189, 1193–1199, 1203, 1220–1226,	50 (0), 1330 (0), 1332 (0), 1354, 1360, 1375a (0), 1377 (0), 1378 (0), 2387, 2506 (0), 2507 (0)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	2353a, 2371, 2372, 2374–2378, 2400d, 2401, 2408, 2410, 2412, 2416, 2417, 2446, 2451, 2458, 2459, 2482, 2488, 2493, 2503, 2504, 2506, 2507, 2517, 2523, 2524, 2524a, 2528, 2535, 2543, 2545, 2546, 2549, 2557a, 2570, 2601a, 2603, 2606, 2610, 2612, 2613, 2622, 2628, 2632, 2635, 2652, 2653, 2658, 2668–2673, 2683, 2688, 2690–2695, 2696, 2717, 2719, 2724, 2737, 2739, 2740, 2744, 2761, 2762, 2767, 2774, 2777, 2792, 2793, 2799a, 2800, 2827–2829, 2831, 2832, 2835–2837, 2839, 2840, 2842–2845, 2848, 2857, 2863, 2869, 2874, 2877, 2878a, 2879, 2880, 2899, 2912, 2919, 2920, 2921, 2924–2927, 2936–2939, 2947, 2951, 2958, 2959, 2966, 2967a, 2969, 2970, 2973–2976, 2980, 2982, 2984–2986, 2998, 3008–3016, 3019, 3021, 3022, 3024, 3025, 3027- 3029, 3035, 3040, 3041, 3044, 3045, 3054, 3056, 3057, 3059, 3072b, 3078, 3087–3089, 3116, 3121a, 3133, 3137, 3139, 3140, 3142, 3143, 3148a, 3156, 3190, 3214, 3227, 3228, 3254, 3255, 3257, 3258, 3265, 3274, 3300, 3302, 3308, 3333, 3370, 3373, 3375, 3378, 3386, 3397, 3398, 3406, 3407, 3410, 3415, 3426, 3443–3446, 3457, 3461, 3454, 3477, 3482, 3491, 3493, 3499, 3505, 3516, 3517, 3521, 3548, 3553, 3557–3559, 3562, 3563, 3570–3572, 3576, 3577, 3585, 3623, 3640, 3658, 3659, 3662, 3670–3672, 3682, 3722, 3731, 3739–3742, 3782–3784, 3790, 3796, 3797, 3803, 3822, 3826, 3833, 3844, 3876, 3884, 3896, 3909, 3910, 3921, 3926, 3928, 3930, 3934, 3936–3939, 3942, 3943, 3952, 3955–3959, 3961, 3972, 3980, 3984, 3990, 3992, 3999, 4009–4011, 4016, 4017, 4039, 4045, 4064, 4065, 4072, 4075, 4076, 4078, 4082, 4103, 4116, 4119–4122, 4127, 4132, 4134, 4137, 4138, 4140–4143, 4162, 4167–4176, 4178–4183, 4189–4191, 4194, 4197, 4198, 4202–4207, 4210, 4211, 4213, 4240, 4248, 4249, 4259, 4264, 4267, 4268, 4273, 4275a, 4285, 4291, 4309, 4310, 4319, 4330, 4363, 4366, 4370, 4385, 4398, 4418, 4529, 4570a, 4636, 4745, 4921, 4994, 5000, 5008, 5013, 5017, 5034, 5035, 5041, 5045, 5047, 5052., 5065, 5068, 5069, 5071, 5079, 5082, 5084, 5099, 5100, 5104, 5112, 5118, 5124, 5129, 5130, 5140, 5159, 5163, 5175, 5166, 5179, 5183, 5189, 5207, 5210, 5211, 5219, 5225, 5226, 5236, 5258, 5259, 5263, 5325, 5343, 5346, 5351, 5390, 5401, 5412, 5414, 5427, 5431, 5443, 5452, 5458–5461, 5470–5472, 5473, 5475, 5476, 5480, 5489, 5507, 5508, 5512, 5520, 5529, 5531, 5532, 5544–5546, 5554, 5558, 5563, 5565, 5643a, 5679, 5706, 5770, 5811b, 5836, 25A84, 25A85	1276, 1324, 1327, 1329, 1330, 1332, 1333, 1361, 1384, 1385, 1388–1390, 1393, 1464, 1492, 1546, 1549, 1550, 1564, 1567a, 1568, 1575, 1577, 1580, 1584, 1606, 1608–1613, 1615, 1624, 1676, 1686, 1702, 1709, 1712, 1719, 1725, 1730, 1746, 1749, 1774, 1811, 1812, 1814, 1836, 1837, 1848, 1853b, 1860a, 1927, 1933a, 1962a, 1990, 2006, 2079, 2104–2111, 2118, 2139, 2146–2150, 2152, 2153, 2164, 2166, 2167, 2191, 2212, 2226, 2263, 2270, 2272, 2273, 2282, 2283, 2290, 2294, 2331a, 2332, 2334, 2337, 2338, 2339a, 2349, 2359, 2372, 2374, 2389, 2417, 2446, 2488, 2503, 2504, 2528, 2529, 2532, 2534, 2543–2545, 2557a, 2606, 2611, 2682,	

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke**	**Tobacco**	**Tobacco Substitute Smoke**
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)		2688, 2689, 2724, 2761, 2762, 2765, 2766, 2786, 2792, 2841, 2844, 2913, 2914, 2917a, 2919, 2920, 2921, 2924–2926, 2938, 2939, 2954 2979–2982, 2989, 3016, 3019, 3022, 3024, 3027, 3028, 3034, 3035, 3041, 3044, 3056, 3059, 3063, 3073, 3074, 3087, 3155, 3188, 3214, 3219, 3254, 3329, 3333, 3375, 3420, 3430, 3444, 3459, 3460, 3476, 3477, 3482, 3491, 3499, 3511, 3512, 3517, 3543, 3549, 3560, 3561, 3570, 3571, 3608a, 3614, 3633, 3634, 3670a, 3705, 3707, 3767a, 3797, 3816, 3905, 3925, 3926, 3928, 3942, 3943b, 3950, 3961, 3972–3974, 3974a, 3974b, 3976, 3980, 3983a, 3999, 4009–4011, 4016, 4017, 4043, 4045,4047, 4051, 4071,	

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)		4073, 4103, 4127, 4159, 4169–4173, 4189, 4207, 4210, 4213, 4218, 4236, 4249, 4266a, 4267, 4370, 4418, 4420, 4529, 4744, 4745, 4817, 4885, 4921, 5000, 5001, 5005, 5018, 5020, 5024, 5033, 5040, 5053, 5079, 5083, 5106, 5107, 5112, 5121, 5122, 5126, 5131, 5133, 5140, 5144, 5146, 5150, 5159, 5161, 5162, 5165, 5171, 5172, 5174, 5189, 5198, 5209, 5213, 5214, 5223, 5229, 5244, 5247, 5258, 5259, 5263, 5267, 5294, 5324, 5331, 5335, 5336, 5339, 5349, 5351, 5366, 5382, 5389, 5390, 5390a, 5391, 5404, 5405, 5416, 5419, 5427, 5430, 5439a, 5444, 5445, 5451–5453, 5463, 5469, 5474, 5477, 5481, 5482, 5487, 5488, 5498, 5499, 5508, 5512,

(*continued*)

TABLE 23.5 (continued)
"Hoffmann Analytes" in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	**Name (per CA Collective Index)**	**Tobacco Smoke**	**Tobacco**	**Tobacco Substitute Smoke**
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)		5528, 5535, 5536, 5542, 5561, 5573, 5582, 5622, 5623, 5634, 5652, 5654–5656, 5663, 5664, 5667, 5676, 5681, 5685, 5701, 5702, 5712, 5725, 5726, 5734, 5735, 5765, 5771, 5772, 5774, 5775, 5790, 5803, 5811b, 5824, 5828, 5848, 5853, 5884, 5886, 5895, 5896, 5901, 5905, 17B05, 17B06, 17B08, 17B11, 17B14, 17B18, 17B20, 17B29, 17B42, 17B43, 17B44, 17B48, 17B61, 17B62, 17B64, 21A07, 21A08, 21A40–21A42,	

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

TABLE 23.6
Reported Yields of "Hoffmann Analytes" in 1R4F (174b, 3190, 3370) and 2R4F (688) Mainstream Smoke; Proposed MSS "Hoffmann Analyte" Yield Analyses (23A06)

		1R4F			1R4F	2R4F	Proposed
		1988	2002	2004	2003		2000
Component	CAS No.	RJRT (3190)	Rustemeier et al. (3370)	Baker et al. [Table 11 in (174b)]	Chen and Moldoveanu (688)		Department of Health (Canada) (23A06)
Polycyclic Aromatic Hydrocarbons							
Benz[*a*]anthracene, ng/cig	56-55-3	10.5	10.1	—	—	—	—
Benzo[*b*]fluoranthene, ng/cig (benzo[*e*] acephenanthrylene)	205-99-2	—	5.63	—	—	—	—
Benzo[*j*]fluoranthene, ng/cig	205-82-3	—		—	—	—	—
Benzo[*k*]fluoranthene, ng/cig	207-08-9	—		—	—	—	—
Benzo[*a*]pyrene, ng/cig	50-32-8	9.2	5.10	6.51	5.51	6.96	×
Chrysene, ng/cig	218-01-9	—	14.4	—	—	—	—
Chrysene, 5-methyl-, ng/cig	3697-24-3	—	<7.60	—	—	—	—
Dibenz[*a,h*]anthracene, ng/cig	53-70-3	—	<0.60	—	—	—	—
Dibenzo[*a,e*]pyrene, ng/cig (naphtho[1,2,3,4-*def*]chrysene)	192-65-4	—	—	—	—	—	—
Dibenzo[*a,h*]pyrene, ng/cig (dibenzo[*b,def*]chrysene)	189-64-0	—	—	—	—	—	—
Dibenzo[*a,i*]pyrene, ng/cig (benzo[*rst*] pentaphene)	189-55-9	—	—	—	—	—	—
Dibenzo[*a,l*]pyrene, ng/cig (dibenzo[*def,p*]chrysene)	191-30-0	—	—	—	—	—	—
Indeno[1,2,3-*cd*]pyrene, ng/cig	193-39-5	—	2.63	—	—	—	—
Aza-Arenes							
Pyridine, µg/cig	110-86-1	2.09	—	7.7	7.47	7.02	×
Quinoline, µg/cig	91-22-5	0.235	—	0.34	0.30	0.23	×
Dibenz[*a,h*]acridine, ng/cig	226-36-8	—	—	—	—	—	—
Dibenz[*a,j*]acridine, ng/cig	224-42-0	—	<2.72	—	—	—	—
7*H*-Dibenzo[*c,g*]carbazole, ng/cig	194-59-2	—	—	—	—	—	—
N-Nitrosamines							
N-Nitrosodimethylamine, ng/cig	62-75-9	ND	<4.40	—	—	—	—
N-Nitrosoethylmethylamine, ng/cig	10595-95-6	ND	—	—	—	—	—
N-Nitrosodiethylamine, ng/cig	55-18-5	ND	—	—	—	—	—
N-Nitrosodi-*n*-propylamine, ng/cig	621-64-7	—	—	—	—	—	—
N-Nitrosodi-*n*-butylamine, ng/cig	924-16-3	—	—	—	—	—	—
N-Nitrosopyrrolidine, ng/cig	930-55-2	14.0	12.5	—	—	—	—
N-Nitrosopiperidine, ng/cig	100-75-4	—	—	—	—	—	—
N-Nitrosodiethanolamine, ng/cig	1116-54-7	—	<4.30	—	—	—	—
N-Nitrososarcosine, ng/cig	13256-22-9	—	—	—	—	—	—
N′-Nitrosonornicotine, ng/cig	16543-55-8	101.0	124	106	107.09	133.11	×
4-(*N*-Methylnitrosamino)-1-(3-pyridyl)-1-butanone, ng/cig	64091-91-4	84.0	138	96	90.69	115.61	×
N′-Nitrosoanabasine, ng/cig	37620-20-5	18.0	18.6	22	19.37	16.28	×
N′-Nitrosoanatabine, ng/cig	71267-22-6	114.0	104.9	96	122.49	119.02	×
N-Nitrosomorpholine	59-89-2	—	—	—	—	—	—
Aromatic Amines							
2-Toluidine, ng/cig	95-53-4	—	—	—	—	—	—
Aniline, 2,6-dimethyl-, ng/cig	87-62-7	—	—	—	—	—	—
1-Naphthylamine, ng/cig	134-32-7	—	—	5.1	15.63	15.06	×
2-Naphthylamine, ng/cig	91-59-8	—	—	12.6	10.40	10.32	×

(*continued*)

TABLE 23.6 (continued)
Reported Yields of "Hoffmann Analytes" in 1R4F (174b, 3190, 3370) and 2R4F (688) Mainstream Smoke; Proposed MSS "Hoffmann Analyte" Yield Analyses (23A06)

		1R4F			1R4F	2R4F	Proposed
		1988	2002	2004	2003		2000
Component	CAS No.	RJRT (3190)	Rustemeier et al. (3370)	Baker et al. [Table 11 in (174b)]	Chen and Moldoveanu (688)		Department of Health (Canada) (23A06)
Biphenyl, 3-amino-, ng/cig	2243-47-2	—	—	3.3	3.20	2.97	×
Biphenyl, 4-amino-, ng/cig	92-67-1	—	—	2.3	1.94	1.73	×
N-Heterocyclic Amines							
AαC, ng/cig	26148-68-5	—	—	—	—	—	—
MeAαC, ng/cig	68006-83-7	—	—	—	—	—	—
Glu-P-1, ng/cig	67730-11-4	—	—	—	—	—	—
Glu-P-2, ng/cig	67730-10-3	—	—	—	—	—	—
PhIP, ng/cig	105650-23-5	—	—	—	—	—	—
IQ, ng/cig	76180-96-6	—	—	—	—	—	—
MeIQ, ng/cig	77094-11-2	—	—	—	—	—	—
Trp-P-1, ng/cig	62450-06-0	—	—	—	—	—	—
Trp-P-2, ng/cig	62450-07-1	—	—	—	—	—	—
Aldehydes and Ketones							
Formaldehyde, µg/cig	50-00-0		16.5	19.5	22.19	21.61	×
Acetaldehyde, µg/cig	75-07-0	—	518	674	623.88	560.48	×
Propionaldehyde, µg/cig	123-38-6	—	—	56.4	51.54	43.92	×
Butyraldehyde, µg/cig	123-72-8	—	—	35.1	33.93	29.58	×
Crotonaldehyde, µg/cig	123-73-9	—	—	24.9	15.90	16.18	×
Acrolein, µg/cig	107-02-8	—	46.3	69.0	60.64	58.77	×
Acetone, µg/cig	67-94-1	—	—	338	293.15	264.74	×
2-Butanone, µg/cig	78-93-3	—	—	80.7	68.08	62.72	
Volatile hydrocarbons							
1,3-Butadiene, µg/cig	106-99-0	—	42.7	30.4	32.10	29.94	×
Isoprene, µg/cig	78-79-5	—	319	361	308.08	297.68	×
Benzene, µg/cig	71-43-2	45.2	39.8	49.3	44.33	43.39	×
Toluene, µg/cig	108-88-5	68.1	67.2	89.6	68.08	64.91	×
Styrene, µg/cig	100-42-5	2.1	—	7.9	6.13	5.11	×
Miscellaneous Organic Compounds							
Acetamide, µg/cig	60-35-5	2.2	—	—	—	—	—
Acrylonitrile, µg/cig	107-13-1	7.6	—	9.4	9.51	8.28	×
Acrylamide, µg/cig	79-06-1	1.1	—	—	—	—	—
Hydrazine, 1,1-dimethyl-, ng/cig	57-14-7	—	—	—	—	—	—
Nitromethane, µg/cig	75-52-5	—	—	—	—	—	—
2-Nitropropane, µg/cig	79-46-9	—	—	—	—	—	—
Nitrobenzene, µg/cig	98-95-3	—	—	—	—	—	—
Vinyl chloride, ng/cig	75-01-4	—	30.0	—	—	—	—
Ethyl carbamate, ng/cig	51-79-6	—	—	—	—	—	—
Ethylene oxide, µg/cig	75-21-8	—	—	—	—	—	—
Propylene oxide, ng/cig	75-56-9	—	—	—	—	—	—
Di(2-ethylhexyl) phthalate, µg/cig	117-81-7	—	—	—	—	—	—
Furan, µg/cig	110-00-9	—	—	—	—	—	—
Benzo[*b*]furan, ng/cig	271-89-6	—	—	—	—	—	—
Phenols							
Phenol, µg/cig	108-95-2	6.8	11.79	9.80	9.63		7.32
o-Cresol, µg/cig	95-48-7	1.8	3.31	3.04	2.62		1.89

TABLE 23.6 (continued)
Reported Yields of "Hoffmann Analytes" in 1R4F (174b, 3190, 3370) and 2R4F (688) Mainstream Smoke; Proposed MSS "Hoffmann Analyte" Yield Analyses (23A06)

		1R4F			1R4F	2R4F	Proposed
		1988	2002	2004	2003		2000
Component	CAS No.	RJRT (3190)	Rustemeier et al. (3370)	Baker et al. [Table 11 in (174b)]	Chen and Moldoveanu (688)		Department of Health (Canada) (23A06)
m-Cresol, µg/cig	103-39-4	1.6	2.55	8.55	7.43	5.84	×
p-Cresol, µg/cig	106-44-5	4.1	6.36				×
Catechol, µg/cig	120-80-9	38.0	53.8	35.3	40.57	37.90	×
Resorcinol, µg/cig	108-46-3	3.0	0.83	<1.1	0.94	0.91	×
Hydroquinone µg/cig	123-31-9	37.0	43.3	34.9	42.77	32.40	×
Methyleugenol, µg/cig	93-15-2	—	—	—	—	—	—
Caffeic acid, µg/cig	331-39-5	—	—	—	—	—	—
Chloroaromatic Compounds							
DDT	50-29-3	—	—	—	—	—	—
DDE	72-55-0		—	—	—	—	—
Polychlorodibenzo-*p*-dioxins	—	—	—	—	—	—	—
Polychlorodibenzofurans	—	—	—	—	—	—	—
Inorganic Components							
Hydrazine	302-01-2	—	—	—	—	—	—
Arsenic, ng/cig	7440-38-2	—	3.33	<15	12.21	10.39	×
Beryllium	7440-41-7	—	—	—	—	—	—
Cobalt	7440-48-4	—	—	—	—	—	—
Nickel, ng/cig	7440-02-0	—	<2.63	<12	6.44	5.12	×
Chromium (VI), ng/cig	7440-47-3	—	<1.32	<5	57.74	73.01	×
Cadmium, ng/cig	7440-43-9	—	24.7	47	55.09	47.82	×
Mercury ng/cig	7439-97-6	—	—	6.5	5.43	3.82	×
Lead, ng/cig	7439-92-1	—	10.1	36	42.51	32.95	×
Selenium ng/cig	7782-49-2	—	—	<20	39.81	34.85	×
Polonium-210	7440-08-6	—	—	—	—	—	—
Additional Components							
Nicotine, mg/cig	54-11-5	0.79	0.74	0.74	0.80	0.75	×
Carbon monoxide, mg/cig	630-08-0	11.3	10.0	—	12.26	11.96	×
Ammonia, µg/cig	7664-41-7	18.0	—	—	12.90	11.02	×
Nitric oxide, µg/cig	10102-43-9	—	—	—	319.88	223.41	×
Nitrogen oxides, µg/cig		234	263	—	348.34	268.98	×
Hydrogen cyanide, µg/cig	74-90-8	89.0	80.8	—	128.93	109.20	×
"Tar", mg/cig		—	—	—	9.38	8.91	×

24 Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

For nearly four decades after the early 1950s, an exceptional amount of information has been generated on the composition of the various types of tobacco, the smoke from many of the types, and the relationship between the two. Although much of the information has been published, much has not. Exemplary in this regard were the research conducted by personnel not only at the R.J. Reynolds Tobacco Company but also at many other tobacco companies. Much information has been published in peer-reviewed journals, and the remainder is available on the Internet. In the early tobacco and tobacco smoke studies, the chemical nature of one or two components was defined by means of classical chemical procedures, e.g., the identification of the terpenoid alcohol solanesol in fluecured tobacco (3359), the phenols eugenol and isoeugenol in the mainstream smoke (MSS) from Oriental tobacco (3280), and maltol in the MSS from an ingredient-free German tobacco blend (1131). However, as analytical methodology became more sophisticated and precise, many more components—sometimes several hundred newly identified in tobacco or smoke—were reported in a single publication.

In 1986, each major U.S. cigarette manufacturer listed the ingredients used at that time in its cigarette products. A combined list was submitted to the U.S. Office on Smoking and Health. That list, comprising 599 additives, was subjected by a panel of eminent toxicologists not only to an extensive literature survey but also to an examination of unpublished data provided by the tobacco industry members on the chemistry and toxicology of the ingredients. The panel assessed the safety of each listed ingredient with regard to its pyrolysate components and its possible effect when added to cigarette tobacco on the chemical and biological properties of the cigarette MSS. The results were summarized in 1994 by Doull et al. (1053). Of the 599 ingredients, 460 (~77%) are individual compounds. The remaining items are mixtures such as natural oils, plant extracts, oleoresins, etc. Many investigators have noted in their publications that numerous compounds on the list of ingredients are tobacco and/or cigarette MSS components. The following pages chronicle such a relationship between individual added components and their presence in untreated tobacco and/or its smoke. While Paschke et al. (2896) attempted to catalog every material ever added to tobacco and its effect on MSS chemical and/or biological properties, the present article deals only with those materials in the list by Doull et al. While some of the additives cataloged by Paschke et al. did reduce the responses in specific bioassays and the levels of some MSS components considered toxic, they also rendered the MSS unacceptable to the consumer. Obviously, the ingredients listed by Doull et al. did not suffer from such a problem since their addition was specifically designed to enhance the consumer acceptability of the MSS from the product.

As a beginning, Doull et al. (1053) in their report noted

> Many of the ingredients added to cigarettes are identical or essentially similar in composition to natural leaf tobacco components.

In their 1998 report of the effect on rats of inhalation of MSS from ingredient-treated tobacco cigarettes, Gaworski et al. (24A04) expressed a similar view:

> The addition of flavoring ingredients to the cigarette prior to smoking did not significantly alter the type or extent of biologic changes normally seen in smoke-exposed rodents. Given the fact that many of the added flavoring ingredients are structurally similar or identical to [*sic*] natural constituents of tobacco leaf or of tobacco smoke itself [Lloyd et al. (2389)], these results are not totally unexpected.

Later, Rustemeier et al. (3370) in their description of the chemistry of MSS from ingredient-treated tobacco cigarettes noted

> Many of these compounds or mixtures are also natural constituents of the tobacco leaf.

Rodgman (3263) concurred with the preceding statements when he wrote

> Many flavorful tobacco additives listed by Doull et al. are structurally identical with or similar to highly polar, volatile components identified in the aqueous alcohol-soluble portion of cigarette MSS and tobacco.

More recently, Rodgman and Green (3300) wrote

> With the capability to isolate and identify highly polar and volatile components of tobacco and its MSS, it was obvious that many were identical with or similar to ingredients of flavor formulations added to specific tobacco blends to impart unique smoking characteristics…Many "top-dressing" components are structurally identical with or similar to identified tobacco components. With no evidence to the contrary, it is assumed that such an individual added flavorant would

behave during the smoking process (in terms of direct transfer to smoke or degradation, reaction, etc.) much in the same manner as the naturally occurring tobacco component.

While many investigators considered many individual compounds added to cigarette tobacco filler to be tobacco and/or tobacco smoke components, it seemed worthwhile to catalog the extent to which this was true. Obviously, if a specific flavorful compound is already a tobacco component, then its addition to tobacco is an attempt to enhance its flavorful effect. If it is a compound generated during the smoking process, then its addition to tobacco enhances the level in the smoke by tobacco-to-smoke transfer.

The compounds added as ingredients to cigarette tobacco may fall into one of the following categories:

- It is a component of one or more of the tobacco types (flue-cured, Oriental, burley, Maryland) commonly used in cigarette blends.
- It is a component of cigarette MSS.
- It is a component of both tobacco and tobacco smoke.
- It is not a component of either the tobaccos or their smoke.

An ingredient compositionally similar to but not identical with a tobacco leaf or smoke component may be categorized as an isomer or a homolog of a compound identified in natural tobacco leaf and/or its smoke. In the broad spectrum of chemistry, biochemistry, and biology, cases exist where the properties of one homolog vary significantly from those of another or where the properties of one isomer differ significantly from those of another.

For example, whether classified as a "Group 2A carcinogen" by the International Agency for Research on Cancer (IARC) (1868a), or a significant carcinogen in cigarette MSS by Hoffmann and Hecht (1727), or overall as a borderline carcinogen by others, e.g., Dipple et al. (983), the specific tumorigenicity of mice skin painted or subcutaneously injected with benz[*a*]anthracene (B[*a*]A) is insignificant compared to that of its homolog, 7,12-dimethylbenz[*a*]anthracene (DMB[*a*]A). The isomeric $C_{20}H_{12}$ polycyclic aromatic hydrocarbons (PAHs) benzo[*a*]pyrene (B[*a*]P) and benzo[*e*]pyrene (B[*e*]P) differ markedly in their specific tumorigenicities in studies involving mouse-skin painting or subcutaneous injection (983). B[*a*]P under appropriate laboratory conditions is one of the most potent tumorigens known, whereas the isomeric B[*e*]P under the same conditions is essentially nontumorigenic.

In the 1950s, the organic solvent extraction of tobacco was studied extensively with the purpose of removing PAH precursors from the tobacco. One process involved an aqueous ethanol–hexane partition to separate the polar, more flavorful tobacco components from the lipophilic PAH precursors. At that time, little was known about the nature of the polar tobacco components, although it was apparent they made a considerable positive contribution to the flavor and aroma of cigarette MSS. Despite the lack of knowledge about the precise nature of the polar components, it was demonstrated they were not significant PAH precursors (3262). The lack of knowledge about the polar tobacco components was due to our inability to separate highly polar compounds in a complex mixture. This situation continued during years of intensive effort on cigarette MSS composition but was finally resolved and utilized by Schumacher et al. (3553) in the 1970s. Among 1490 MSS components identified by Schumacher et al. (3553), Newell et al. (2769), and Heckman and Best (1587) were over 1125 components new to the tobacco smoke literature, many of which were highly polar. By glass capillary gas chromatography, Grob (1416) also identified many polar components in the MSS from cigarettes containing additive-free tobacco. Later, it was shown that some of the identified polar components reported in MSS by Grob are also in the Doull et al. list.

With regard to tobacco, Lloyd et al. (2389) identified 275 previously unidentified components of additive-free flue-cured tobacco, 132 new to all tobacco types. Many of these compounds were highly polar and considered significant contributors to MSS flavor and aroma. Similar studies were conducted on the composition of burley (3219), Oriental (3561), and Maryland (3550) tobaccos. Later, it became apparent that many of the highly polar components of tobacco and tobacco smoke were identical with or similar to many of the components used in the flavor additive formulations, i.e., the "top dressing," added to a specific tobacco blend to impart its unique smoking characteristics (1053).

As previously mentioned, in the mid-1980s, each major U.S. cigarette manufacturer listed the ingredients added to its cigarette products at that time. In 1986, a combined list, comprising 599 entities, was submitted to the U.S. Office on Smoking and Health. From an extensive literature survey and examination of much unpublished data from the cigarette manufacturers on the chemistry and toxicology of the ingredients, a panel of eminent toxicologists assessed the safety of each listed ingredient with regard to its pyrolysis products and its possible effect when added to cigarette tobacco on the chemical and biological properties of cigarette MSS. Subsequently, Doull et al. (1053) listed the ingredients assessed and summarized the conclusions of the panel on their effect on the chemical and biological properties of cigarette smoke.

In their assessment of available information on these ingredients variously used as cigarette tobacco ingredients, Doull et al. concluded that none of the materials used as flavorants on smoking tobacco products, particularly cigarettes marketed by U.S. manufacturers, imparted any significant adverse chemical or biological properties to the MSS from the ingredient-treated tobacco. However, Doull et al. did not publish an overview of the studies and reports they had examined or provide any details on their analysis. In their detailed assessment of reported chemical and biological properties of the MSS from cigarettes fabricated with tobacco with or without one or more additives, Paschke et al. (2895) reached a similar conclusion; namely, that in general, no significant

increase in the biological activity of tobacco was reported from cigarettes containing specifically described added ingredients. In his examination of extensive laboratory data generated from additives and additive-treated cigarettes between the mid-1950s and the late 1970s, Rodgman (3263, 3264) reached a conclusion similar to that of Doull et al. (1053) and Paschke et al. (2896).

Previously [see Table 1 in (3266)], the individual compounds listed by Doull et al. (1053) as possible U.S. cigarette ingredients were assigned a number somewhat indicative of the alphabetical order in which the 460 individual components were listed by Doull et al. That numerical listing is listed in Table 24.1. A similar number assignment [see Table 7A in (3266)] was made in the case of individual components used as tobacco ingredients by cigarette manufacturers outside of the United States. That numerical listing appears in Table 24.2. In each case, a few citations on the identification of the component in tobacco and/or smoke were included in the previous publication [see Tables 1 and 7A in (3266)] to indicate that the ingredient was indeed a tobacco and/or tobacco smoke component. A more complete listing of citations on the identification of the ingredient in tobacco and/or smoke is included in Table 24.3. Examination of Reference column in Table 24.3 indicates that the number of references for many of the tobacco and/or tobacco smoke components used as ingredients is substantial. They include not only reports on the identification of the component in additive-free tobacco and/or its tobacco smoke but also reports on the effect of the added ingredient on MSS composition, particularly references dealing with "Hoffmann analyte" yields. In several instances, ingredients not previously included as tobacco and/or smoke components in (3266) are cataloged in Table 24.3 because of their identification in tobacco after the publication of (3266), e.g., previously unidentified 2-hexenol and several naphthalene derivatives identified in tobacco by Peng et al. (2917a), several esters identified in tobacco by Leffingwell and Alford (2339a).

Examination of the data presented previously [see Tables 1 and 7A in (3266)] permits verification of the statements by numerous investigators that many of the ingredients in the Doull et al. list have been identified as components in untreated tobacco types and/or the MSS from cigarettes containing such tobaccos. Such an examination also permits an assessment of the effect of a number of the listed ingredients that have been reported in a variety of studies to not adversely affect the chemical or biological properties of the MSS from cigarettes containing such ingredients or the chemical properties of the pyrolysates from individual ingredients.

Table 24.3 catalogs those individual compounds that have been identified in untreated tobacco and/or its tobacco smoke and are listed by Doull et al. (1053) as tobacco additives used by U.S. cigarette manufacturers in and prior to 1994. The references cited are pertinent not only to their tobacco/tobacco smoke identification but also to their effect on the chemical and biological properties of the MSS from cigarettes containing ingredient-treated tobacco. The components are cross-referenced to the numbers assigned to their listing in the Doull et al. (1053) and Baker et al. (174b, 174c, 24A01) articles (see Tables 24.1 and 24.2). Over 260 of the 460 individual compounds (57%) listed by the Doull et al. and 19 of the 50 compounds (38%) in the Baker et al. list have been identified as components in additive-free tobacco and/or its smoke.

In 1957, Wynder (4296) proposed that reduction of the per cigarette "tar" yield by about 50% would have beneficial health-related results. By the late 1970s, early 1980s, the tobacco industry had exceeded the suggested reduction by generating the low-"tar" and ultralow-"tar" cigarette. This led to the criticisms and assertions that (1) some commercial low-"tar" brands might have additive levels much higher than those in previous high- and medium-"tar" cigarettes and (2) the fates during the cigarette smoking process of many individual added components were unknown.

The criticisms and assertions of the early 1980s about tobacco additives were not new but an extension of those made earlier, e.g., in 1967, Wynder and Hoffmann wrote about additives [see pp. 488 and 628 in (4332)]:

> The importance of flavor-enhancing agents as contributors to the tumorigenicity in the experimental animals varies for different tobacco products. For cigarettes it may be a minor factor compared to the overwhelming effects of other constituents and variables. Nevertheless, one should emphasize that further studies on the toxicity of flavorants and their combustion products could provide a scientific basis for the selection of less harmful additives… In evaluating the effect of tobacco additives, we need to consider whether such additions may contribute to the production of tumorigenic agents during the smoking of a tobacco product. If an additive increases the formation of carcinogenic substances during smoking to an analytically significant extent, it would, of course, be most undesirable. If, however, an additive should inhibit the production of tumorigenic agents during smoking and at the same time not yield other types of toxic substances, it may represent an effective and useful agent.

However, the proponents of problems with added tobacco ingredients became more vocal when the nearly 70% reduction in sales-weighted MSS "tar" yield achieved by 1985 not only answered the "tar" criticisms of the late 1950s, early 1960s, but exceeded the goal that halving the "tar" yield was a means to lower lung cancer incidence in cigarette smokers (4296).

In 1980, LaVoie et al. (24A06) wrote

> The development of the low-tar, low-nicotine cigarette required cigarette fillers with a potential for smoke flavor contribution to make these cigarettes acceptable to the consumer. Such products can be realized either by selecting tobaccos rich in flavor or by addition of tobacco extracts or certain plant extracts, addition of synthetic flavor compounds, or a combination of several of these factors…New cigarettes should be assayed for toxicity and tumorigenicity, so that the reduction of toxic and tumorigenic effects in the smoke of low-tar, low-nicotine cigarettes is not offset by the introduction of unknown factors.

TABLE 24.1
As Listed by Doull et al. (1053), Individual Ingredient Components Used in U.S. Smoking Products

Assigned No.	Name in Doull et al. (1053)	Assigned No.	Name in Doull et al. (1053)	Assigned No.	Name in Doull et al. (1053)
1[a]	Acetanisole	**52**	2-Butanone	101	5,7-Dihydro-2-methylthieno[3,4-*d*] pyrimidine
2	Acetic acid	**53**	4-(2-Butylidene-3,5,5-trimethyl)-2-cyclohexen-1-one	102	*m*-Dimethoxybenzene
3	Acetoin	**54**	Butyl acetate	**103**	*p*-Dimethoxybenzene
4	Acetophenone	55	Butyl butyrate	**104**	2,6-Dimethoxyphenol
5	6-Acetoxydihydrotheaspirane	56	Butyl butyryl lactate	**105**	Dimethyl succinate
6	2-Acetyl-3-ethylpyrazine	57	Butyl isovalerate	**106**	3,4-Dimethyl-1,2-cyclopentanedione
7	2-Acetyl-5-methylfuran	58	Butyl phenylacetate	**107**	3,5-Dimethyl-1,2-cyclopentanedione
8	Acetylpyrazine	59	Butyl undecylenate	**108**	3,7-Dimethyl-1,3,6-octatriene
9	2-Acetylpyridine	60	3-Butylidenephthalide	109	4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one
10	3-Acetylpyridine	61	Butyric acid		
11	2-Acetylthiazole	62	Cadinene	**110**	6,10-Dimethyl-5,9-undecadien-2-one
12	Aconitic acid	63	Caffeine	111	3,7-Dimethyl-6-octenoic acid
13	*dl*-Alanine	64	Calcium carbonate	112	2,4-Dimethylacetophenone
14	Allyl hexanoate	**65**	Camphene	**113**	α,*p*-Dimethylbenzyl alcohol
15	Allylionone	**66**	Carbon dioxide	114	α,α-Dimethylphenethyl acetate
16	Ammonia	**67**	β-Carotene *cis*-*trans*-	115	α,α-Dimethylphenethyl butyrate
17	Ammonium bicarbonate			**116**	2,3-Dimethylpyrazine
18	Ammonium hydroxide	**68**	Carvacrol	**117**	2,5-Dimethylpyrazine
19	Ammonium phosphate dibasic	**69**	4-Carvomenthenol	**118**	2,6-Dimethylpyrazine
20	Ammonium sulfide	**70**	1-Carvone	119	Dimethyltetrahydrobenzofuranone
21	Amyl alcohol	**71**	β-Caryophyllene	120	δ-Dodecalactone
22	Amyl butyrate	**72**	β-Caryophyllene oxide	121	γ-Dodecalactone
23	Amyl formate	**73**	Cellulose	122	*p*-Ethoxybenzaldehyde
24	Amyl octanoate	**74**	Cinnamaldehyde	123	Ethyl 10-undecenoate
25	α-Amylcinnamaldehyde	**75**	Cinnamic acid	**124**	Ethyl 2-methylbutyrate
26	Anethole *trans*-	76	Cinnamyl acetate	**125**	Ethyl acetate
27	Anisyl acetate	**77**	Cinnamyl alcohol	126	Ethyl acetoacetate
28	Anisyl alcohol	**78**	Cinnamyl cinnamate	**127**	Ethyl alcohol
29	Anisyl formate	**79**	Cinnamyl isovalerate	**128**	Ethyl benzoate
30	Anisyl phenylacetate	80	Cinnamyl propionate	**129**	Ethyl butyrate
31	*l*-Arginine	**81**	Citral	**130**	Ethyl cinnamate
32	Ascorbic acid	**82**	Citric acid	**131**	Ethyl decanoate
33	*l*-Asparagine monohydrate	**83**	*dl*-Citronellol	132	Ethyl fenchol
34	*l*-Aspartic acid	84	Citronellyl butyrate	133	Ethyl furoate
35	Benzaldehyde	85	Citronellyl isobutyrate	134	Ethyl heptanoate
36	Benzaldehyde glyceryl acetal	**86**	Cuminaldehyde	**135**	Ethyl hexanoate
37	Benzoic acid	**87**	*p*-Cymene	**136**	Ethyl isovalerate
38	Benzoin	**88**	*l*-Cysteine	**137**	Ethyl lactate
39	Benzophenone	**89**	*trans*, *trans*-2,4-Decadienal	**138**	Ethyl laurate
40	Benzyl alcohol	90	δ-Decalactone	139	Ethyl levulinate
41	Benzyl benzoate	**91**	γ-Decalactone	**140**	Ethylmaltol
42	Benzyl butyrate	**92**	Decanal	141	Ethyl methylphenylglycidate
43	Benzyl cinnamate	**93**	Decanoic acid	**142**	Ethyl myristate
44	Benzyl propionate	**94**	1-Decanol	**143**	Ethyl nonanoate
45	Benzyl salicylate	95	3-Decenal	**144**	Ethyl octadecanoate
46	Bisabolene	96	Dehydromenthofurolactone	**145**	Ethyl octanoate
47	Borneol	97	Diethyl malonate	**146**	Ethyl oleate
48	Bornyl acetate	98	Diethyl sebacate	**147**	Ethyl palmitate
49	1,3-Butanediol	**99**	Diethylpyrazine (three isomers)	**148**	Ethyl phenylacetate
50	2,3-Butanedione	100	Dihydroanethole	**149**	Ethyl propionate
51	1-Butanol				

TABLE 24.1 (continued)
As Listed by Doull et al. (1053), Individual Ingredient Components Used in U.S. Smoking Products

Assigned No.	Name in Doull et al. (1053)	Assigned No.	Name in Doull et al. (1053)	Assigned No.	Name in Doull et al. (1053)
150	Ethyl salicylate	200	3-Hexen-1-ol	**247**	Lauric acid
151	Ethyl *trans*-2-butenoate	201	*cis*-3-Hexen-1-yl acetate	248	Lauric aldehyde
152	Ethyl valerate	**202**	2-Hexenal	**249**	*l*-Leucine
153	Ethylvanillin	203	2-Hexenoic acid	**250**	Levulinic acid
154	2-Ethyl-3-methoxypyrazine	**204**	3-Hexenoic acid	**251**	Linalool
155	2-Ethyl-5-methoxypyrazine	205	3-Hexenyl formate	**252**	Linalool oxide
156	2-Ethyl-6-methoxypyrazine	206	Hexyl 2-methylbutyrate	**253**	Linalyl acetate
157	2-Methyl-3-methoxypyrazine	**207**	Hexyl acetate	**254**	*l*-Lysine
158	2-Methyl-5-methoxypyrazine	**208**	Hexyl alcohol	**255**	Malic acid
159	2-Methyl-6-methoxypyrazine	209	Hexyl phenylacetate	**256**	Maltol
160	2-Ethyl-1-hexanol	**210**	*l*-Histidine	257	Maltyl isobutyrate
161	3-Ethyl-2-hydroxy-2-cyclopenten-1-one	211	5-Hydroxy-2,4-decadienoic acid δ-lactone	258	*p*-Mentha-8-thiol-3-one
162	2-Ethyl-3,5-dimethylpyrazine	212	2,5-Dimethyl-4-hydroxy-3(2*H*)-furanone	**259**	*l*-Menthol; *l*-menthol (synthetic)
163	2-Ethyl-3,6-dimethylpyrazine			**260**	*l*-Menthone
164	5-Ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone	213	2-Hydroxy-3,5,5-trimethyl-2-cyclohex-1-one	261	Menthyl acetate
				262	*dl*-Methionine
165	2-Ethyl-3-methylpyrazine	**214**	4-Hydroxy-3-pentenoic acid lactone	**263**	Methoprene
166	4-Ethylbenzaldehyde			**264**	2-Methoxy-4-methylphenol
167	4-Ethylguaiacol	215	2-Hydroxy-4-methylbenzaldehyde	**265**	2-Methoxy-4-vinylphenol
168	*p*-Ethylphenol			**266**	*p*-Methoxybenzaldehyde
169	3-Ethylpyridine	216	4-Hydroxybutanoic acid lactone	267	1-(*p*-Methoxyphenyl)-1-penten-3-one
170	Eucalyptol	217	Hydroxycitronellal	268	4-(*p*-Methoxyphenyl)-2-butanone
171	Farnesol	218	6-Hydroxydihydrotheaspirane	269	1-(*p*-Methoxyphenyl)-2-propanone
172	*d*-Fenchone	**219**	4-(*p*-Hydroxyphenyl)-2-butanone	270	Methoxypyrazine
173	Furfurylmercaptan	**220**	α-Ionone	**271**	Methyl 2-furoate
174	4-(2-Furyl)-3-buten-2-one	**221**	β-Ionone	272	Methyl 2-octynoate
175	Geraniol	222	α-Irone	**273**	Methyl 2-pyrrolyl ketone
176	Geranyl acetate	**223**	Isoamyl acetate	274	Methyl anisate
177	Geranyl butyrate	224	Isoamyl benzoate	**275**	Methyl anthranilate
178	Geranyl formate	225	Isoamyl butyrate	**276**	Methyl benzoate
179	Geranyl isovalerate	**226**	Isoamyl cinnamate	**277**	Methyl cinnamate
180	Geranyl phenylacetate	**227**	Isoamyl formate	278	Methyl dihydrojasmonate
181	*l*-Glutamic acid	228	Isoamyl hexanoate	**279**	Methyl isovalerate
182	*l*-Glutamine	**229**	Isoamyl isovalerate	**280**	Methyl linoleate
183	Glycerol	230	Isoamyl octanoate	**281**	Methyl linolenate
184	Glycyrrhizin, ammoniated	**231**	Isoamyl phenylacetate	**282**	Methyl naphthyl ketone
185	Guaiacol	232	Isobornyl acetate	**283**	Methyl nicotinate
186	2,4-Heptadienal	233	Isobutyl acetate	**284**	Methyl phenylacetate
187	γ-Heptalactone	**234**	Isobutyl alcohol	**285**	Methyl salicylate
188	Heptanoic acid	235	Isobutyl cinnamate	286	Methyl sulfide
189	2-Heptanone	236	Isobutyl phenylacetate	287	3-Methylcyclopentadecanone
190	3-Hepten-2-one	237	Isobutyl salicylate	288	4-Methyl-1-phenyl-2-pentanone
191	2-Hepten-4-one	238	2-Isobutyl-3-methoxypyrazine	289	5-Methyl-2-phenyl-2-hexenal
192	4-Heptenal	239	α-Isobutylphenethyl alcohol	**290**	5-Methyl-2-thiophenecarboxaldehyde
193	2-Heptenal	**240**	Isobutyraldehyde	**291**	6-Methyl-3,5-heptadien-2-one
194	Heptyl acetate	**241**	Isobutyric acid		
195	ω-6-Hexadecenlactone	**242**	*dl*-Isoleucine	292	2-Methyl-(*p*-isopropylphenyl)-propionaldehyde
196	γ-Hexalactone	243	α-Isomethylionone	**293**	5-Methyl-3-hexen-2-one
197	Hexanal	**244**	2-Isopropylphenol	294	4-Isopropyl-3-methoxy-1-methylbenzene
198	Hexanoic acid	**245**	Isovaleric acid		
199	2-Hexen-1-ol	**246**	Lactic acid	**295**	4-Methyl-3-penten-2-one

(*continued*)

TABLE 24.1 (continued)
As Listed by Doull et al. (1053), Individual Ingredient Components Used in U.S. Smoking Products

Assigned No.	Name in Doull et al. (1053)
296	2-Methyl-4-phenylbutyraldehyde
297	6-Methyl-5-hepten-2-one
298	4-Methyl-5-thiazoleethanol
299	4-Methyl-5-vinylthiazole
300	Methyl-α-ionone
301	Methyl-2-butenoic acid, *Z*-, *E*
302	4-Methylacetophenone
303	*p*-Methylanisole
304	α-Methylbenzyl acetate
305	α-Methylbenzyl alcohol
306	2-Methylbutyraldehyde
307	3-Methylbutyraldehyde
308	2-Methylbutyric acid
309	α-Methylcinnamaldehyde
310	Methylcyclopentenolone
311	2-Methylheptanoic acid
312	2-Methylhexanoic acid
313	3-Methylpentanoic acid
314	4-Methylpentanoic acid
315	2-Methylpyrazine
316	5-Methylquinoxaline
317	2-Methyltetrahydrofuran-3-one
318	Methyl methylthiopyrazine
319	3-Methylthiopropionaldehyde
320	Methyl 3-methylthiopropionate
321	2-Methylvaleric acid
322	Myristaldehyde
323	Myristic acid
324	β-Naphthyl ethyl ether
325	Nerol
326	Nerolidol
327	2,6-Nonadienal
328	2,6-Nonadien-1-ol
329	γ-Nonalactone
330	Nonanal
331	Nonanoic acid
332	2-Nonanone
333	2-Nonen-1-ol
334	2-Nonenal
335	Nonyl acetate
336	9,12-Octadecadienoic acid
337	9,12,15-Octadecatrienoic acid
338	δ-Octalactone
339	γ-Octalactone
340	Octanal
341	Octanoic acid
342	1-Octanol
343	2-Octanone
344	3-Octen-2-one
345	1-Octen-3-ol
346	1-Octen-3-yl acetate
347	2-Octenal
348	Octyl isobutyrate
349	Oleic acid
350	Palmitic acid
351	ω-Pentadecalactone
352	2,3-Pentanedione
353	2-Pentanone
354	4-Pentenoic acid
355	2-Pentylpyridine
356	α-Phellandrene
357	2-Phenethyl acetate
358	Phenethyl alcohol
359	Phenethyl butyrate
360	Phenethyl cinnamate
361	Phenethyl isobutyrate
362	Phenethyl isovalerate
363	Phenethyl phenylacetate
364	Phenethyl salicylate
365	1-Phenyl-1-propanol
366	3-Phenyl-1-propanol
367	2-Phenyl-2-butenal
368	4-Phenyl-3-buten-2-ol
369	4-Phenyl-3-buten-2-one
370	Phenylacetaldehyde
371	Phenylacetic acid
372	*l*-Phenylalanine
373	3-Phenylpropionaldehyde
374	3-Phenylpropionic acid
375	3-Phenylpropyl acetate
376	3-Phenylpropyl cinnamate
377	2-(3-Phenylpropyl) tetrahydrofuran
378	Phosphoric acid
379	α-Pinene
380	β-Pinene
381	*d*-Piperitone
382	Piperonal
383	Potassium sorbate
384	*l*-Proline
385	5-Propenylguaethol
386	Propionic acid
387	Propyl acetate
388	Propyl *p*-hydroxybenzoate
389	Propylene glycol
390	3-Propylidenephthalide
391	Pyridine
392	Pyroligneous acid
393	Pyrrole
394	Pyruvic acid
395	Rhodinol
396	Salicylaldehyde
397	Sclareolide
398	Skatole
399	Sodium acetate
400	Sodium benzoate
401	Sodium bicarbonate
402	Sodium carbonate
403	Sodium chloride
404	Sodium citrate
405	Sodium hydroxide
406	Solanone
407	Sucrose octaacetate
408	Sugar alcohols
409	Sugars[b]
410	Tannic acid
411	*d*-Tartaric acid
412	α-Terpineol
413	Terpinolene
414	α-Terpinyl acetate
415	5,6,7,8-Tetrahydroquinoxaline
416	1,5,5,9-Tetramethyl-13-oxatricyclo[8,3,0,0(4,9)]tridecane
417	2,3,4,5-Tetramethylethylcyclohexanone
418	3,4,5,6-Tetramethylethylcyclohexanone
419	2,3,5,6-Tetramethylpyrazine
420	Thiamine hydrochloride
421	Thiazole
422	*l*-Threonine
423	Thymol
424	α-Tocopherol
425	*o*-Tolualdehyde
426	*m*-Tolualdehyde
427	*p*-Tolualdehyde
428	*p*-Tolyl 3-methylbutyrate
429	*p*-Tolylacetaldehyde
430	*p*-Tolyl acetate
431	*p*-Tolyl isobutyrate
432	*p*-Tolyl phenylacetate
433	Triacetin
434	2-Tridecanone
435	2-Tridecenal
436	Triethyl citrate
437	3,5,5-Trimethyl-1-hexanol
438	*p*,α,α-Trimethylbenzyl alcohol
439	4-(2,6,6-Trimethylcyclohex-2-enyl)-but-2-en-4-one
440	2,6,6-Trimethylcyclohex-2-ene-1,4-dione
441	2,6,6-Trimethylcyclohexa-1,3-dienyl-methane

TABLE 24.1 (continued)
As Listed by Doull et al. (1053), Individual Ingredient Components Used in U.S. Smoking Products

Assigned No.	Name in Doull et al. (1053)	Assigned No.	Name in Doull et al. (1053)	Assigned No.	Name in Doull et al. (1053)
442	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-but-2-en-4-one	**449**	2-Undecanone	**456**	Valine
		450	10-Undecenal	**457**	Vanillin
443	2,6,6-Trimethylcyclohexanone	**451**	Urea	**458**	Veratraldehyde
444	2,3,5-Trimethylpyrazine	**452**	Valencene	**459**	Water
445	*l*-Tyrosine	**453**	Valeraldehyde	**460**	3,4-Xylenol
446	δ-Undecalactone	**454**	Valeric acid		
447	γ-Undecalactone	**455**	γ-Valerolactone		
448	Undecanal				

Note: The assigned numbers are those assigned by Rodgman (3266) to the individual component ingredients listed alphabetically in their more or less common name by Doull et al. (1053).

[a] A number in bold print indicates the component has been identified as a tobacco and/or a tobacco smoke component (see Table 24.3).

[b] Sugars include glucose, fructose, sucrose, galactose, and mannose.

TABLE 24.2
As Listed by Baker et al. (174a), Individual Ingredient Components Not Used in U.S. Smoking Products but Used Outside of the United States

Assigned No.	Name in Baker et al. (174a)	Assigned No.	Name in Baker et al. (174a)	Assigned No.	Name in Baker et al. (174a)
1A	Ambroxide	18A	Ethyl isobutyrate	**35A**	Methylcyclopentenolone
2A	Ammonium glycyrrhizinate[a]	**19A**	Hexen-2-al	36A	6-Methyl-5-hepten-2-one
3A	Amyl hexanoate	**20A**	2-Hexenol	37A	Methyl 2-octynate
4A[b]	Anisole	**21A**	2-Hexenyl acetate	38A	4-Methyl-5-thiazole ethanol
5A	Anisyl propionate	**22A**	Ionone	39A	Neryl acetate
6A	Benzyl formate	23A	Isoamyl propionate	40A	δ-Nonalactone
7A	Benzyl isobutyrate	**24A**	Isoamyl salicylate	**41A**	Pectin
8A	Benzyl isovalerate	25A	Isobutyl butyrate	**42A**	Pent-4-en-4-olide
9A	Bornyl isovalerate	26A	*dl*-Isomenthone	43A	Potassium citrate
10A	Butyl valerate	27A	Isopropyl myristate	44A	Rose oxide
11A	*d*-Carvone	28A	Linalyl benzoate	45A	Sodium ethyl 4-hydroxybenzoate
12A	Cinnamyl isobutyrate	29A	Linalyl isobutyrate	46A	Sodium methyl 4-hydroxybenzoate
13A	Citronellal	**30A**	Methional	47A	Sodium propyl 4-hydroxybenzoate
14A	Citronellyl acetate	31A	5*H*-5-Methyl-6,7-dihydrocyclopenta-[*b*]pyrazine	**48A**	Sorbic acid
15A	Cyclamen aldehyde	32A	Menthyl isovalerate	**49A**	Sorbitol
16A	Dextrin	**33A**	Methyl anthranilate[c]	50A	Tetradecalactone
17A	3-Ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone	34A	1-Methyl-2,3-cyclohexadione		

[a] The Doull et al. list does not include this item per se but does include glycyrrhizin, ammoniated (see Table 24.1, item No. 184).

[b] A number in bold print indicates the component has been identified as a tobacco and/or a tobacco smoke component (see Table 24.3).

[c] Methyl anthranilate, a component in the Doull et al. list, was inadvertently listed in Table 7A in (3266).

TABLE 24.3
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
1.	64-19-7 [2]	Acetic acid CH_3-COOH	18, 126a, 126b, 167, 172, 237, 239, 424, 563, 565, 568b, 722, 916, 937, 938, 960, 966, 1023, 1063–1066, 1068–1074, 1099, 1132, 1140, 1232, 1263, 1348, 1350, 1354, 1360, 1364, 1365, 1375, 1375a, 1375b, 1377, 1388–1390, 1437, 1445, 1586, 1668, 1674, 1744, 1842, 1882, 1884, 1903, 1904, 1917, 2043, 2079, 2086, 2088, 2133, 2170, 2195, 2200, 2203, 2253, 2270, 2293, 2310, 2337, 2387, 2414, 2475, 2529, 2543, 2545, 2570, 2582, 2601a, 2619, 2623, 2628, 2702, 2765, 2767, 2777, 2799a, 2821, 2855, 2857, 2858, 2934, 2939, 3060, 3064, 3105, 3187, 3255, 3257, 3263, 3266, 3300, 3302, 3308, 3324, 3384, 3394, 3397, 3403, 3452, 3495, 3553, 3557, 3559, 3797, 3799, 3876, 3973, 3992, 4064, 4065, 4249, 4301, 4304, 4319, 4332, 4342, 4406, 4570a, 5079, 5189, 5359, 5512, 5811b, 5835	120, 212, 404, 565, 568b, 647, 937, 938, 1053, 1063, 1085, 1087, 1276, 1550, 1893b, 1705, 1982, 1999, 2014, 2079, 2154, 2270, 2283, 2293, 2337, 2338, 2339a, 2386, 2389, 2529, 2544, 2862a, 2917a, 2939, 3052, 3188, 3266, 3328, 3374, 3507, 3549, 3550, 3655b, 3787, 3797, 3905, 3973, 3974a, 3983a, 4064, 4249, 5079, 5114, 5165, 5189, 5381, 5419, 5478, 5695, 5708, 5709, 5712, 5735, 5811b, 5846, 5896	1228, 1354, 1360, 1375a, 1377, 2244, 2387, 3393, 3401, 3402, 3404, 3405
2.	123-86-4 [54]	Acetic acid, butyl ester {butyl acetate} CH_3-COO-C_4H_9	222–224, 568b, 1140, 1416, 1422, 1445, 3266, 3302, 3797, 4249, 5811b	172a, 174b, 568b, 1053, 1063, 2339a, 3186, 3188, 3266, 3905, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

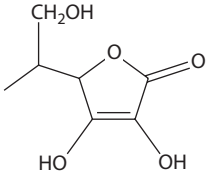
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
3.	141-78-6 [125]	Acetic acid, ethyl ester {ethyl acetate} CH_3-COO-C_2H_5	565, 1140, 1375, 1375a, 1375b, 1377, 1378, 1413, 1414, 1416, 1418, 1445, 1449, 1590, 1903–1905, 1907, 2088, 2782, 2804, 2858, 2939, 3254, 3266, 3308, 3508, 3530, 3553, 3797, 4249, 4319, 5811b	120, 1053, 1063, 1590, 2339a, 2389, 2544, 2861a, 2939, 3266, 3797, 3973, 3974a, 4249, 5811b	1375a, 1377, 1378
4.	142-92-7 [207]	Acetic acid, hexyl ester {hexyl acetate} CH_3-COO-$(CH_2)_5$-CH_3	1157, 4249	172a, 174b, 1053, 1063, 1157, 3266, 3370, 4249	
5.	123-92-2 [223]	Acetic acid, 3-methylbutyl ester CH_3-COO-$(CH_2)_2$-CH═$(CH_3)_2$		404, 1053, 2339a, 3266	
6.	103-45-7 [357]	Acetic acid, 2-phenylethyl ester {2-phenethyl acetate} CH_3-COO-$(CH_2)_2$-C_6H_5	568b, 937, 3224, 3266, 3302, 3794, 4249, 5811b	120, 172a, 174b, 404, 568b, 937, 1053, 1063, 2339a, 2386, 2389, 2544, 2611, 2861a, 2917a, 2939, 3266, 3354, 3370, 3543, 3547, 3560, 3561, 3905, 3973, 3974a, 4249, 5811b	
7.	109-60-4 [387]	Acetic acid, propyl ester {propyl acetate} CH_3-COO-$(CH_2)_2$-CH_3	568b, 2544, 4249	172a, 174b, 568b, 1053, 1590, 2339a, 2389, 2544, 3266, 4249, 5811b	
8.	6898-94-8 [13]	Alanine	1910, 1914, 2858, 2939, 3266, 3555, 3797	1053, 1086, 2079, 3266, 3555, 3797	
9.	107-95-9 [13]	β-Alanine H_2N-$(CH_2)_2$-COOH	1083, 1351, 1910, 1914, 2858, 2939, 3224, 3266, 3302, 3491, 3797, 4249, 4319, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2270, 2337, 2338, 2359, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5603, 5785, 5827, 5811b, 5831, 5881, 5905	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

	CAS No.	Name (per CA Collective Index)	References		
			Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
10.	7664-41-7 [16]	Ammonia	30, 31, 50, 126b, 129, 167, 172, 173a, 174a, 174b, 174c, 195, 197, 198, 213, 237, 239, 364, 365, 375, 376, 402, 407, 408, 424, 472, 473, 475, 480, 491, 688, 827, 916, 985–987, 989, 1051, 1063–1066, 1068–1075, 1091, 1099, 1100, 1128b, 1137, 1140, 1222, 1245, 1263, 1277, 1293, 1335, 1348–1351, 1354, 1369, 1375a, 1386, 1388–1390, 1437, 1442, 1445, 1469, 1489, 1492, 1522, 1524, 1531, 1532, 1539, 1580, 1589, 1673, 1674, 1709, 1741, 1744, 1808, 1841, 1842, 1853b, 1884, 1902, 1911, 1966, 2079, 2083–2085, 2133, 2134a, 2142, 2161, 2170, 2217, 2224, 2263, 2267, 2270, 2326, 2330, 2338, 2342, 2342a, 2343, 2368, 2480, 2524, 2529, 2541, 2543, 2545, 2607, 2627, 2688, 2691–2695, 2724, 2761, 2762, 2775, 2777, 2781, 2782, 2804, 2858, 2919, 2927, 2928, 2934, 2936, 2937, 2939, 2973, 2986–2988, 3007, 3022, 3029, 3059, 3140, 3187, 3190, 3213, 3214, 3251, 3254, 3255, 3257, 3266, 3300, 3302, 3306, 3308, 3324, 3369, 3385, 3482, 3491, 3493, 3583, 3584, 3623, 3659, 3693, 3695, 3797, 3844,	129, 174b, 212, 385, 555, 622, 677b, 826a, 856, 927, 989, 1053, 1063–1066, 1068–1074, 1128b, 1189, 1222, 1244, 1263, 1329, 1330, 1332, 1333, 1335, 1351, 1369, 1493, 1527, 1835b, 1941, 2079, 2313a, 2330, 2337, 2338, 2339b, 2356, 2381, 2394a, 2453, 2529, 2543, 2545, 2607, 2746, 2761, 2762, 2765, 2766, 2787, 2914, 2919, 2939, 2987, 3022, 3214, 3254, 3261, 3266, 3385, 3420, 3491, 3499, 3693, 3707, 3780, 3797, 3974a, 3974b, 4244, 4249, 4837a, 5018, 5079, 5126, 5165, 5186, 5189, 5194, 5298, 5382, 5389, 5396, 5669, 5712, 5803, 5811b, 5872, 5907, 17B40	50, 1354, 1375a, 4052, 4056

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

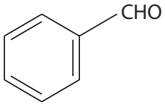
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
		Ammonia (cont.)	3909, 3910, 3934, 3955, 3956, 3973, 3992, 4005–4007, 4009–4011, 4041, 4052, 4056, 4060–4062, 4064, 4065, 4136, 4226, 4245, 4249, 4301, 4319, 4332, 4406, 4636, 4686, 4743, 5042, 5049, 5082, 5079, 5099, 5100, 5129, 5189, 5263, 5359, 5382, 5389, 5512, 5546, 5811b, 5836, 5869a,19A02		
11.	74-79-3 [31]	*L*-Arginine $H_2N\text{-}C(=NH)\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$	3797, 5811b	120, 158, 555a, 555b, 622, 749, 751–756, 1053, 1063–1066, 1068–1074, 1305a, 1329, 1330, 1332, 1351, 1918, 1919, 2079, 2270, 2283, 2337, 2338, 2394a, 2453, 2532, 2597a, 2722, 2795, 2911c, 2939, 3266, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4244, 4249, 5811b	
12.	50-81-7 [32]	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-} 	3257, 3266, 3685, 4249, 4751a	120, 174b, 379, 486, 557, 1053, 1971, 2079, 2270, 2489, 2532, 2939, 3266, 3707, 3922, 4236, 4249, 5079, 5267a, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
13.	7006-34-0 [33]	Asparagine H_2N-CO-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 1965, 2724, 3266, 4159, 4249, 5811b	120, 480, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1223, 1305a, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2532, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4224, 4226, 4244, 4249, 4398c, 5048, 5079, 5126, 5189, 5437, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	
14.	56-84-8 [34]	*L*-Aspartic acid HOOC-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3797, 4159, 4249	120, 158, 480, 555a, 555b, 622, 749, 751–756, 826a, 927, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4159, 4224, 4226, 4244, 4249, 4359, 4398b, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5905, 5907	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

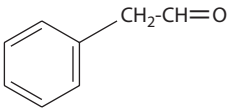
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
15.	100-52-7 [35]	Benzaldehyde 	156, 157, 239, 299, 568b, 2544, 4249591, 830a, 966, 1168, 1215, 1238, 1313, 1360, 1364, 1365, 1368, 1371, 1375a, 1377, 1426, 1427, 1437, 1884, 1949, 1971, 2079, 2088, 2089, 2170, 2270, 2337, 2387, 2506, 2507, 2543, 2545, 2702, 2731, 2735, 2761, 2762, 2765, 2766, 2773–2775, 2799a, 2912, 2939, 3255, 3266, 3302, 3308, 3410, 3555, 3648, 3797, 3876, 4155, 4159, 4249, 4304, 4570a, 5034, 5079, 5811b	120, 404, 568b, 2544, 4249937, 984, 1053, 1063–1066, 1068–1074, 1189, 1368, 1379, 1550, 1590a, 1615, 1854, 1949, 2282, 2337, 2339a, 2386, 2389, 2544, 2611, 2702, 2860a, 2862, 2917a, 2939, 3188, 3194, 3205, 3217, 3219, 3266, 3354, 3539, 3543, 3547, 3550, 3555, 3560, 3561, 3648, 3797, 3905, 3973, 3974a, 4098a, 4249, 5811b	1360, 1375a, 1377, 2387, 2506, 2507, 3401, 3402, 3404
16.	120-14-9 [458]	Benzaldehyde, 3,4-dimethoxy- {veratraldehyde}	568b, 1238, 4249	172a, 174b, 568b, 938, 1053, 1254, 1256, 3266, 3370, 3767a, 4249, 5811b	
17.	121-32-4 [153]	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}	568b, 2731, 2735, 3266, 3712, 4050, 4249, 4566	568b, 633, 1053, 2281, 2282, 2478, 2699, 3266, 3643, 3894, 4050, 4249	
18.	90-02-8 [396]	Benzaldehyde, hydroxy- Benzaldehyde, 2-hydroxy- {salicylaldehyde}	5034 414, 568b, 1238, 1378, 1586, 1626, 1789, 1884, 1906, 2088, 2327c, 2939, 3059, 3266, 3302, 3308, 3557, 3559, 3712, 3797, 4249, 4313, 4317, 4319, 4332, 5811b	120, 172a, 174b, 568b, 937, 1053, 2339a, 2862, 2939, 3059, 3266, 3370, 3973, 3974a, 4249, 5811b	1378, 3395, 3401, 3402, 3404

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
19.	121-33-5 [457]	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}	568b, 1105, 1238, 1352, 1358, 1360, 1361, 1364, 1375, 1375a, 1375b, 1586, 2042–2044, 2327c, 2339, 2570, 2601a, 2640, 2762, 2765, 2767, 3224, 3266, 3302, 3308, 3553, 3557, 3712, 3745, 3797, 4050, 4249, 4379, 5034, 5811b	172a, 174b, 404, 568b, 633, 935, 1053, 1063–1066, 1068–1074, 1105, 1352, 1379, 1590a, 1825, 2281, 2338, 2339, 2339a, 2478, 2389, 2544, 2611, 2699, 2917a, 3159, 3215, 3219, 3266, 3370, 3550, 3643, 3767a, 3797, 3973, 3974a, 4050, 4249, 5811b	1360, 1375a, 3395
20.	123-11-5 [266]	Benzaldehyde, 4-methoxy- {*p*-anisaldehyde}	278, 568b, 1884, 3266, 4036, 4249, 5811b	45, 120, 172a, 174b, 568b, 1053, 1379, 2862, 2917a, 2939, 3059, 3266, 3370, 3797, 3905, 3973, 3974a, 4249, 5811b	
21.	529-20-4 [425]	Benzaldehyde, 2-methyl- {*o*-tolualdehyde}	299, 568b, 937, 3266, 3404, 3797, 4249, 5811b	568b, 937, 172a, 174b, 1053, 3266, 3370, 3797, 4249, 5811b	3402, 3404
22.	620-23-5 [426]	Benzaldehyde, 3-methyl- {*m*-tolualdehyde}	568b, 1884, 3266, 3302, 3794, 5811b	120, 172a, 174b, 524, 568b, 1053, 2389, 2544, 2722, 2862, 2939, 3266, 3370, 3547, 3797, 3974a, 4249, 5811b	3402, 3404
23.	104-87-0 [427]	Benzaldehyde, 4-methyl- {*p*-tolualdehyde}	299, 568b, 1526, 1427, 3266, 4249, 5811b	172a, 174b, 404, 568b, 1053, 2917a, 3266, 3370, 3547, 3905, 4249	3402, 3404
24.	122-03-2 [86]	Benzaldehyde, 4-(1-methylethyl)- {cuminaldehyde}	568b, 1238, 3266, 4249	172a, 174b, 568b, 937, 1053, 1156, 3266, 4090, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
25.	150-78-7 [103]	Benzene, 1,4-dimethoxy-	297, 568b, 3266, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370, 3547, 4249	
26.	100-66-3 [4A]	Benzene, methoxy- {anisole}	568b, 616, 1140, 1416, 1419, 1422, 1427, 1626, 2114, 2939, 3266, 3302, 4249, 5034	172a, 174b, 568b, 1379, 3266	
27.	104-93-8 [303]	Benzene, 1-methoxy-4-methyl- {*p*-methylanisole}	568b, 615, 795, 796, 1426, 1427, 1626, 2939, 3266, 4249, 5811b	172a, 174b, 404, 568b, 1053, 3266	
28.	104-46-1 [26]	Benzene, 1-methoxy-4-(1-propenyl)- {anethole}	1884, 3193, 3266, 3555, 4249	1053, 1254, 1256, 2339a, 3266, 3547, 3555, 3905, 4249, 5811b	
29.	99-87-6 [87]	Benzene, 1-methyl-4-(1-methylethyl)- {*p*-cymene}	143, 299, 568b, 798, 1140, 1313, 1365, 1419, 2767, 3224, 3255, 3266, 3308, 3557, 3797, 4249, 5811b	568b, 1053, 1157, 3266, 3370, 4082, 4249, 5811b	
30.	122-78-1 [370]	Benzeneacetaldehyde {phenylacetaldehyde} 	299, 568b, 1238, 1949, 2769, 3266, 4159, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1063–1066, 1068–1074, 1590a, 1662, 1949, 2282, 2286, 2337, 2389, 2544, 2917a, 3266, 3370, 3543, 3547, 3549, 3550, 3560, 3561, 4249, 5811b	
31.	4411-89-6 [367]	Benzeneacetaldehyde, α-ethylidene- {2-phenyl-2-butenal}	568b, 1587, 3266, 4249, 5811b	174b, 568b, 943, 1053, 2389, 2544, 3266, 3547, 3561, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

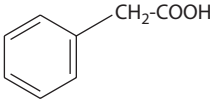
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
32.	103-82-2 [371]	Benzeneacetic acid {phenylacetic acid} 	172, 568b, 1132, 1063–1066, 1068–1074, 1099, 1165, 1359, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1587a, 1882, 1886, 2270, 2338, 2387, 2529, 2543, 2570, 2601a, 2641–2643, 2758, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3266, 3302, 3308, 3394, 3410, 3553, 3557, 4249, 5811b	120, 212, 172a, 174b, 404, 568b, 848, 908, 1053, 1165, 1587a, 1590a, 1620, 1999, 2014, 2270, 2283, 2338, 2386, 2389, 2529, 2544, 2758, 2862a, 2939, 3215, 3219, 3266, 3329, 3332, 3532, 3543, 3549, 3560, 3561, 3767a, 3973, 3974a, 3974b, 4249, 5708, 5811b	1360, 1375a, 2387
33.	101-97-3 [148]	Benzeneacetic acid, ethyl ester {ethyl phenylacetate}	222–224, 568b, 4249	174b, 568b, 1053, 2389, 2544, 3266, 3555, 4249, 5811b	
34.	101-41-7 [284]	Benzeneacetic acid, methyl ester {methyl phenylacetate}	568b, 2543, 2761, 2762, 2766, 2773, 3266, 4249, 4570a	172a, 174b, 568b, 1053, 1254, 1256, 1662, 2339a, 2389, 2544, 3186, 3188, 3266, 3370, 3547, 3905, 4249, 5811b	
35.	102-19-2 [231]	Benzeneacetic acid, 3-methylbutyl ester	2487	172a, 174b, 404, 1053, 3266, 3370	
36.	102-20-5 [363]	Benzeneacetic acid, 2-phenylethyl ester	2487	172a, 174b, 404, 1053, 3266, 3370	
37.	60-12-8 [358]	Benzeneethanol {phenethyl alcohol} C_6H_5-CH_2CH_2-OH [Occasionally listed as 1321-27-3 Ethyl, phenyl-]	172, 568b, 1215, 1360, 1364, 1371, 1375a, 1586, 1882, 1905, 1907, 1949, 1971, 2270, 2387, 2400a, 2422, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858,	120, 172a, 174b, 404, 543a, 568b, 937, 1053, 1063–1066, 1068–1074, 1550, 1587a, 1590a, 1949, 1980, 2282,	1360, 1375a, 2387

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Benzeneethanol {phenethyl alcohol} (cont.)	3059, 3193, 3224, 3255, 3266, 3302, 3410, 3553, 3555, 3557, 3797, 4159, 4249, 4319, 5811b	2283, 2338, 2339a, 2386, 2389, 2422, 2544, 2611, 2861a, 2917a, 2939, 3059, 3188, 3198, 3215, 3219, 3266, 3350, 3370, 3539, 3543, 3547, 3549, 3550, 3555, 3560, 3561, 3797, 3905, 3973, 3974a, 4098a, 4249, 5811b	
38.	100-51-6 [40]	Benzenemethanol {benzyl alcohol} C_6H_5-CH_2OH	155, 172, 568b, 1360, 1371, 1375a, 1426, 1427, 1586, 1882, 1884, 1905, 1907, 2079, 2270, 2387, 2506, 2507, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3059, 3255, 3266, 3302, 3410, 3553, 3555, 3557, 3648, 3794, 3797, 3812, 4159, 4202, 4249, 4319, 4570a, 5079, 5811b	120, 404, 568b, 1053, 1063–1066, 1068–1074, 1550, 1587a, 1590a, 2282, 2283, 2338, 2339a, 2386, 2389, 2544, 2611, 2861a, 2917a, 2939, 3059, 3186, 3188, 3193, 3198, 3215, 3219, 3266, 3350, 3539, 3543, 3547, 3550, 3555, 3560, 3561, 3648, 3797, 3905, 3973, 3974a, 4073b, 4098a, 4202, 4249, 5079, 5811b	1360, 1375a, 2387, 2506, 2507
39.	105-13-5 [28]	Benzenemethanol, 4-methoxy- {anisyl alcohol}		172a, 174b, 568b, 1053, 3266, 3370, 3893, 4249	
40.	1197-01-9 [438]	Benzenemethanol, α,α,4-trimethyl- {*p*,α,α-trimethylbenzyl alcohol} C_6H_5-$C(CH_3)_2OH$	568b, 2570, 4249	568b, 1053, 1156, 2389, 2544, 3266, 4090, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

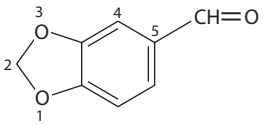
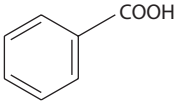
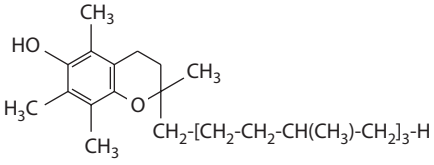
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
41.	536-50-5 [113]	Benzenemethanol, α,4-dimethyl-		937, 1053, 1156, 2389, 3266, 4090	
42.	98-85-1 [305]	Benzenemethanol, α-methyl- C_6H_5-CH(CH_3)OH	568b, 2387, 3266, 4249, 5811b	568b, 967, 1053, 2283, 2386, 2389, 2544, 3266, 3547, 4249, 5811b	2387
43.	104-21-2 [27]	Benzenemethanol, 4-methoxy-, acetate {anisyl acetate}	568b, 3553, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370, 3893, 4249	
44.	501-52-0 [374]	Benzenepropanoic acid {3-phenylpropionic acid; hydrocinnamic acid}	568b, 1360, 1364, 1371, 1375a, 2543, 2761, 2762, 2765, 2766, 2773, 2775, 3266, 3308, 3410, 3506, 3553, 3555, 4249, 5811b	172a, 174b, 568b, 1053, 2092, 3266, 3555, 3973, 4249, 5811b	1360, 1375a
45.	122-97-4 [366]	Benzenepropanol {3-phenyl-1-propanol} C_6H_5-CH_2-CH_2-CH_2OH	1367, 3266, 4249	172a, 174b, 1053, 3266, 4249	
46.	120-57-0 [382]	1,3-Benzodioxole-5-carboxaldehyde {piperonal; heliotropin} 	1238, 2478, 3266, 3894, 4249	172a, 174b, 1053, 1254, 1256, 1590a, 1662, 2478, 3266, 3370, 3643, 3894, 4249, 5811b	
47.	65-85-0 [37]	Benzoic acid {benzenecarboxylic acid} 	126b, 172, 237, 395, 563, 565, 568b, 966, 1063–1066, 1068–1074, 1099, 1132, 1233, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1445, 1586, 1668, 1674, 1882, 1884, 1903, 1904, 2079, 2133, 2170, 2270, 2529, 2543, 2545, 2601a, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2873, 2939, 3059, 3255, 3266, 3302, 3308, 3394, 3410, 3496, 3553, 3555, 3557, 3559, 3876, 4202, 4249, 4304, 4319, 4342, 4354, 5034, 5079, 5207, 5811b	120, 565, 568b, 848, 908, 1053, 1590a, 1620, 1999, 2014, 2283, 2338, 2339a, 2356, 2386, 2389, 2529, 2544, 2862a, 2917a, 2939, 3194, 3217, 3219, 3266, 3329, 3332, 3543, 3547, 3549, 3555, 3560, 3561, 3767a, 3973, 3974a, 4249, 5708, 5709, 5811b	1360, 1375a, 1377, 3393, 3402
48.	93-89-0 [128]	Benzoic acid, ethyl ester {ethyl benzoate}	568b, 1998, 1999, 3266, 4249	174b, 568b, 1053, 2339a, 2389, 2544, 3266, 4249, 5811b	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
49.	93-58-3 [276]	Benzoic acid, methyl ester {methyl benzoate}	568b, 1371, 2487, 2543, 2722, 2773, 3266, 3410, 4249, 5811b	172a, 174b, 568b, 937, 1053, 2339a, 2389, 2544, 3266, 3905, 4249, 5811b	
50.	120-51-4 [41]	Benzoic acid, phenylmethyl ester {benzyl benzoate}	568b, 2543, 2553, 2773, 3263, 3266, 3308, 3485, 3504, 3506, 3797, 4249, 5811b	568b, 1053, 3266, 3547, 3797, 3988, 4249, 5811b	
51.	134-20-3 [275, 33A]	Benzoic acid, 2-amino-, methyl ester {methyl anthranilate}		1053, 1254, 3266, 3370, 4249	
52.	118-61-6 [150]	Benzoic acid, 2-hydroxy-, ethyl ester {ethyl salicylate}		172a, 174b, 1053, 2386, 2995, 3266, 4249, 5811b	
53.	119-36-8 [285]	Benzoic acid, 2-hydroxy-, methyl ester {methyl salicylate}	568b, 1586, 4249	120, 172a, 174b, 568b, 908, 1053, 2094, 2389, 2544, 2611, 2862, 2939, 3059, 3266, 3370, 3547, 3973, 3974a, 3988, 3974a, 4249, 5811b	
54.	87-20-7 [24A]	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester {isoamyl salicylate}		174b, 1256, 2339a, 3266, 4249	
55.	1406-66-2 59-02-9 [424]	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl) {tocopherol}		5811	
		2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]-{α-tocopherol} 	1360, 1373, 1375a, 1842, 1884, 2601a, 2939, 3059, 3170, 3251, 3255, 3257, 3265, 3266, 3271, 3286, 3295, 3300, 3302, 3655a, 3684, 3685, 3797, 3875, 4159c, 4249	120, 174b, 486, 557, 667, 840, 1053, 1651, 2270, 2939, 3059, 3155, 3156, 3170, 3266, 3295, 3347, 3349, 3357, 3484, 3493, 3616, 3655a, 3707, 3755, 3797, 3811, 3875, 3971, 3973, 3974a, 4098a, 4236, 4249, 5079, 5811b	1360, 1375a

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

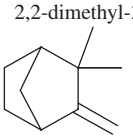
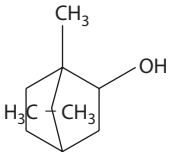
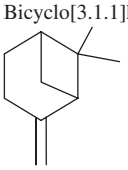
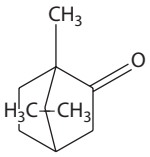
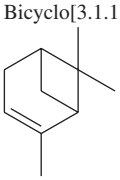
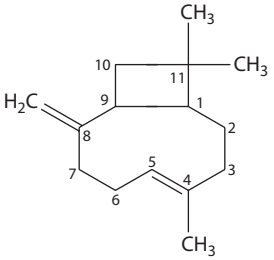
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
56.	79-92-5 [65]	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- {camphene} 	3266, 3302, 4249	1053, 2282, 3266, 3370, 4249	
57.	507-70-0 [47]	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *endo*- {borneol} 	568b, 1971, 3266, 3302, 4249, 4319	120, 909, 1053, 1156, 1971, 2270, 2939, 3266, 3374, 3797, 3971, 3974a, 4090, 4249, 5079, 5811b	
58.	127-91-3 18172-67-3 [380]	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- {β-pinene} 	314, 1140, 1168, 1365, 1375, 1375b, 1416, 1422, 1613, 3224, 3254, 3266, 3302, 3794, 3797, 4249, 5811b	134, 172a, 174b, 909, 1053, 2282, 2339a, 3266, 4249, 5811b	
59.	76-22-2	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- {camphor} 		568b, 1156, 1254, 1256, 2095, 2389, 2544, 4090, 4249, 5811b	
60.	80-56-8 7785-26-4 [379]	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- {α-pinene} 	1168, 1375, 1375b, 1822, 2870, 2939, 3254, 3266, 3451, 4249, 4259, 5811b	123, 172a, 174b, 909, 1053, 1157, 2282, 2339a, 3266, 3547, 3971, 4249	
61.	87-44-5 [71]	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4*E*,9S*)]- {β-caryophyllene} 		172a, 174b, 937, 1053, 1156, 1254, 1256, 2611, 3266, 3370, 4073b, 4090, 4249, 5811b	
62.	96-17-3 [306]	Butanal, 2-methyl- {2-methylbutyraldehyde} $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH{=}O$	299, 314, 568b, 1221, 1063–1066, 1068–1074, 1221, 1360, 1375a, 1418, 1419, 1999, 2337, 2545, 2767, 3219, 3266, 3308, 3508, 4249, 4570a, 5770, 5811b	172a, 174b, 568b, 1053, 1550, 2337, 2339a, 2917a, 3186, 3188, 3266, 4249, 5811b	1360, 1375a

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
63.	590-86-3 [307]	Butanal, 3-methyl- {3-methylbutyraldehyde; isovaleraldehyde} $(H_3C)_2$═CH-CH_2-CH═O	173a, 299, 314, 405, 407, 408, 568b, 605, 1039, 1063–1066, 1068–1074, 1140, 1238, 1348–1350, 1354, 1360, 1365, 1375, 1375a, 1375b, 1412–1414, 1416, 1418, 1419, 1884, 2003, 2293, 2337, 2573–2375, 2767, 2782, 2804, 2927, 3254, 3266, 3302, 3308, 3413, 3508, 3557, 3794, 3817, 4052, 4056, 4162, 4249, 4319, 4570, 5034, 5770, 5811b	172a, 174b, 568b, 647, 909, 937, 1053, 1157, 1550, 1615, 2337, 2339a, 2914, 2917a, 2939, 3188, 3266, 3350, 3370, 3626, 3797, 3974a, 4223, 4225, 4249, 5811b	1354, 1360, 1375a, 4052, 4056
64.	106-65-0 [105]	Butanedioic acid, dimethyl ester {dimethyl succinate}	1235, 3266, 3553, 4249	1053, 3266	
65.	6915-15-7 [255]	Butanedioic acid, hydroxy- {malic acid} HOOC-CHOH-CH_2-COOH	565, 1371, 2939, 3059, 3061, 3224, 3266, 3302, 3308, 3496, 3555, 3741, 3743, 4249, 5811b	120, 172a, 256, 385, 543a, 555, 634, 677b, 722, 826a, 835, 836, 838, 839, 840, 963, 1053, 1063–1066, 1068–1074, 1279, 1289, 1305a, 1330, 1332, 1333, 1548 1923, 1933a, 1982, 2014, 2079, 2270, 2283, 2356, 2529, 2532, 2543, 2545, 2688, 2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3052, 3107, 3194, 3266, 3353, 3476, 3486, 3555, 3655b, 3656, 3667, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 3974b, 3976, 3984, 4103, 4131, 4249, 4275, 5079, 5109, 5126, 5189, 5244, 5342, 5381, 5384, 5389, 5419, 5430, 5477, 5478, 5745, 5749, 5753, 5811b, 5832, 5896, 17B17	3393

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
66.	526-83-0 [411]	Butanedioic acid, 2,3-dihydroxy- {tartaric acid} HOOC-CHOH-CHOH-COOH	1268, 1270, 3266, 3555, 4249	1053, 1268, 1270, 1982, 3266, 3555, 4249, 5529, 5764	
67.	107-88-0 [49]	1,3-Butanediol {1,3-butylene glycol} H_3C-CHOH-CH_2-CH_2OH	627, 2246, 2548, 2549, 2790, 3266, 3302, 3308, 3553, 3689, 4249	627, 1053, 2188, 2195, 2196, 3264, 3266, 4249, 5811b	
68.	431-03-8 29350-67-2 [50]	2,3-Butanedione {diacetyl; biacetyl} H_3C-CO-CO-CH_3	111, 112, 314, 480, 568b, 605, 966, 1140, 1067, 1153, 1231, 1232, 1238, 1239, 1348–1352, 1354, 1374, 1375, 1375a, 1375b, 1377, 1378, 1416, 1418, 1419, 1491, 1586, 1587, 1589, 1637, 1884, 1947, 1966, 2063, 2079, 2091, 2170, 2220, 2270, 2293, 2310, 2337, 2469, 2506, 2507, 2543, 2545, 2559, 2559a, 2570, 2704, 2765, 2767, 2775, 2777, 2782, 2804, 2822, 2857, 2866, 2939, 3059, 3105, 3254, 3255, 3266, 3300, 3302, 3308, 3341, 3413, 3475, 3557, 3794, 3876, 3897, 4005–4007, 4052, 4056, 4249, 4257, 4259, 4319, 4360, 4570a, 4732, 5034, 5079, 5680, 5811b, 5835	120, 174b, 568b, 1053, 1550, 2283, 2293, 2337, 2339a, 2704, 3186, 3188, 3266, 3561, 4249, 5079, 5371, 5372, 5811b	1354, 1375a, 1377, 1378, 2244, 2506, 2507, 3401, 3404, 4052, 4056
69.	107-92-6 [61]	Butanoic acid {butyric acid} H_3C-$(CH_2)_2$-COOH	526, 563, 565, 568b, 960, 1063–1066, 1068–1074, 1132, 1140, 1360, 1364, 1365, 1371, 1375a, 1388–1390, 1586, 1587a, 1638, 1884, 1886, 1903, 1904, 1917, 2043, 2079, 2088, 2170, 2270, 2337, 2338, 2387, 2493, 2543, 2570, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3263, 3266, 3302, 3308, 3410, 3452, 3495, 3553, 3799, 3800, 3809, 3910, 3912, 4052, 4056, 4064, 4065, 4185, 4249, 4304, 4319, 4406, 5079, 5189, 5811b	172a, 174b, 404, 568b, 647, 848, 981a, 1053, 1085, 1087, 1276, 1587a, 1590a, 1982, 1999, 2014, 2092, 2337, 2338, 2570, 2649, 2722, 3266, 3328, 3370, 3507, 3655b, 3809, 3973, 3974a, 3974b, 4064, 4249, 5079, 5381, 5708, 5735, 5811b, 5845	1360, 1375a, 2387, 3393, 3401, 3402, 4052, 4056
70.	105-54-4 [129]	Butanoic acid, ethyl ester {ethyl butyrate} H_3C-$(CH_2)_2$-COO-C_2H_5	565, 1140, 1971, 2088, 2858, 2939, 3266, 3302, 3308, 3797, 4249, 4319, 5811b	174b, 1053, 2939, 3266, 3797, 3974a, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
71.	103-37-7 [42]	Butanoic acid, phenylmethyl ester {benzyl butyrate} $H_3C\text{-}(CH_2)_2\text{-}COO\text{-}CH_2C_6H_5$	568b, 3263, 3266, 3485, 3504, 3506, 3557, 3797, 4249	172a, 174b, 568b, 1053, 2389, 2544, 3266, 3370, 3561, 3797, 4249, 5811b	
72.	116-53-0 600-07-7 [308]	Butanoic acid, 2-methyl- {2-methylbutyric acid} $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}COOH$	568b, 1140, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1587a, 1999, 2270, 2338, 2387, 2543, 2545, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2939, 3266, 3410, 3452, 3553, 3797, 4249, 5811b	120, 172a, 174b, 404, 568b, 848, 937, 938, 1053, 1587a, 1590a, 1999, 2014, 2283, 2288, 2291, 2338, 2339a, 2386, 2389, 2544, 2570, 2722, 2862, 2917a, 2939, 3219, 3266, 3329, 3370, 3537, 3547, 3550, 3560, 3561, 3973, 3974a, 4249, 5708, 5811b, 5831	1360, 1375a, 2387
73.	7452-79-1 [124]	Butanoic acid, 2-methyl-, ethyl ester		172a, 174b, 1053, 2339a, 3266, 3370	
74.	503-74-2 [245]	Butanoic acid, 3-methyl- {isovaleric acid} $(H_3C)_2{=}CH\text{-}CH_2\text{-}COOH$	563, 565, 775, 960, 1063–1066, 1068–1074, 1132, 1360, 1371, 1375, 1375a, 1375b, 1388–1390, 1418, 1586, 1587a, 1668, 1886, 1903, 1904, 2043, 2079, 2270, 2337, 2338, 2387, 2543, 2570, 2619, 2623, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 3224, 3266, 3302, 3308, 3410, 3452, 3553, 3557, 3794, 3799, 3800, 3809, 4249, 4319, 4997, 5811b	120, 172a, 174b, 404, 563, 565, 908, 909, 981a, 1053, 1085, 1221, 1587a, 1590a, 1982, 1999, 2014, 2079, 2283, 2291, 2337, 2338, 2339a, 2386, 2389, 2544, 2570, 2611, 2816, 2817, 2917a, 2939, 3215, 3219, 3266, 3507, 3537, 3545, 3547, 3550, 3560, 3561, 3809, 3973, 3974a, 3974b, 4249, 5079, 5180, 5708, 5735, 5811b, 5846	1360, 1375a, 2387, 3393

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
75.	140-26-1 [362]	Butanoic acid, 3-methyl-, 2-phenylethyl ester {phenethyl isovalerate}	318	172a, 174b, 318, 947, 1053, 2339a, 2386, 3266, 3370, 4249	
76.	103-38-8 [8A]	Butanoic acid, 3-methyl-, phenylmethyl ester {benzyl isovalerate}		174b, 2386, 2389, 2544, 3266, 3561, 4249, 5811b	
77.	108-64-5 [136]	Butanoic acid, 3-methyl-, ethyl ester {ethyl isovalerate} $(H_3C)_2$═CH-CH_2-COO-C_2H_5	565, 1903, 1904, 2858, 2939, 3266, 4249, 4319, 5811b	908, 1053, 2339a, 2389, 2544, 3266, 3974a, 4249, 5811b	
78.	556-24-1 [279]	Butanoic acid, 3-methyl-, methyl ester {methyl isovalerate} $(H_3C)_2$═CH-CH_2-COO-CH_3		568b, 908. 1053, 2339a, 2389, 2544, 3266, 3370, 4249, 5811b	
79.	659-70-1 [229]	Butanoic acid, 3-methyl-, 3-methylbutyl ester {isoamyl isovalerate}	1379, 2487, 5811b	172a, 174b, 1053, 1379, 3266, 3370	
80.	140-27-2 [79]	Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester	2487	1053, 3266, 3370	
81.	76-50-6 [9A]	Butanoic acid, 3-methyl-, 1,7,7-trimethylbicyclo[2.2.1] hept-2-yl ester, endo- {bornyl isovalerate}		174b, 1590a, 3266, 4249, 4787	
82.	71-36-3 [51]	1-Butanol {*n*-butyl alcohol} H_3C-$(CH_2)_2$-CH_2OH	172, 568b, 1140, 1218, 1373, 1375a, 1377, 1378, 1416, 2559, 2559a, 3255, 3257, 3265, 3266, 3302, 3559, 3797, 4249, 5811b	568b, 1053, 1550, 2339a, 3186, 3188, 3266, 3328, 3905, 3973, 4249	1375a, 1377, 1378
83.	78-93-3 [52]	2-Butanone {methyl ethyl ketone} H_3C-CO-CH_2-CH_3	37, 38, 111, 112, 172, 173a, 174b, 174c, 299, 314, 480, 544–546, 564, 568b, 605, 643, 645, 688, 764a, 778, 966, 1038, 1050, 1063–1074, 1140, 1153, 1154, 1215, 1238, 1284, 1348–1352, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1412–1414, 1416, 1418, 1419, 1427, 1495, 1586, 1589, 1590, 1637, 1668,	404, 568b, 647, 984, 1053, 1590, 2337, 2339a, 2914, 2939, 3266, 3555, 3626, 3797, 3974a, 4223, 4225, 4249, 5811b	1354, 1375a, 1377, 1378, 2244, 2387, 2506, 2507, 3401, 4052, 4056

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		2-Butanone {methyl ethyl ketone} (cont.)	1875, 1947, 1966, 2002, 2003, 2063, 2079, 2089, 2091, 2270, 2293, 2310, 2337, 2387, 2483, 2506, 2507, 2520, 2543, 2545, 2559, 2559a, 2570, 2591, 2765, 2767, 2777, 2782, 2804, 2822, 2857, 2858, 2866, 2939, 2942, 3007, 3059, 3105, 3132, 3135, 3136, 3254, 3255, 3266, 3300, 3308, 3396, 3413, 3431, 3436, 3438, 3482, 3493, 3530, 3551, 3555, 3557, 3692, 3794, 3797, 3817, 3876, 3897, 3901, 3939, 4005–4007, 4052, 4056, 4078, 4104, 4162, 4249, 4257, 4290, 4319, 4360, 4570a, 5034, 5049, 5770, 5811b, 5836		
84.	513-86-0 [3]	2-Butanone, 3-hydroxy- {acetoin} $H_3C\text{-}CO\text{-}CHOH\text{-}CH_3$	568b, 1063–1066, 1068–1074, 1426, 1427, 1882, 2337, 2761, 2762, 2765, 2766, 2777, 3266, 3410, 3555, 3559, 4249, 5811b	174b, 404, 568b, 1053, 2339a, 2339b, 2386, 2917a, 3266, 3549, 4249, 5811b	2244, 3401, 3402, 3404
85.	5471-51-2 [219]	2-Butanone, 4-(4-hydroxyphenyl)- {4-(*p*-hydroxyphenyl)-2-butanone}	374, 568b, 3266, 3712, 4249	172a, 174b, 568b, 1053, 3266, 3370	
86.	13201-46-2 [301]	2-Butenoic acid, 2-methyl-, (*Z*)- {angelic acid}	565, 568b, 1586, 1886, 2767, 2769, 3266, 3553, 3557, 4249, 5811b	120, 172a, 174b, 404, 568b, 937, 938, 1053, 2270, 2283, 2611, 2917a, 3266, 3153, 3547, 4249, 5811b	3393
87.	80-59-1 [301]	2-Butenoic acid, 2-methyl-, (*E*)- {tiglic acid}	565, 1586, 1886, 2767, 2769, 3266, 3553, 3557, 4249	120, 172a, 174b, 404, 937, 938, 1053, 2270, 2283, 2611, 2917a, 3266, 3153, 3547, 4249	3393

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

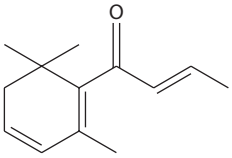
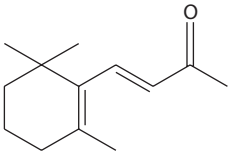
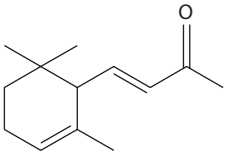
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
88.	541-47-9 [301]	2-Butenoic acid, 3-methyl-	568b, 2767, 3266, 3553, 4249, 5811b	404, 568b, 1053, 2611, 3186, 3266, 3547, 3550, 4249	
89.	23726-93-4 23696-85-7 [442]	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)- {β-damascenone} 	568b, 775, 1371, 1663, 1949, 2765, 2766, 2773, 3266, 3410, 4249, 4570a	172a, 174b, 404, 543a, 568b, 936, 937, 1053, 1063–1066, 1068–1074, 1156, 1254, 1256, 1590a, 1949, 2338, 2339a, 2339b, 2386, 2389, 2544, 2611, 2917a, 3218, 3266, 3370, 3547, 3549, 4090, 4098a, 4159, 4249, 5811b	
90.	80111-68-8 23770-92-3 35044-68-9 [439]	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)- {damascone}	568b, 1075, 2545, 4249	172a, 174b, 568b, 911, 937, 1053, 1063–1066, 1068–1074, 1156, 1254, 1256, 1590a, 2339a, 2339b, 2386, 2389, 2544, 3218, 3266, 3370, 3547, 3549, 4090, 4098a, 4249, 5811b	
91.	623-15-4 [174]	3-Buten-2-one, 4-(2-furanyl)-	568b, 1238, 1587, 3266, 4249, 5811b	568b, 1053, 3266, 3893, 4249	
92.	122-57-6 [369]	3-Buten-2-one, 4-phenyl- C_6H_5-CH═CH-CO-CH_3	568b, 642, 2570, 3266, 4249	568b, 1053, 2389, 2544, 3266, 4249, 5811b	
93.	14901-07-6 [221] [22A]	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- {β-ionone} 	297, 568b, 1949, 3266, 4249	172a, 174b, 404, 543a, 568b, 908, 911, 937, 1053, 1156, 1254, 1854, 1949, 2338, 2339a, 2339b, 2386, 2389, 2544, 2611, 2917a, 3217, 3218, 3266, 3354, 3370, 3545, 3547, 3560, 3561, 3647, 4090, 4159, 4249, 5811b	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
94.	127-41-3 8013-90-9 [220]	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- {α-ionone} 	3266, 4249, 5811b	172a, 174b, 404, 908, 1053, 1156, 1254, 1256, 2338, 2339a, 2339b, 2389, 2544, 2611, 2917a, 2939, 3218, 3266, 3370, 3560, 3561, 3647, 3973, 4090, 4249, 5811b	
95.	124-38-9 [66]	Carbon dioxide	28, 30, 31, 90, 126a, 126b, 162–170, 172, 174, 217, 199, 220, 222–224, 238, 239, 337, 375, 403, 421, 445, 474, 480, 491, 499, 544–546, 568b, 621, 686, 722, 855, 857, 916, 918a, 920, 957, 966, 1048a, 1051, 1063–1074, 1099, 1119, 1140, 1202, 1205, 1208, 1243, 1263, 1284, 1329, 1330, 1332–1334, 1348–1350, 1352, 1354, 1373, 1375a, 1377, 1378, 1388–1390, 1413, 1419, 1420, 1437, 1442, 1445, 1464, 1466, 1468, 1477, 1478, 1492, 1541, 1589, 1600, 1664, 1668, 1673, 1674, 1693, 1709, 1744, 1760, 1803, 1837, 1842, 1924, 1935–1937, 1963, 1966, 1977, 2029, 2059, 2060, 2062, 2066, 2068, 2079, 2117, 2124, 2133, 2134a, 2142, 2170, 2183, 2196, 2198, 2252, 2263, 2265, 2270, 2293, 2310, 2326, 2342, 2343, 2348, 2457, 2506, 2507, 2524, 2537, 2543, 2545, 2548, 2549, 2555, 2571, 2582, 2624, 2634, 2659, 2662, 2683, 2761, 2762, 2777, 2780, 2782, 2798, 2799, 2799a, 2804, 2866, 2867, 2913, 2919, 2920–2922, 2928, 2939, 2942, 2973, 3059, 3088, 3102, 3116, 3120, 3121, 3132, 3190, 3224, 3254, 3255, 3257, 3266, 3302, 3308, 3317, 3324, 3336, 3378,	212, 256, 568b, 1053, 1206a, 2079, 3266, 4249, 4577, 4795, 4926, 5079, 5132, 5165, 5189, 5192, 5193, 5811b, 17B40	1228, 1330, 1332, 1354, 1375a, 1377, 1378, 2506, 2507, 3192, 4052, 4056, 4249

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

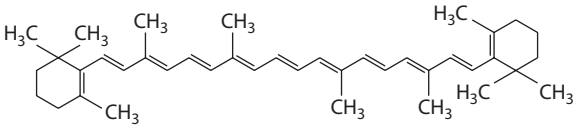
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Carbon dioxide (cont.)	3412, 3482, 3493, 3511, 3516, 3522, 3548, 3564, 3640, 3795, 3870, 3876, 3880, 3882, 3883, 3897, 3909, 3910, 3929, 3930, 3939, 3973, 3987, 3992, 4052, 4055, 4056, 4064, 4067, 4078a, 4079, 4145, 4162, 4212, 4215, 4249, 4251, 4319, 4332, 4360, 4364, 4365, 4406, 4418, 5047, 5079, 5140, 5207, 5359, 5512, 5811b		
96.	7235-40-7 [67]	β,β-Carotene {β-carotene, all-*trans*} 	3257	120, 367, 433, 543a, 585, 830a, 832, 835, 838, 922b, 943, 971, 972, 1053, 1063–1066, 1068–1074, 1110, 1156, 1254, 1256, 1927a, 1941, 1956, 2079, 2270, 2283, 2338, 2339b, 2543, 2545, 2611, 2761, 2762, 2765, 2766, 2939, 3059, 3194, 3218, 3266, 3616, 3645, 3797, 3971, 3973, 3974a, 4090, 4159, 4222, 4249, 4286, 5079, 5189, 5300, 5811b	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

	CAS No.	Name (per CA Collective Index)	References		
			Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
97.	9004-34-6 [73]	Cellulose		120, 172, 248, 277, 337, 385, 385a, 420, 451, 535, 539, 601, 602, 629, 665, 722, 1053, 1063–1066, 1068–1074, 1077, 1228, 1289, 1329, 1330, 1333, 1352, 1878a, 1885, 1887, 1933a, 2014, 2042, 2044, 2046, 2070, 2079, 2154, 2195, 2270, 2283, 2338, 2356, 2454, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2913, 2919, 2939, 3029, 3059, 3087, 3192, 3264, 3266, 3305, 3371, 3372, 3393, 3395, 3401, 3402, 3404, 3405, 3409, 3430, 3449, 3450, 3462, 3468, 3551, 3665a, 3702, 3797, 3871, 3973, 3974a, 3975, 3976, 4104, 4151, 4249, 4261, 4262, 4418, 4999, 5079, 5189, 5344, 5811b, 5841	
98.	99-83-2 1329-99-3 [356]	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- {α-phellandrene}	1154, 3266, 4249	172a, 174b, 1053, 3266	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

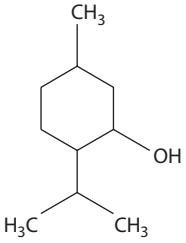
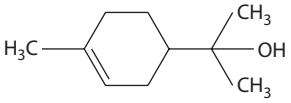
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
99.	4221-98-1 [356]	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)-, (R)- {α-phellandrene}	568b, 3266, 4249	172a, 174b, 568b, 1053, 3266	
100.	89-78-1 [259]	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {menthol} 	172, 174e, 309, 315, 355, 391, 409, 449, 568b, 873, 874, 1104, 1106–1108, 1269, 1360, 1361, 1375a, 1377, 1426, 1427, 1448, 1482, 1627, 1637, 1874, 1933, 1936, 1949, 2020, 2062, 2143, 2242, 2299, 2410, 2415, 2522, 2562, 2628, 2761, 2762, 2765, 2766, 2770–2773, 2775–2777, 2800, 2923, 2939, 3072b, 3132, 3153, 3154, 3187, 3193, 3228, 3266, 3302, 3308, 3553, 3603, 3662, 4103, 4249, 4259, 4268, 4319, 5055, 5058, 5079, 5506, 5530, 5544, 5545, 5549, 5556, 5575	172a, 174b, 309, 315, 355, 449, 568b, 722, 873, 1053, 1104, 1106–1108, 1156, 1482, 1627, 1874, 1933a, 1936, 1949, 2020, 2242, 2284, 2339a, 2356, 2386, 2389, 2402, 2415, 2544, 2562, 2761, 2762, 2770–2772, 2776, 2800, 2923, 2939, 3153, 3154, 3266, 3354, 3370, 3476, 3497, 3547, 3549, 3560, 3561, 3603, 3905, 3974a, 3988, 4090, 4103, 4249, 4259, 5058, 5079, 5506, 5549, 5811b	1360, 1375a, 1377
101.	2408-37-9 [443]	Cyclohexanone, 2,2,6-trimethyl- {2,6,6-trimethylcyclohexanone}		404, 1053, 2339a, 2389, 2544, 3218, 3266, 3547, 4249	
102.	89-80-5 10458-16-7 [260]	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}	309, 568b, 1238, 1361, 1936, 3266, 4247, 4248	172a, 174b, 568b, 1053, 2339a, 2385a, 3266, 3370, 4249	
103.	14073-97-3	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, (*L*) {*L*-menthone}	5811, 5811a, 5811b		
104.	1125-21-9 [440]	2-Cyclohexene-1,4-dione, 2,6,6-trimethyl- {4-ketoisophorone; 4-oxoisophorone}	568b, 1360, 1375a, 1949, 2543, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 3266, 4249, 5811b	404, 568b, 937, 1053, 1254, 1590a, 1949, 2338, 2386, 2389, 2544, 2917a, 3188, 3215, 3219, 3266, 3543, 3545, 3560, 3561, 3905, 4249	1360, 1375a

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
105.	98-55-5 10482-56-1 [412]	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {α-terpineol} 	568b, 1054, 2543, 2773, 3266, 3555, 4249	172a, 174b, 568b, 1053, 1254, 1256, 2389, 2544, 2917a, 3215, 3266, 3370, 3547, 3550, 3555, 4249, 5811b	
106.	80-26-2 [414]	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate {α-terpinyl acetate}	3266, 4249	172a, 174b, 1053, 1156, 2389, 2544, 3266, 3370, 4090, 4249, 5811b	
107.	562-74-3 [69]	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- {4-carvomenthenol}	3266, 3555, 4249	131, 172a, 174b, 1053, 2339a, 3266, 3370, 3555, 4249	
108.	99-49-0 6485-40-1 [70]	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*l*-carvone}	568b, 2570, 2769, 3266, 3557, 4249, 5811, 5811a, 5811b	172a, 174b, 568b, 1053, 1156, 1254, 1256, 2339a, 2389, 2544, 3188, 3266, 3370, 4090, 4249, 5811, 5811a, 5811b	
109.	89-81-6 [381]	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- {*D*-piperitone}	5811b	404, 568b, 1053, 1156, 2095, 2389, 2544, 3266, 3370, 3547, 4090, 4098a, 4249, 5811b	
110.	13215-88-8 [53]	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-	1075, 2570, 2777, 3266, 3288, 3302, 3410, 3553, 3557, 5811b	922b, 943a, 1053, 1063–1066, 1068–1074, 1254, 1256, 1590a, 1854, 2338, 2389, 2544, 3266, 3288, 3355, 3547, 4098a, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

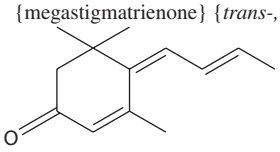
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
111.	5164-78-3 [53]	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-,(*E,E*)- {megastigmatrienone} {*trans-, trans*-K_{1a}} 	568b, 775, 1063–1066, 1068–1074, 1352, 1364, 1365, 1371, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2766, 2767, 2773, 2775, 3251, 3288, 3308, 3397, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2282, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249, 5811b	2387
112.	5298-13-5 [53]	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*E,Z*)- {megastigmatrienone} {*trans*-, *cis*-K_{2a}}	568b, 775, 1063–1066, 1068–1074, 1352, 1360, 1364, 1365, 1371, 1375a, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 3251, 3288, 3308, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249	1360, 1375a, 2387
113.	5492-79-5 [53]	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-,(*Z,E*)- {megastigmatrienone}{*cis*-, *trans*-K_{1b}}	568b, 775, 1063–1066, 1068–1074, 1352, 1360, 1364, 1365, 1371, 1375a, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3251, 3288, 3308, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249, 5811b	1360, 1375a, 2387

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
114.	5164-79-4 [53]	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,Z*)- {megastigmatrienone}{*cis*-, *cis*-K_{2b}}	568b, 775, 1063–1066, 1068–1074, 1352, 1364, 1365, 1371, 1586, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 3251, 3288, 3308, 3410, 3553, 3557, 4249, 4380, 4570a	404, 543a, 568b, 908, 911, 943, 1063–1066, 1068–1074, 1149, 1149a, 1254, 1256, 1352, 1590a, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3205, 3215, 3219, 3354, 3355, 3543, 3547, 3549, 3550, 3560, 3561, 3760a, 3905, 4098a, 4159, 4249, 5811b	2387
115.	13494-06-9 [106]	1,2-Cyclopentanedione, 3,4-dimethyl-	91, 568b, 1063–1066, 1068–1074, 1215, 1352, 1586, 2543, 2545, 2767, 3266, 3553, 3557, 4249, 4570a, 5811b	172a, 174b, 568b, 1053, 4266	
116.	13494-07-0 [107]	1,2-Cyclopentanedione, 3,5-dimethyl-	91, 568b, 1352, 1375, 1375b, 1378, 1586, 2327c, 2767, 3266, 3553, 3557, 4249, 5811b	568b, 1053, 3266	1378
117.	765-70-8 [35A]	1,2-Cyclopentanedione, 3-methyl- {cyclotene}	91, 172, 568b, 775, 1063–1066, 1068–1074, 1352, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1377, 1378, 1744, 1842, 1882, 2387, 2543, 2545, 2570, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3266, 3394, 3397, 3410, 3553, 3557, 4570a, 5512	174b, 568b, 2386, 2389, 2544, 3266, 3905, 4249, 5811b	1360, 1375a, 1377, 1378, 2387, 3401, 3402, 3405
118.	80-71-7 [310]	2-Cyclopenten-1-one, 2-hydroxy-3-methyl- {methylcyclopentenolone}	92, 93, 596, 597, 1099, 1133, 1375, 1375b, 1586, 1958, 1960, 2327c, 2337, 2387, 2493, 2601a, 3255, 3266, 3553, 3555, 3557, 4249, 5034, 5811b	174b, 1053, 2337, 2389, 2544, 3266, 3370, 3430, 3555, 4249, 5811b	2387, 3402, 3404

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
119.	52-90-4 [88]	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto-(R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1274, 3265, 3266, 4249	120, 158, 172, 342, 722, 927, 1053, 1128b, 1305a, 1351, 1918, 2049, 2337, 2939, 3266, 3491, 3729, 3797, 3974a, 3978, 4224, 4249, 4398c, 5079, 5189, 5376, 5811b, 5874, 5881	
120.	25152-84-5 [89]	2,4-Decadienal, (*E,E*)-	568b, 3266, 3553, 4249	568b, 1053, 3186, 3188, 3266, 4249	
121.	112-31-2 [92]	Decanal {capraldehyde}	60, 568b, 1238, 3302, 4249, 5811b	172a, 174b, 404, 568b, 937, 1053, 2337, 2389, 2544, 2913a, 3266, 3370, 4249, 5811b	
122.	334-48-5 [93]	Decanoic acid {capric acid} $H_3C\text{-}(CH_2)_8\text{-}COOH$	60, 563, 565, 568b, 809, 1132, 1232, 1348, 1360, 1375, 1375a, 1375b, 1668, 1884, 1917, 2418, 2939, 3266, 3293, 3308, 3553, 3797, 4249, 4993, 5079, 5811b	60, 120, 172a, 174b, 404, 524, 568b, 848, 908, 565, 1053, 1893a, 1893b, 2270, 2356, 2283, 2389, 2544, 2592, 2611, 2917a, 3266, 3370, 3543, 3545, 3547, 3560, 3561, 3633, 3767a, 3974a, 4249, 4993, 5657, 5695, 5811b	1360, 1375a
123.	110-38-3 [131]	Decanoic acid, ethyl ester {ethyl caprate} $H_3C\text{-}(CH_2)_8\text{-}COO\text{-}C_2H_5$	3266, 4249	172a, 174b, 908, 1053, 2389, 2544, 3266, 3370, 4249, 5811b	
124.	112-30-1 [94]	1-Decanol {capric alcohol} $H_3C\text{-}(CH_2)_8\text{-}CH_2OH$	172, 568b, 1333, 1365, 3255, 3559, 4249, 5811b	568b, 1053, 1157, 1333, 2650a, 2650b, 3266, 3370, 3633, 3811a, 3973, 3977, 4098a, 4249, 5811b	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
125.	9004-53-9 [16A]	Dextrin		120, 174b, 2079, 2283, 2939, 2947b, 2947c, 3266, 3449, 4249, 5079, 5189, 5344, 5449, 5811b	
126.	40596-69-8 [263]	2,4-Dodecadienoic acid, 11-methoxy-3,7,11-trimethyl-, 1-methylethyl ester, (*E,E*)- {Methoprene®; Altosid®} $(H_3C)_2$═$C(OCH_3)$-$(CH_2)_3$-$CH(CH_3)$-CH_2-CH═CH-$C(CH_3)$═CH-COO-$CH(CH_3)_2$	1242, 1243, 21A19	1053, 1242, 1243, 1588, 2483a, 3266, 3633, 21A19	
127.	143-07-7 [247]	Dodecanoic acid {lauric acid} H_3C-$(CH_2)_{10}$-COOH	60, 172, 257, 258, 568b, 765, 809, 1132, 1232, 1375, 1586, 1785, 1906, 1917, 2418, 2529, 2570, 2767, 2939, 3266, 3293, 3302, 3308, 3557, 4030, 4249, 4319, 4993, 5079, 5811b	60, 101, 120, 172a, 174b, 404, 568b, 908, 1053, 1785, 1893a, 1893b, 2092, 2093, 2270, 2283, 2339a, 2356, 2529, 2862, 2917a, 3194, 3266, 3370, 3547, 3633, 3973, 3974a, 4249, 4280, 4993, 5695	
128.	106-33-2 [138]	Dodecanoic acid, ethyl ester {ethyl laurate} H_3C-$(CH_2)_{10}$-COO-C_2H_5		172a, 174b, 568b, 908, 1053, 2389, 2544, 3266, 3370, 4249	
129.	7212-44-4 [326]	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- {nerolidol}	3224, 3266, 4249	172a, 174b, 1053, 2389, 2544, 2611, 3266, 4098a, 4249, 5811b	
130.	4602-84-0 3790-71-4 [171]	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- {farnesol}	1586, 2601a, 2767, 3224, 3251, 3266, 3284, 3285, 3302, 3557, 4249, 4570a, 5811b	172a, 174b, 404, 909, 1053, 2386, 2917a, 3266, 4249	
131.	64-17-5 [127]	Ethanol {ethyl alcohol}	37, 38, 172, 222–224, 314, 568b, 605, 916, 1140, 1375a, 1377, 1378, 1412–1414, 1416, 1419, 1422, 1449, 1481, 1905, 1907, 2088, 2270, 2634, 2858, 2939, 3224, 3255, 3257, 3265, 3302, 3308, 3530, 3692, 3797, 3882, 3901, 4005–4007, 4052, 4056, 4162, 4249, 4319, 4570a, 5811b	120, 172a, 174b, 568b, 1053, 1481, 1550, 2702a, 2339a, 2861a, 2939, 3266, 3328, 3370, 3797, 3973, 3974a, 4249, 5079, 5811b	1375a, 1377, 1378, 4052, 4056

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
132.	1072-83-9 [273]	Ethanone, 1-(1*H*-pyrrol-2-yl)- {2-acetylpyrrole; methyl 2-pyrrolyl ketone}	568b, 1360, 1371, 1375a, 1375, 1375b, 1428, 1586, 1587a, 2337, 2387, 2543, 2545, 2570, 2731, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3059, 3266, 3397, 3410, 3444, 3553, 3555, 3557, 4249, 4407, 5811b	120, 172a, 174b, 404, 568b, 937, 965, 1053, 1063–1066, 1068–1074, 1590a, 1854, 2337, 2386, 2389, 2544, 2861a, 2862, 2917a, 2939, 3188, 3198, 3215, 3217, 3266, 3354, 3543, 3545, 3547, 3555, 3560, 3561, 3797, 3905, 3974a, 4249, 5811b	1360, 1375a, 2387
133.	1122-62-9 [9]	Ethanone, 1-(2-pyridinyl)- {2-acetylpyridine}	1099, 1360, 1371, 1375a, 1587, 1949, 2234, 2543, 2727, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2939, 3056, 3255, 3266, 3398, 3491, 3557, 4249, 4570a, 5034	937, 1053, 1949, 2336, 2337a, 2339a, 2359, 2724, 2917a, 2939, 3056, 3204, 3215, 3266, 3491, 3550, 3974a, 4159a, 4249	1360, 1375a
134.	350-03-8 [10]	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine; methyl 3-pyridyl ketone}	568b, 761, 1075, 1078, 1083, 1360, 1364, 1371, 1375a, 2224, 2234, 2270, 2493, 2543, 2724, 2731, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 2939, 3054, 3058, 3059, 3062, 3255, 3266, 3308, 3386, 3397, 3398, 3410, 3499, 3505, 3553, 3797, 4249, 5034, 5811b	120, 404, 568b, 937, 1053, 1086, 1223, 1225, 1662, 1854, 2339a, 2359, 2386, 2389, 2544, 2917a, 2939, 3266, 3430, 3547, 3905, 3973, 3974a, 3983a, 4249, 5079, 5720, 5811b	1360, 1375a
135.	100-06-1 [1]	Ethanone, 1-(4-methoxyphenyl)- {acetanisole}	336, 616, 1626, 2939, 3224, 3266, 4249, 5811b	172a, 174b, 336, 1053, 2389, 2544, 3266, 3370, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
136.	122-00-9 [302]	Ethanone, 1-(4-methylphenyl)- {4-methylacetophenone}	568b, 1132, 1360, 1371, 1375, 1375a, 1375b, 1426, 1427, 2387, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3266, 3410, 3557, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 937, 1053, 1156, 2339a, 2386, 2389, 2544, 2917a, 3266, 3370, 3547, 3973, 4090, 4249	1360, 1375a, 2387
137.	1193-79-9 [7]	Ethanone, 1-(5-methyl-2-furanyl)- {2-acetyl-5-methylfuran}	568b, 1427, 1586, 2337, 2570, 2731, 2735, 2767, 2775, 3553, 3555, 3557, 4249, 4570a, 5811b	404, 568b, 965, 1053, 1662, 2337, 2339a, 2386, 2389, 2544, 3188, 3205, 3219, 3266, 3543, 3547, 3555, 3560, 3561, 3905, 4249, 5811b	
138.	1333-52-4 93-08-3 [282]	Ethanone, 1-(naphthalenyl)- {methyl naphthyl ketone}	568b, 626, 2761, 2762, 3266, 3797, 4249	568b, 1053, 3266, 4249	
139.	98-86-2 [4]	Ethanone, 1-phenyl- {acetophenone}	37, 38, 568b, 1075, 1238, 1360, 1364, 1371, 1375a, 1426, 1427, 1586, 1949, 2337, 2387, 2506, 2507, 2731, 2735, 2767, 2773, 2775, 2777, 2799a, 3266, 3397, 3410, 3553, 3557, 3559, 4036, 4249, 4570a, 5811b	172a, 174b, 568b, 937, 984, 1053, 1254, 1256, 1662, 1949, 1980, 2283, 2337, 2339, 2339a, 2386, 2389, 2544, 2917a, 3188, 3205, 3219, 3266, 3370, 3543, 3547, 3560, 3561, 3905, 4249, 5811b	1360, 1375a, 2387, 2506, 2507, 3401
140.	22047-25-2 [8]	Ethanone, 1-pyrazinyl- {acetylpyrazine}	568b, 1587, 1587a, 2470, 3266, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1207, 2337, 3204, 3202, 3205, 3215, 3219, 3266, 3370, 3491, 3547, 3550, 4249, 5811b	
141.	110-45-2 [227]	Formic acid, 3-methylbutyl ester		1053, 2339a, 3266, 3370	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

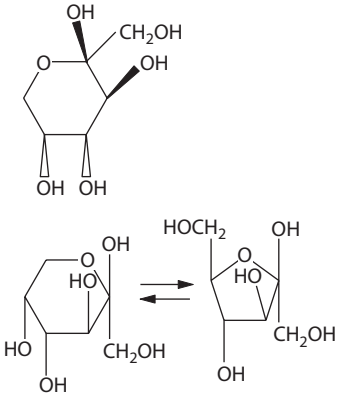
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
142.	104-57-4 [6A]	Formic acid, phenylmethyl ester {benzyl formate}	5811b	174b, 404, 937, 2339a, 2389, 2544, 3266, 3547, 4249, 5811b	
143.	57-48-7 [409]	*D*-Fructose {levulose} 	1089a, 1352, 1360, 1361, 1375a, 1587, 1887a, 1944, 2079, 2145, 2321, 2524a, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	71, 120, 321b, 480, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1141, 1142, 1289, 1352, 1361, 1435a, 1916, 1971, 2070, 2270, 2283, 2313a, 2337, 2338, 2381, 2532, 2818, 2911c, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3462, 3551, 3555, 3580, 3667, 3797, 3871, 3913, 3973, 3974a, 3974b, 4159, 4249, 4275, 4411, 5079, 5105, 5108, 5109, 5114, 5189, 5344, 5387, 5449, 5562, 5652, 5748, 5768, 5811b, 5819	1360, 1375a
144.	611-13-2 1334-76-5 [271]	2-Furancarboxylic acid, methyl ester {methyl 2-furoate}	568b, 1884, 3266, 4249, 5811b	568b, 984, 1053, 3266, 4249, 5811b	
145.	5989-33-3 60047-17-8 [252]	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*Z*)- {*cis*-linalool oxide}		172a, 174b, 404, 568b, 1053, 2336, 2338, 2339a, 2386, 2389, 2544, 2917a, 3266, 3555, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
146.	104-50-7 [339]	2(3*H*)-Furanone, 5-butyldihydro- {γ-octalactone}		172a, 174b, 404, 568b, 1053, 1980, 2339a, 2389, 2544, 3219, 3266, 3370, 3543, 3553, 3555, 3560, 3561, 4098a, 4249	
147.	96-48-0 [216]	2(3*H*)-Furanone, dihydro- {butyrolactone}	126a, 126b, 237, 568b, 642, 1063–1066, 1068–1074, 1099, 1371, 1375, 1375a, 1375b, 1377, 1445, 1586, 1674, 1881, 1958, 1960, 2387, 2418, 2493, 2506, 2507, 2570, 2731, 2735, 2767, 2775, 2777, 2799a, 3255, 3266, 3300, 3302, 3397, 3553, 3555, 3557, 3559, 4032, 4249, 5811b	404, 568b, 1053, 1590a, 2339a, 2386, 2389, 2544, 2917a, 3188, 3266, 3549, 3550, 3555, 4098a, 4249, 5811b	1375a, 1377, 2387, 2506 (0), 2507 (0), 3401, 3402, 3404, 3405
148.	695-06-7 [196]	2(3*H*)-Furanone, dihydro-5-ethyl- {γ-hexalactone}	568b, 4249, 4407	172a, 174b, 404, 568b, 1053, 1256, 1980, 2339a, 2389, 2544, 3219, 3266, 3370, 4249, 5811b	
149.	706-14-9 [91]	2(3*H*)-Furanone, dihydro-5-hexyl- {γ-decalactone}	5811b	172a, 174b, 568b, 1053, 1248, 2611, 3266, 3370, 3545, 3560, 3561, 4249	
150.	108-29-2 [455]	2(3*H*)-Furanone, dihydro-5-methyl- {γ-valerolactone}	1360, 1371, 1375a, 1883, 2731, 2735, 2775, 3266, 4249, 5770	172a, 174b, 404, 1053, 2389, 2544, 2917a, 3219, 3266, 3370, 4249, 5811b	1360, 1375a
151.	104-61-0 [329]	2(3*H*)-Furanone, dihydro-5-pentyl- {γ-nonalactone}	5811b	172a, 174b, 404, 568b, 1053, 2337a, 2339a, 2389, 2544, 3215, 3266, 3370, 3543, 3547, 3555, 3560, 3561, 4098a, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

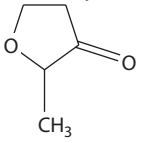
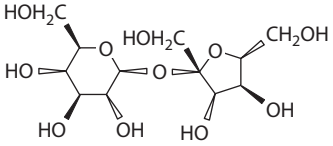
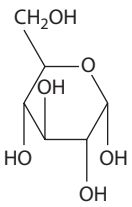
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
152.	105-21-5 [187]	2(3*H*)-Furanone, dihydro-5-propyl- {γ-heptalactone}	568b, 2601a, 4249	120, 172a, 174b, 568b, 1053, 2283, 2270, 3266, 4249	
153.	591-12-8 [214] [42A]	2(3*H*)-Furanone, 5-methyl- {4-hydroxy-3-pentenoic acid lactone; α-angelica lactone}	568b, 2570, 2769, 2775, 3255, 3257, 3265, 3266, 3553, 3557, 4032, 4407, 5811b	172a, 174b, 568b, 1053, 1980, 2336, 2337a, 2389, 2544, 3266, 4249, 5811b	3401
154.	3188-00-9 [317]	3(2*H*)-Furanone, dihydro-2-methyl- {2-methyltetrahydrofuran-3-one} 	1371, 2735, 3266, 3410, 4249, 5770, 5811b	172a, 174b, 984, 1053, 1590a, 2336, 2389, 2544, 2917a, 3188, 3266, 3370, 3547, 3555, 4249, 5811b	3404, 4249
155.	59-23-4 [409]	*D*-Galactose	3266, 4249, 5580	120, 158, 344a, 933, 1053, 1263, 2070, 2270, 2338, 2939, 3075, 3266, 3555, 3797, 3973, 3974a, 4249, 4411, 5079, 5114, 5768, 5785, 5811b	
156.	57-50-1 [409]	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose} 	1264, 1265, 1361, 4249, 5811b	71, 120, 172c, 248, 321b, 840, 933, 1053, 1063–1066, 1068–1074, 1128a, 1264, 1265, 1289, 1361, 1933a, 1958, 1960, 1971, 2070, 2079, 2270, 2283, 2313a, 2337, 2532, 2818, 2911c, 2939, 2947c, 3059, 3075, 3266, 3370, 3398, 3409, 3449, 3461, 3462, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3973, 3974a, 3974b, 4249,	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

	CAS No.	Name (per CA Collective Index)	References		
			Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
				4411, 4990, 5079, 5108, 5109, 5126, 5189, 5449, 5562, 5679, 5692, 5748, 5768, 5811b, 5819, 5836, 5896	
157.	50-99-7 26655-34-5 [409]	α-*D*-Glucose 	1264, 1265, 1352, 1360, 1361, 1371, 1375a, 1883, 1944, 2145, 2761, 2762, 2765, 2766, 2777, 2939, 3266, 3300, 3302, 3555, 3797, 4249, 5580, 5811b	72, 120, 172c, 174b, 248, 321b, 480, 727, 840, 924, 933, 1053, 1063–1066, 1068–1074, 1077b, 1128a, 1141, 1142, 1264, 1265, 1289, 1352, 1361, 1835b, 1835d, 1863, 1916, 1933a, 1971, 2070, 2079, 2270, 2283, 2313a, 2338, 2339b, 2381, 2394a, 2532, 2704a, 2850, 2911c, 2913, 2939, 3059, 3075, 3266, 3305, 3409, 3461, 3551, 3555, 3580, 3667, 3767, 3797, 3871, 3913, 3973, 3974a, 4103, 4159, 4249, 4275, 4411, 4999, 5079, 5108, 5109, 5126, 5189, 5255, 5344, 5449, 5562, 5655, 5656, 5698, 5748, 5768, 5774, 5811b, 5819, 5831	1360, 1375a

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
158.	6899-05-4 [181]	Glutamic acid $HOOC-(CH_2)_2-CH(NH_2)-COOH$	562, 563, 1083, 1351, 1910, 1914, 2079, 2724, 2858, 2939, 3059, 3061, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 563, 622, 749, 751–756, 826a, 927, 966, 1033, 1034, 1053, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2026, 2270, 2283, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 4422, 5079, 5699, 5785, 5827, 5896, 5905, 5907	
159.	56-85-9 [182]	*L*-Glutamine	480, 562, 563, 1351, 1668, 1910, 1914, 1965, 2079, 2724, 2858, 2939, 3059, 3266, 3302, 3491, 3797, 4159, 4249	120, 480, 563, 622, 749, 751–756, 1033, 1034, 1053, 1063–1066, 1068–1074, 1223, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2453, 2529, 2532, 2939, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 5079, 5189, 5434, 5437, 5699, 5785, 5811b, 5827, 5831, 5881, 5905, 5907	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
160.	4313-03-5 5910-85-0 [186]	2,4-Heptadienal O═CH-CH═CH-CH═CH-CH_2-CH═O		172a, 174b, 404, 937, 1053, 1854, 2389, 2544, 2917a, 3266, 3370, 3547, 4249, 5811b	
161.	1604-28-0 [291]	3,5-Heptadien-2-one, 6-methyl-, (*E*)- $(H_3C)_2$═C═CH-CH═CH-CO-CH_3	568b, 2506, 2507, 2570, 4249, 5811b	172a, 174b, 404, 568b, 937, 1053, 1156, 2338, 2339a, 2386, 2389, 2544, 3186, 3188, 3266, 3370, 3905, 3547, 4090, 4098a, 4249, 5811b	2506 (0), 2507 (0)
162.	111-14-8 [188]	Heptanoic acid {enanthic acid} H_3C-$(CH_2)_5$-COOH	172, 526, 563, 565, 1132, 1360, 1364, 1365, 1371, 1375a, 1917, 2079, 2271, 2543, 2545, 2761, 2762, 2765, 2766, 2777, 2939, 3263, 3266, 3302, 3308, 3555, 3797, 3799, 3800, 4249, 4319, 4993, 5079, 5811b	172a, 174b, 848, 1053, 1085, 1590a, 1982, 1999, 2014, 2094, 2271, 2338, 2339a, 2356, 2389, 2544, 2570, 2722, 2917a, 3266, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3767a, 3797, 3973, 3974a, 3974b, 4131, 4249, 4993, 5811b, 5846	1360, 1375a, 3393
163.	110-43-0 [189]	2-Heptanone {methyl pentyl ketone}	1238, 2002, 2461, 2773, 3266, 4249	172a, 174b, 1053, 2337, 2339a, 2389, 2544, 3186, 3188, 3266, 3370, 4249, 5811b	
164.	2463-63-0 [193]	2-Heptenal H_3C-$(CH_2)_3$-CH═CH-CHO		404, 1053, 3266	4249, 4856

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
165.	110-93-0 [297]	5-Hepten-2-one, 6-methyl-	568b, 1371, 1949, 2545, 2773, 2775, 3410, 4249, 5811b	172a, 404, 568b, 937, 984, 1053, 1063–1066, 1068–1074, 1256, 1590a, 1615, 1854, 1949, 2015, 2095, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3188, 3266, 3370, 3905, 3547, 4249, 5811b	
166.	57-10-3 [350]	Hexadecanoic acid {palmitic acid} $H_3C\text{-}(CH_2)_{14}\text{-}COOH$	60, 101, 172, 239, 257, 258, 722, 723, 765, 809, 966, 1132, 1063–1066, 1068–1074, 1231, 1329, 1330, 1332, 1333, 1348, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1377, 1388–1390, 1437, 1448, 1449, 1582, 1586, 1651, 1744, 1785, 1944, 2387, 2418, 2529, 2543, 2545, 2570, 2601a, 2683, 2761, 2762, 2766, 2767, 2773, 2775, 2777, 2799a, 2857, 2939, 3265, 3266, 3293, 3302, 3308, 3384, 3410, 3447, 3454, 3457, 3496, 3553, 3555, 3557, 3608, 3876, 4005–4007, 4030, 4249, 4280, 4319, 4354, 4570a, 5512, 5552, 5811b	60, 101, 120, 172a, 174b, 404, 634, 637, 722, 835, 836, 838, 891, 908, 1053, 1329, 1330, 1332, 1333, 1388–1390, 1590a, 1651, 1785, 1848, 1893a, 1893b, 1982, 2079, 2270, 2283, 2338, 2339a, 2356, 2386, 2389, 2529, 2544, 2570, 2593, 2862, 2917a, 2939, 3155, 3194, 3219, 3266, 3328, 3329, 3332, 3349, 3430, 3511, 3543, 3545, 3547, 3549, 3550, 3555, 3560, 3561, 3608, 3755, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 5079, 5189, 5367, 5380, 5388, 5695, 5811b	1330, (0) 1332 (0), 1375a, 1377, 2387

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

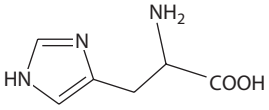
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
167.	628-97-7 [147]	Hexadecanoic acid, ethyl ester {ethyl palmitate} H_3C-$(CH_2)_{14}$-COO-CH_2-CH_3	1371, 2601a, 2775, 3266, 3410, 4249	172a, 174b, 908, 1053, 1157, 2389, 2544, 3266, 3547, 3555, 4249	
168.	110-44-1 22500-92-1 [48A]	2,4-Hexadienoic acid, (*E,E*)- {sorbic acid}	1371, 1886, 2543, 2773, 2873, 3308, 4249, 5811b	454, 742, 1547, 2092, 3266, 3547, 3767a, 4249, 5018, 5811b	3393
169.	66-25-1 [197]	Hexanal {caproic aldehyde} H_3C-$(CH_2)_4$-CH═O	568b, 1140, 1238, 1416, 1418, 1419, 2270, 2337, 2939, 3266, 3302, 3308, 3452, 3797, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 1053, 1550, 1615, 1893b, 2337, 2339b, 3186, 3188, 3266, 3370, 3973, 4249	
170.	50-70-4 [49A]	Hexane, hexahydroxy- {sorbitol; glucitol} $HOCH_2$-$(CHOH)_4$-CH_2OH	627, 1360, 1375a, 1586, 2761, 2762, 2765–2767, 2777, 2850, 5580	120, 174b, 627, 773, 933, 1221, 1971, 2079, 2195, 2705, 2939, 3075, 3163, 3264, 3266, 3667, 3797, 3973, 3974a, 5079, 5180, 5216, 5811b	1360, 1375a
171.	142-62-1 [198]	Hexanoic acid {caproic acid} H_3C-$(CH_2)_4$-COOH	172, 526, 563, 565, 568b, 960, 1132, 1140, 1232, 1360, 1364, 1365, 1371, 1375a, 1586, 1587a, 1668, 1903, 1917, 2079, 2088, 2170, 2271, 2338, 2543, 2545, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3263, 3266, 3308, 3410, 3555, 3557, 3797, 3799, 3800, 3809, 4064, 4065, 4249, 4319, 4993, 5079, 5811, 5811b	120, 172a, 174b, 404, 563, 568b, 848, 908, 1053, 1085, 1587a, 1590a, 1982, 1999, 2014, 2079, 2271, 2283, 2338, 2356, 2386, 2389, 2544, 2570, 2611, 2722, 2862a, 2917a, 2939, 3219, 3266, 3329, 3370, 3507, 3545, 3547, 3549, 3555, 3560, 3561, 3633, 3767a, 3797, 3973, 3974b, 4131, 4249, 4993, 5695, 5708, 5811, 5811b, 5846	1360, 1375a, 3393
172.	123-66-0 [135]	Hexanoic acid, ethyl ester {ethyl caproate} H_3C-$(CH_2)_4$-COO-C_2H_5	565, 568b, 1140, 1416, 1903, 1904, 2858, 2939, 3266, 3302, 4249, 4259, 4319, 5811b	172a, 174b, 568b, 1053, 2389, 2544, 3266, 3370, 3905, 3974a, 4249	
173.	4536-23-6 [312]	Hexanoic acid, 2-methyl- {2-methylhexanoic acid}	568b, 1132, 1884, 3266, 3302, 3553, 3557, 3797, 4249	568b, 1053, 2337a, 2389, 2544, 3266, 3370, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
174.	111-27-3 [208]	1-Hexanol {caproyl alcohol} $H_3C\text{-}(CH_2)_4\text{-}CH_2OH$	172, 568b, 1419, 3555, 4249, 5811b	172a, 174b, 568b, 937, 1053, 2339a, 2917a, 3266, 3547, 3555, 4249, 5811b	
175.	104-76-7 [160]	1-Hexanol, 2-ethyl-	1445, 2570, 2767, 2769, 3266, 3557, 4249, 5811b	1053, 1550, 2917a, 3266, 3547, 4249, 5811b	
176.	505-57-7 [19A]	2-Hexenal $H_3C\text{-}(CH_2)_2\text{-}CH{=}CH\text{-}CH{=}O$	568b, 2444, 3266, 3559, 4249, 5811b	174b, 404, 568b, 1590a, 2339b, 2917a, 3188, 3266, 4249	
177.	6728-26-3 [202]	2-Hexenal, (*E*)-	568b, 2444, 3266, 4249	172a, 568b, 1053, 1157, 3266, 3370, 4249, 5811b	
178.	4219-24-3 [204]	3-Hexenoic acid {hydrosorbic acid} $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}CH_2\text{-}COOH$	60, 1586, 2663, 2767, 3266, 3557, 4249	172a, 174b, 1053, 2092, 3186, 3188, 3266, 3547, 4249	
179.	928-95-0 [199]	2-Hexen-1-ol, (*E*)-		172a, 174b, 1053, 2917a, 3266	
180.	2497-18-9 [21A]	2-Hexen-1-ol, acetate, (*E*)-		172a, 174b, 1053, 3266	
181.	928-97-2 [200]	3-Hexen-1-ol, (*E*)-		404, 1053, 1157, 2389, 2544, 3266, 3547, 4249	
182.	928-96-1 [200]	3-Hexen-1-ol, (*Z*)- {leaf alcohol}	297, 316, 568b, 3186, 4249	297, 316, 404, 568b, 740, 1053, 1590a, 2339a, 2339b, 2386, 2389, 2544, 2914, 3186, 3188, 3219, 3266, 3354, 4098a, 4249, 5811b	
183.	5166-53-0 [293]	3-Hexen-2-one, 5-methyl-	1360, 1375a, 2761, 2765, 3266, 4249	1053, 1662, 2336, 3186, 3188, 3266, 3550, 4249	1360, 1375a

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

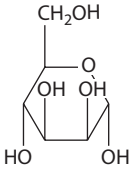
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
184.	71-00-1 [210]	*L*-Histidine 		120, 158, 553, 622, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5478, 5699, 5785, 5811b, 5831	
185.	83-34-1 [398]	1*H*-Indole, 3-methyl- {skatole}	293, 568b, 722, 918a, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1360, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1388–1390, 1426, 1427, 1580, 1586, 1744, 1765, 1778, 1842, 1880, 1898, 2387, 2510, 2537, 2545, 2683, 2724–2727, 2732, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2939, 3081, 3082, 3251, 3255, 3266, 3279, 3286, 3302, 3308, 3386, 3397, 3410, 3491, 3504, 3506, 3553, 3557, 3559, 3650, 3797, 3886, 3887, 4249, 4407, 5512, 5811b	568b, 1053, 3266, 4249	1330, 1332, 1360, 1375a, 2387

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
186.	73-32-5 [242]	*L*-Isoleucine $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(NH_2)\text{-}COOH$		120, 158, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1971, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 5811b	
187.	7005-03-0 [249]	Leucine $(H_3C)_2{=}CH\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1083, 1351, 1910, 1914, 2724, 2858, 3266, 3302, 3491, 3797, 4249	120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5699, 5785, 5827, 5831, 5881, 5905	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
188.	56-87-1 [254]	*L*-Lysine $H_2N\text{-}(CH_2)_4\text{-}CH(NH_2)\text{-}COOH$		120, 158, 480, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2902, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 4224, 4226, 4244, 4249, 5811b	
189.	31103-86-3 [409]	Mannose 	1587, 2761, 2762, 2765, 2766, 2777, 3266, 3555, 4249	1053, 2070, 3266, 3555, 3797, 3973, 3974a, 4249, 5768	
190.	119-61-9 [39]	Methanone, diphenyl- {benzophenone} $C_6H_5\text{-}CO\text{-}C_6H_5$	278, 568b, 3266, 4249	172a, 174b, 568b, 1053, 2339a, 3266, 3370	
191.	63-68-3 [262]	*L*-Methionine $H_3C\text{-}S\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$		116, 120, 158, 172, 622, 722, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1127b, 1305a, 1329, 1330, 1332, 1351, 1493, 2049, 2270, 2337, 2359, 2532, 2597a, 2795, 2939, 3186, 3188, 3266, 3491, 3499, 3705, 3729, 3797, 3973, 3974a, 3978, 4226, 4249, 4398c, 5079, 5376, 5811b, 5907	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

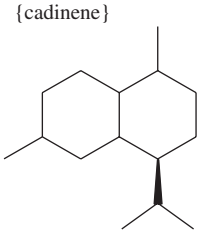
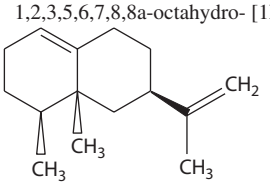
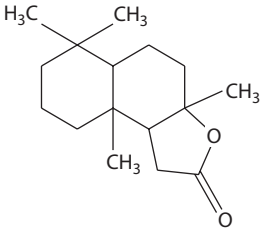
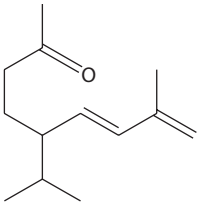
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
192.	29350-73-0 [62]	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)- {cadinene} 		1053, 2339a, 2917a, 3266, 4249	
193.	4630-07-3 [452]	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)- 1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7β,8a α] {valencene} 		172a, 404, 568b, 1053, 2917a, 3266	
194.	93-18-5 [324]	Naphthalene, 2-ethoxy- {β-naphthyl ethyl ether}	5811b	1053, 1248, 3266, 4249, 5811b	
195.	564-20-5 [397]	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {1,5,5,9-tetramethyl-13-oxatricyclo[8,3,0,0(4,9)]tridecane} {sclareolide} 	568b, 775, 2292, 2756, 2767, 3251, 3267, 3272, 3295, 3557, 4249, 5811b	120, 174e, 568b, 1053, 1296, 1590a, 2292, 2308, 2338, 2386, 2611, 2756, 3198, 3263, 3266, 3267, 3295, 3370, 3533, 3534, 3545, 3547, 3560, 3561, 4249, 5811b	
196.	557-48-2 [327]	2,6-Nonadienal, (*E,Z*)-		1053, 2336, 3266, 3370, 3547, 4249, 5811b	
197.	1937-54-8 [406]	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [S-(*E*)]- {solanone} 	69, 568b, 802, 803, 1352, 1360, 1364, 1365, 1375, 1375a, 1375b, 1586, 2045, 2387, 2506, 2507, 2545, 2570, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2799a, 2857, 2871, 3224, 3266, 3297, 3302, 3308, 3410, 3557, 3559, 3648, 4249, 4336, 5811b	9, 69, 404, 537, 543a, 568b, 671, 908, 909, 911, 943, 1053, 1063–1066, 1068–1074, 1149, 1149a, 1156, 1254, 1256, 1257, 1352, 1550, 1590a, 1591, 1961, 2282, 2338, 2339a,	1360, 1375a, 2387, 2506, 2507

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

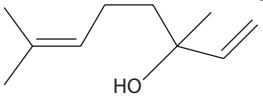
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [S-(*E*)]-{solanone} (cont.)		2386, 2389, 2544, 2786, 2914, 3188, 3198, 3215, 3219, 3266, 3354, 3543, 3545, 3547, 3549, 3550, 3560, 3561, 3648, 3905, 3973, 4090, 4098a, 4249, 4336, 5811b	
198.	124-19-6 [330]	Nonanal {pelargonaldehyde} H_3C-$(CH_2)_7$-CH═O	568b, 1238, 4249, 5811b	172a, 174b, 568b, 1053, 2282, 3153, 3266, 3370, 3547, 4249, 5811b	
199.	112-05-0 [331]	Nonanoic acid {pelargonic acid} H_3C-$(CH_2)_7$-COOH	172, 563, 565, 568b, 809, 1132, 1348, 1364, 1371, 1886, 1917, 1999, 2079, 2545, 2939, 3266, 3293, 3302, 3555, 3797, 4249, 4993, 5079, 5811b	172a, 174b, 404, 568b, 848, 908, 1053, 1590a, 1999, 2014, 2338, 2339a, 2356, 2389, 2544, 2722, 2917a, 3219, 3266, 3370, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3767a, 3974b, 3973, 3974a, 4131, 4249, 4993, 5811b	
200.	123-29-5 [143]	Nonanoic acid, ethyl ester H_3C-$(CH_2)_7$-COO-C_2H_5		172a, 174b, 908, 1053, 2389, 2544, 3266, 3370, 4249, 5811b	
201.	821-55-6 [332]	2-Nonanone H_3C-$(CH_2)_6$-CO-CH_3	297, 568b, 3266, 4249	172a, 174b, 568b, 1053, 1662, 2339a, 3266, 3626, 4249	
202.	2463-53-8 [334]	2-Nonenal H_3C-$(CH_2)_5$-CH═CH-CH═O	568b, 3255, 4249	404, 568b, 1053, 2336, 3153, 3266, 3547, 3550, 3850, 4249	
203.	18829-56-6 [334]	2-Nonenal, (*E*)-		404, 1053, 2336, 3153, 3205, 3266, 4249, 4332, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
204.	506-21-8 [336]	9,12-Octadecadienoic acid, (*E,E*)- {linoleic acid} H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COOH	60, 101, 257, 258, 723, 765, 966, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1448, 1582, 1586, 1651, 1744, 1842, 1944, 2529, 2543, 2570, 2683, 2767, 2777, 2939, 3122, 3266, 3302, 3308, 3384, 3454, 3457, 3557, 3608, 3876, 4005–4007, 4115, 4249, 4280, 4570a, 5512, 5552	60, 101, 120, 634, 722, 836, 838, 891, 908, 966, 981a, 1053, 1329, 1330, 1332, 1333, 1651, 1731, 1893a, 1893b, 1982, 2079, 2270, 2283, 2338, 2389, 2529, 2544, 2570, 2593, 2939, 3155, 3219, 3266, 3329, 3435, 3461, 3543, 3549, 3608, 3755, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 5079, 5189, 5367, 5388	1330, 1332, 1360, 1375a
205.	112-63-0 [280]	9,12-Octadecadienoic acid (*Z,Z*)-, methyl ester {methyl linoleate}	60, 568b, 2773, 3224, 3266, 4249	60, 568b, 908, 1053, 1590a, 2386, 2389, 2544, 3219, 3266, 3547, 3549, 4249, 5811b	
206.	111-61-5 [144]	Octadecanoic acid, ethyl ester {ethyl stearate} H_3C-$(CH_2)_{16}$-COO-CH_2-CH_3	568b, 2601a, 4249, 5811b	568b, 1053, 2389, 2544, 3266, 3547, 4249, 5811b	
207.	463-40-1 [337]	9,12,15-Octadecatrienoic acid, (*Z,Z,Z*)- {linolenic acid} H_3C-$(CH_2CH═CH)_3$-$(CH_2)_7$-COOH	101, 257, 258, 723, 765, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1448, 1582, 1586, 1651, 1744, 1785, 1842, 2529, 2543, 2570, 2601a, 2683, 2767, 2799a, 2939, 3204, 3122, 3266, 3302, 3308, 3384, 3454, 3457, 3557, 3608, 3797, 4005–4007, 4031, 4249, 4280, 4570a, 5079, 5512, 5811b	101, 120, 404, 634, 835, 836, 838, 891, 908, 1053, 1329, 1330, 1332, 1333, 1651, 1785, 2092, 2270, 2283, 2338, 2389, 2529, 2544, 2570, 2593, 2917a, 2939, 3266, 3329, 3435, 3461, 3608, 3755, 3797, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 4774, 5079, 5380, 5695, 5811b	1330, 1332, 1360, 1375a
208.	301-00-8 [281]	9,12,15-Octadecatrienoic acid, methyl ester, (*Z,Z,Z*)- {methyl linolenate} H_3C-$(CH_2CH═CH)_3$-$(CH_2)_7$-COO-CH_3	2543, 2545, 2601a, 2773, 3266, 4249	1053, 1590a, 2917a, 3266, 3547, 4249, 5811b	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
209.	26764-26-1 [349]	Octadecenoic acid {oleic acid}	60, 101, 257, 258, 723, 765, 966, 1063–1066, 1068–1074, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1448, 1582, 1586, 1651, 1744, 1785, 1842, 2529, 2543, 2570, 2683, 2767, 2939, 2773, 2777, 3122, 3266, 3302, 3308, 3384, 3454, 3457, 3557, 3608, 3876, 4030, 4280, 4354, 4570a, 5512, 5552	60, 101, 120, 297, 634, 722, 835, 836, 838, 891, 981a, 1053, 1329, 1330, 1332, 1333, 1651, 1785, 1893b, 2079, 2270, 2283, 2338, 2339a, 2389, 2529, 2544, 2552, 2570, 2593, 2649, 2917a, 2939, 3155, 3266, 3435, 3461, 3543, 3545, 3608, 3755, 3812, 3973, 3974a, 4131, 4249, 4280, 5811b	1330, 1332, 1360, 1375a
210.	111-62-6 [146]	9-Octadecenoic acid (*Z*)-, ethyl ester {ethyl oleate} $H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}COO\text{-}C_2H_5$	2601a	908, 1053, 2389, 2544, 3266, 3547, 4249, 5811b	
211.	141-27-5 5392-40-5 [81]	2,6-Octadienal, 3,7-dimethyl- {citral}	278, 568b, 3266, 4249, 5811	172a, 174b, 568b, 1053, 3266, 3370, 5811	
212.	78-70-6 [251]	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool} 	317, 568b, 1360, 1375a, 1949, 2761, 2762, 2765, 2766, 3193, 3266, 3302, 3555, 3971, 4249	120, 172a, 174b, 317, 404, 568b, 909, 937, 1053, 1254, 1590a, 1949, 2270, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 2939, 3188, 3205, 3215, 3217, 3219, 3266, 3354, 3370, 3374, 3547, 3555, 3797, 3971, 3973, 3974a, 4098a, 4249, 5079, 5811b	1360, 1375a

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

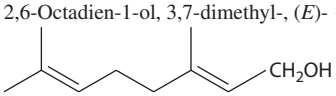
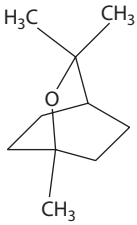
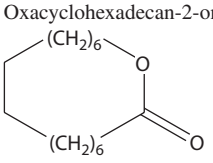
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
213.	115-95-7 [253]	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate {linalyl acetate}		172a, 174b, 1053, 2339a, 3198, 3219, 3266, 3354, 3370, 4249	
214.	106-24-1 [175]	2,6-Octadien-1-ol, 3,7-dimethyl-, (*E*)- {geraniol} 	568b, 1586, 2761, 2762, 2765–2767, 2775, 3193, 3224, 3266, 3302, 3555, 3557, 4249, 5811b	172a, 174b, 568b, 937, 1053, 1156, 1254, 1256, 2389, 2544, 2611, 2917a, 3215, 3266, 3370, 3555, 3797, 3988, 4090, 4249	
215.	106-25-2 [325]	2,6-Octadien-1-ol, 3,7-dimethyl-, (*Z*)- {nerol}	568b, 3557, 4249	172a, 174b, 568b, 937, 1053, 1254, 1256, 2389, 2544, 3266, 3370, 4249	
216.	124-13-0 [340]	Octanal $H_3C\text{-}(CH_2)_6\text{-}CH{=}O$	568b, 1238, 4249, 5770, 5811b	172a, 174b, 404, 568b, 1053, 3266, 3370	
217.	124-07-2 [341]	Octanoic acid {caprylic acid} $H_3C\text{-}(CH_2)_6\text{-}COOH$	172, 563, 565, 568b, 722, 809, 1132, 1232, 1348, 1364, 1371, 1587a, 1668, 1917, 1971, 2079, 2338, 2543, 2545, 2765, 2773, 2775, 2939, 3266, 3293, 3302, 3308, 3410, 3555, 3797, 4064, 4065, 4249, 4319, 4993, 5079, 5811b	120, 172a, 174b, 404, 568b, 848, 908, 1053, 1085, 1221, 1587a, 1590a, 1893a, 1893b, 1982, 1999, 2014, 2079, 2270, 2283, 2338, 2356, 2389, 2544, 2570, 2611, 2649, 2722, 2917a, 3219, 3266, 3370, 3507, 3543, 3545, 3547, 3555, 3560, 3561, 3633, 3767a, 3797, 3973, 3974a, 3974b, 4131, 4249, 4993, 5079, 5180, 5363, 5695, 5811b, 5846	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
218.	106-32-1 [145]	Octanoic acid, ethyl ester {ethyl caprylate}	1949	172a, 174b, 908, 1053, 1949, 2389, 2544, 3266, 3370, 4249, 5811b	
219.	111-87-5 [342]	1-Octanol {caprylic alcohol}	172, 568b, 4249, 5811b	172a, 174b, 404, 568b, 1053, 2389, 2544, 2913a, 3266, 3547, 3811a, 3973, 4098a, 4249, 5811b	
220.	111-13-7 [343]	2-Octanone {hexyl methyl ketone}	568b, 1371, 3105, 3219, 3224, 3266, 3308, 4249	59, 568b, 1053, 2339a, 3266, 4249, 4434	
221.	13877-91-3 [108]	1,3,6-Octatriene, 3,7-dimethyl- {ocimene} $H_2C{=}CH\text{-}C(CH_3){=}CH\text{-}CH_2\text{-}CH{=}C(CH_3)_2$	1365, 1371, 3266, 4249, 4579	1053, 3266, 4249	
222.	106-23-0 [13A]	6-Octenal, 3,7-dimethyl- {citronellal} $(H_3C)_2{=}C{=}CH\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH{=}O$	568b, 1238, 3193, 3266, 3302, 4249	174b, 568b, 1156, 2917a, 3266, 4090, 4249	
223.	3391-86-4 [345]	1-Octen-3-ol		172a, 174b, 568b, 937, 1053, 3266, 3555, 4098a, 4249	
224.	106-22-9 [83]	6-Octen-1-ol, 3,7-dimethyl- {*dl*-citronellol}	568b, 2775, 3266, 4249	172a, 174b, 568b, 1053, 1254, 1256, 3266, 3370, 4249, 5811b	
225.	470-82-6 [170]	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- {eucalyptol; 1,8-cineole} 	568b, 3193, 3266, 3302, 4249	172a, 174b, 568b, 1053, 1247, 1254, 1256, 1662, 2339a, 2389, 2544, 3266, 3370, 4249, 5811b	
226.	106-02-5 [351]	Oxacyclohexadecan-2-one {ω-pentadecalactone; exaltolide} 		172a, 174b, 947, 1053, 3266, 3370, 4249	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

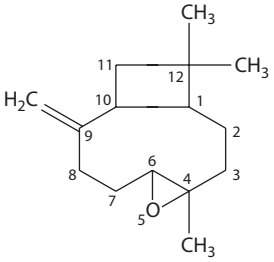
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
227.	1139-30-6 [72]	5-Oxatricyclo[8.2.0.04,6]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- {β-caryophyllene oxide} 		172a, 174b, 568b, 1053, 1156, 1157, 1662, 3266, 4090, 4249, 5811b	
228.	9000-69-5 [41A]	Pectin		120, 172, 174b, 176, 248, 344a, 385, 385a, 535, 722, 1063–1074, 1077, 1263, 1289, 1361, 1435a, 1887, 1933a, 2070, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2529, 2543, 2545, 2761, 2762, 2764–2766, 2850, 2851, 2939, 2947c, 3029, 3042, 3059, 3266, 3305, 3372, 3429, 3450, 3468, 3551, 3651, 3665a, 3702, 3767, 3797, 3871, 3973, 3974a, 3974b, 4151, 4249, 4279, 4396, 4999, 5079, 5114, 5189, 5234, 5306, 5344, 5811b, 5831	
229.	110-62-3 [453]	Pentanal {valeraldehyde} CH_3-$(CH_2)_3$-CH═O	568b, 605, 1039, 1140, 1238, 1365, 1374, 1375, 1375b, 1412–1414, 1416, 1418, 1419, 1615, 2002, 2337, 2573–2575, 2782, 2804, 2887, 3254, 3266, 3302, 3308, 3413, 3557, 3797, 3817, 4249, 4319, 4570a, 5811b, 5896	172a, 174b, 404, 568b, 1053, 1550, 1615, 1893b, 2337, 2914, 3186, 3188, 3266, 3370, 3547, 3626, 3797, 3973, 3974a, 4223, 4225, 4249, 5811b, 5896	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
230.	600-14-6 [352]	2,3-Pentanedione $H_3C\text{-}CH_2\text{-}CO\text{-}CO\text{-}CH_3$	314, 568b, 1140, 1232, 1238, 239, 1348–1350, 1354, 1374, 1375a, 1375a, 1377, 1378, 1418, 1419, 1586, 1589, 1590, 2002, 2079, 2337, 2387, 2469, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 2939, 3266, 3302, 3308, 3341, 3557, 3559, 3797, 3901, 4249, 4570a, 5570, 5811b, 5896	172a, 174b, 568b, 1053, 2917a, 3266, 5811b, 5896	1354, 1375a, 1375a, 1377, 1378 2244, 2387, 2506, 2507, 3401, 3402, 3404
231.	109-52-4 [454]	Pentanoic acid {valeric acid} $H_3C\text{-}(CH_2)_3\text{-}COOH$	526, 563, 565, 568b, 960, 1132, 1063–1066, 1068–1074, 1140, 1263, 1364, 1371, 1375, 1375b, 1586, 1587a, 1646, 1668, 1886, 1917, 2043, 2079, 2088, 2170, 2270, 2271, 2338, 2543, 2570, 2619, 2623, 2702, 2761, 2762, 2765–2767, 2858, 2939, 3061, 3263, 3266, 3308, 3393, 3410, 3553, 3557, 3799, 3800, 3809, 4064, 4065, 4079, 4249, 4319, 4993, 5079, 5811b	120, 172a, 174b, 404, 568b, 848, 908, 981a, 1053, 1085, 1087, 1263, 1587a, 1590a, 1893b, 1982, 1999, 2014, 2092, 2270, 2271, 2283, 2338, 2389, 2544, 2570, 2611, 2917a, 2939, 3219, 3266, 3328, 3329, 3370, 3507, 3547, 3717, 3809, 3973, 3974a, 3974b, 4064, 4249, 4993, 5079, 5364, 5695, 5708, 5811b, 5846	3393
232.	539-82-2 [152]	Pentanoic acid, ethyl ester {ethyl valerate} $H_3C\text{-}(CH_2)_3\text{-}COO\text{-}C_2H_5$	565, 1903, 1904, 2858, 2939, 3266, 3302, 4249, 5811b	172a, 174b, 174b, 1053, 3266, 3797, 3973, 3974a, 4249	
233.	97-61-0 [321]	Pentanoic acid, 2-methyl- {2-methylvaleric acid}	565, 568b, 2761, 2858, 3266, 3393, 3405, 4249, 5811b	172a, 174b, 174b, 848, 568b, 1053, 3266, 3370, 3560, 3561, 3974b, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
234.	105-43-1 [313]	Pentanoic acid, 3-methyl- {β-methylvaleric acid; 3-methylpentanoic acid}	172, 526, 565, 568b, 775, 1063–1066, 1068–1074, 1099, 1132, 1140, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1587a, 1881, 1884, 1886, 1903, 1904, 1999, 2092, 2270, 2338, 2387, 2493, 2543, 2545, 2570, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2816, 2817, 2858, 2939, 3224, 3255, 3266, 3302, 3308, 3015, 3410, 3529, 3553, 3557, 3795, 3799, 3800, 3809, 3827, 4249, 4319, 5811b	51, 120, 172a, 174b, 404, 568b, 848, 908, 981a, 1053, 1087, 1587a, 1590a, 1982, 1999, 2014, 2270, 2283, 2288, 2291, 2338, 2339a, 2386, 2389, 2544, 2570, 2611, 2862a, 2863, 2917a, 2939, 3215, 3219, 3266, 3328, 3329, 3507, 3537, 3543, 3545, 3547, 3549, 3809, 3973, 3974a, 3974b, 4575, 4997, 5079, 5364, 5708, 5811b, 5846	1360, 1375a, 2387, 3393
235.	646-07-1 [314]	Pentanoic acid, 4-methyl- {isocaproic acid}	568b, 1132, 1364, 1371, 1879, 1881–1884, 2543, 2765, 3266, 3302, 3308, 3410, 3553, 3797, 3799, 3800, 3809, 4249, 5811b	404, 568b, 848, 1053, 1085, 1087, 2092, 2270, 2570, 2722, 2917a, 3266, 3547, 3809, 3973, 3974a, 4249, 5846	3393
236.	123-76-2 [250]	Pentanoic acid, 4-oxo- {levulinic acid} $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}COOH$	565, 568b, 741, 1099, 1103, 1237, 1238, 1360, 1375, 1375a, 1375b, 1586, 1882, 2088, 2570, 2761, 2762, 2765–2767, 2939, 3059, 3060, 3061, 3224, 3255, 3266, 3302, 3308, 3394, 3496, 3553, 3557, 4249, 4319, 4897, 5811b	307, 568b, 569, 570, 833, 1053, 1103, 1312, 3060, 3266, 4249, 5811b	1360, 1375a, 3393, 3402, 3404, 3405
237.	71-41-0 [21]	1-Pentanol {amyl alcohol} $H_3C\text{-}(CH_2)_3\text{-}CH_2OH$	172, 568b, 4249, 5811b	404, 568b, 937, 1053, 1590a, 2282, 2339a, 3186, 3188, 3266, 3547, 3555, 3973, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
238.	107-87-9 [353]	2-Pentanone $H_3C\text{-}(CH_2)_2\text{-}CO\text{-}CH_3$	112, 173a, 299, 299, 568b, 1063–1066, 1068–1074, 1140, 1238, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1378, 1412–1414, 1416, 1418, 1419, 1586, 1589, 1637, 1947, 2337, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 2782, 2804, 2858, 2939, 3254, 3255, 3266, 3302, 3308, 3508, 3530, 3557, 3901, 4052, 4056, 4162, 4249, 4319, 5770, 5811b	172a, 174b, 568b, 647, 1053, 2337, 2389, 2544, 2722, 3266, 3797, 3973, 3974a, 4249, 5811b	1354, 1375a, 1378, 2506, 2507, 2244, 4052, 4056
239.	591-80-0 [354]	4-Pentenoic acid	2761, 3266, 4249	848, 1053, 3266, 4092, 4093, 4249	
240.	141-79-7 [295]	3-Penten-2-one, 4-methyl- {mesityl oxide} $(H_3C)_2{=}C{=}CH\text{-}CO\text{-}CH_3$	1053, 1238, 3266, 4249, 5770	404, 1053, 2339a, 3217, 3266, 4249	
241.	90-05-1 [185]	Phenol, 2-methoxy- {guaiacol}	50, 376, 568b, 615, 723, 765, 789, 789a, 804, 830a, 851, 859, 966, 1063–1066, 1068–1074, 1089a, 1099, 1140, 1232, 1235, 1236, 1292, 1360, 1364, 1371, 1375, 1375a, 1375b, 1427, 1586, 1626, 1882, 1884, 1887a, 1906, 1928, 1963, 1995, 2042–2045, 2079, 2142, 2195, 2270, 2298, 2302, 2307, 2311, 2327c, 2379a, 2387, 2524a, 2545, 2577, 2598, 2601a, 2761, 2762, 2765–2767, 2777, 2858, 2939, 3059, 3090, 3255, 3266, 3302, 3308, 3394, 3410, 3453, 3457, 3462, 3555, 3557, 3559, 3719, 3746, 3747, 3764, 3767, 3797, 3876, 3952, 4248, 4249, 4313, 4317, 4319, 4414, 4796, 4999, 5011, 5034, 5079, 5811b	120, 172a, 174a, 174b, 404, 568b, 937, 952, 1053, 1063–1066, 1068–1074, 1102, 1590a, 1825, 1876, 1877a, 1980, 2338, 2379a, 2611, 2862, 2917a, 2939, 3059, 3090, 3194, 3266, 3350, 3430, 3543, 3547, 3555, 3560, 3561, 3797, 3973, 3974a, 4202, 4249, 5079, 5811b	50, 1360, 1375a, 2387, 3395

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
242.	93-51-6 [264]	Phenol, 2-methoxy-4-methyl- {4-methylguaiacol}	568b, 1063–1066, 1068–1074, 1360, 1364, 1371, 1375, 1375a, 1375b, 1586, 2327c, 2543, 2767, 2773, 2775, 3266, 3410, 3553, 3557, 3712, 4249, 4796, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877a, 2014, 3266, 3370, 3430, 4249, 5811b	1360, 1375a
243.	88-69-7 [244]	Phenol, 2-(1-methylethyl)- {2-isopropylphenol}	568b, 1378, 1884, 2543, 2773, 3559, 3712, 3746, 3747, 4248, 4249, 5811b	568b, 1053, 3266, 4249	1378
244.	499-75-2 [68]	Phenol, 2-methyl-5-(1-methylethyl)- {carvacrol}	2195, 3266, 3308, 3555, 3712, 4249	172a, 174b, 1053, 3266, 5811b	
245.	7786-61-0 [265]	Phenol, 4-ethenyl-2-methoxy- {4-vinylguaiacol}	101, 1063–1066, 1068–1075, 1089a, 1364, 1586, 1879, 1881, 1883, 1884, 1887a, 2524a, 2545, 2570, 2767, 3255, 3266, 3397, 3410, 3557, 3712, 3746, 3747, 4159, 4249, 5811b	172a, 174b, 937, 1053, 1587a, 1590a, 1876, 1877a, 1878, 2338, 2389, 2544, 2917a, 3266, 3430, 3547, 3549, 4249, 5811b	
246.	123-07-9 [168]	Phenol, 4-ethyl- {*p*-ethylphenol}	50, 568b, 723, 851, 1075, 1360, 1364, 1371, 1375, 1375a, 1375b, 1426, 1427, 1586, 1626, 1709, 1766, 1789, 1791, 1803, 1882, 1884, 1981, 1995, 2543, 2545, 2598, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2800, 2876, 3088, 3095, 3266, 3302, 3308, 3397, 3410, 3493, 3555, 3557, 3559, 3712, 3716–3719, 3746, 3747, 3764, 3765, 3797, 3800, 4249, 4313, 4317, 4319, 4350, 4796, 5011, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877a, 2389, 2544, 2917a, 3266, 3430, 3547, 3555, 4249, 5811b	50, 1360, 1375a, 3395

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
247.	89-83-8 [423]	Phenol, 5-methyl-2-(1-methylethyl)- {thymol}	568b, 1884, 2577, 3266, 3308, 3555, 3559, 3797, 4249, 5811b	172a, 174b, 568b, 1053, 1156, 1254, 1256, 2611, 3266, 4090, 4249, 5811b	
248.	91-10-1 [104]	Phenol, 2,6-dimethoxy- {syringol}	568b, 1063–1066, 1068–1074, 1360, 1364, 1365, 1371, 1375, 1375a, 1375b, 1586, 1879, 1884, 2043, 2045, 2327c, 2387, 2543, 2545, 2598, 2601a, 2761, 2762, 2765–2767, 2773, 2775, 3266, 3302, 3394, 3410, 3553, 3557, 3712, 3797, 4249, 5811b	172a, 174b, 568b, 952, 1053, 1876, 1877, 2339, 2386, 2917a, 3266, 3430, 4249, 5811b	1360, 1375a, 2387, 3395
249.	95-65-8 [460]	Phenol, 3,4-dimethyl- {3,4-xylenol}	50, 155, 414, 568b, 830a, 1360, 1375a, 1378, 1426, 1427, 1586, 1626, 1789, 1879, 1881, 1883, 1884, 1928, 1995, 2005, 2387, 2447, 2598, 2628, 2761, 2762, 2765–2767, 2876, 3224, 3255, 3266, 3302, 3308, 3452, 3453, 3488, 3557, 3712, 3716–3719, 3746, 3747, 3764, 3797, 4249, 4317, 4319, 4407, 4414, 4796, 5011, 5811b	568b, 952, 1053, 1876, 1877a, 3266, 4249, 5811b	50, 1360, 1375a, 1378, 2387, 3395
250.	63-91-2 [372]	*L*-Phenylalanine C_6H_5-CH_2-CH(NH_2)-COOH	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3797, 4159, 4249, 5811b	120, 158, 622, 722, 749, 751–756, 826a, 927, 1053, 1063–1066, 1068–1074, 1102, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1971, 2079, 2270, 2337, 2338, 02359, 2394a,	

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TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

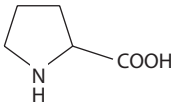
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		L-Phenylalanine (cont.)		2453, 2532, 2597a, 2795, 2903, 2905, 2911c, 2914, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3829, 3973, 3974a, 3975, 3978, 4098a, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5785, 5811b, 5831, 5905, 5907	
251.	147-85-3 [384]	*L*-Proline 	1351, 1910, 1914, 1933, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249, 4319, 5048, 5811b	120, 158, 480, 486, 749, 751–756, 826a, 927, 1033, 1053, 1063–1066, 1068–1074, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1933a, 1971, 2133, 2270, 2337, 2394a, 2395, 2453, 2529, 2532, 2592, 2597a, 2795, 2858, 2911c, 2914, 2939, 3059, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3974b, 3975, 3978, 3984, 4226, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 4422, 5079, 5699, 5785, 5811b, 5827, 5831, 5881, 5896, 5905, 5907	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
252.	78-84-2 [240]	Propanal, 2-methyl- {isobutyraldehyde} $(H_3C)_2$═CH-CH═O	111, 299, 314, 568b, 605, 1038, 1039, 1063–1066, 1068–1074, 1140, 1238, 1284, 1338, 1348–1350, 1354, 1365, 1374, 1375, 1375a, 1375b, 1377, 1378, 1412–1414, 1415, 1418, 1419, 1495, 1586, 1589, 1634, 1875, 2002, 2003, 2270, 2293, 2301, 2310, 2313a, 2337, 2506, 2507, 2543, 2545, 2570, 2765, 2767, 2777, 2782, 2804, 2939, 3105, 3132, 3254, 3257, 3266, 3302, 3308, 3396, 3413, 3557, 3793, 3817, 3901, 3935, 4052, 4056, 4104, 4162, 4249, 4290, 4319, 4570a, 5770, 5811b	120, 172a, 174b, 568b, 984, 1053, 1157, 1550, 2282, 2293, 2337, 2339a, 2860a, 2914, 2939, 3186, 3188, 3194, 3266, 3350, 3370, 3626, 3797, 3935, 3974a, 4223, 4225, 4249, 5811b, 5896	1354, 1375a, 1377, 1378, 2244, 2506, 2507, 4052, 4056
253.	3268-49-3 [319][30A]	Propanal, 3-(methylthio)- {methional}	568b, 1365, 3255, 3266, 3854, 4249, 5770	174b, 568b, 1053, 3266, 4249	
254.	57-55-6 [389]	1,2-Propanediol {propylene glycol} H_3C-CHOH-CH_2OH	167, 173a, 174e, 239, 409, 568b, 627, 966, 1350, 1352, 1354, 1360, 1364, 1371, 1373, 1375, 1375a, 1375b, 1382, 1427, 1437, 1445, 1586, 1603, 1944, 1963, 2144, 2300, 2387, 2410, 2543, 2545, 2570, 2601a, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 3190, 3255, 3266, 3302, 3308, 3410, 3551, 3553, 3557, 3559, 3603, 3797, 3835, 3876, 3992, 4249, 4259, 4337, 5770, 5811b	172a, 174b, 320, 568b, 569, 570, 27, 830a, 858, 865, 974, 1024, 1053, 1294, 1295, 383, 2009, 2188, 2195, 2196, 2246, 2313a, 2788, 2790, 2917a, 2939, 3163, 3264, 3266, 3370, 3549, 3550, 3551, 3603, 3707, 3797, 3974a, 4249, 4259, 4337, 5009, 5639, 5811b, 5817	1354, 1360, 1375a, 2387

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TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

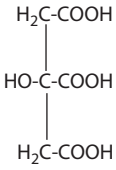
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
255.	77-92-9 [82]	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid} 	2079, 3029, 3302, 3324, 3555, 5079, 5447, 5811b	69, 120, 172a, 256, 305, 385, 543a, 555, 634, 677b, 826a, 835, 836, 838, 839, 963, 840, 1053, 1063–1066, 1068–1074, 1289, 1305a, 1330, 1332, 1333, 1548, 1923, 1933a, 1982, 2014, 2079, 2154, 2270, 2283, 2337, 2338, 2356, 2374, 2529, 2532, 2688, 2761–2763, 2765, 2766, 2891, 2939, 2947c, 3029, 3052, 3107, 3194, 3266, 3353, 3370, 3476, 3486, 3555, 3660, 3655b, 3701a, 3748, 3749, 3751, 3797, 3973, 3974a, 3974b, 3976, 4249, 4275, 5079, 5108, 5109, 5126, 5244, 5381, 5389, 5419, 5477, 5478, 5745, 5749, 5753, 5764, 5811b, 5832, 5896, 5909	
256.	18996-35-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monosodium salt		4249, 4760, 5548	
257.	77-93-0 [436]	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester {triethyl citrate}	3190, 3992	172a, 174b, 1053, 2386, 3266, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
258.	56-81-5 [183]	1,2,3-Propanetriol {glycerol} $HOCH_2$-CHOH-CH_2OH	50, 167, 172, 173a, 174e, 409, 568b, 607, 627, 636, 723, 849, 966, 1089a, 1209, 1218, 1332, 1333, 1348, 1350, 1352, 1354, 1364, 1373, 1375, 1375a, 1375b, 1378, 1382, 1427, 1450, 1586, 1603, 1744, 1819, 1842, 1882, 1887a, 1944, 1963, 2079, 2144, 2170, 2270, 2300, 2380, 2387, 2410, 2493, 2524a, 2545, 2547, 2570, 2601a, 2691–2695, 2767, 2774, 2799a, 2857, 2939, 3190, 3255, 3266, 3302, 3308, 3454, 3551, 3553, 3557, 3559, 3603, 3835, 3876, 3992, 3999, 4103, 4249, 4319, 4337, 5034, 5079, 5189, 5286, 5512, 5811b	120, 172a, 174b, 300–302, 310, 311, 319, 568b, 627, 830a, 858, 865, 1053, 1124, 1024, 1221, 1294–1296, 1332, 1383, 1819, 1933a, 2079, 2188, 2192, 2196, 2270, 2313a, 2380, 2481, 2547, 2761, 2762, 2765, 2766, 2788, 2790, 2789, 2913, 2939, 3163, 3266, 3370, 3551, 3603, 3689, 3707, 3797, 3813, 3876, 3973, 3974a, 4103, 4249, 4337, 5009, 5079, 5180, 5228, 5286, 5388, 5679, 5682, 5692, 5811b, 5817, 5836	50, 1354, 1375a, 1378, 2387
259.	102-76-1 [433]	1,2,3-Propanetriol, triacetate {triacetin}	173a, 332, 568b, 1063–1066, 1068–1074, 1302, 1340, 1364, 1365, 1371, 1586, 2410, 2487, 2506, 2507, 2522, 2543, 2545, 2601a, 2761, 2762, 2765, 2773, 2777, 3228, 3255, 3266, 3308, 3559, 3797, 3835, 4249, 4259, 4268, 4570a, 5811b	172a, 174b, 568b, 1053, 2410, 3266, 3354, 3370, 3593, 3905, 4249, 4259, 4751, 5018, 5089, 5543, 5555, 5811b	2506, 2507

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
260.	79-09-4 [386]	Propanoic acid {propionic acid} $H_3C\text{-}CH_2\text{-}COOH$	563, 565, 568b, 916, 960, 1023, 1063–1066, 1068–1074, 1132, 1140, 1232, 1263, 1360, 1364, 1365, 1371, 1375a, 1388–1390, 1586, 1587a, 1668, 1842, 1882, 1903, 1904, 1917, 2043, 2079, 2088, 2265, 2270, 2337, 2338, 2339b, 2387, 2493, 2529, 2543, 2545, 2570, 2619, 2623, 2761, 2762, 2765–2767, 2773, 2775, 2777, 2858, 2939, 3060, 3105, 3255, 3263, 3266, 3300, 3302, 3308, 3410, 3495, 3553, 3555, 3557, 3799, 3973, 4064, 4065, 4249, 4304, 4319, 5079, 5512, 5811b	120, 172a, 174b, 404, 563, 565, 568b, 647, 848, 937, 1053, 1085, 1087, 1263, 1587a, 1590a, 1923, 1999, 2014, 2092, 2283, 2337, 2338, 2339, 2386, 2389, 2544, 2570, 2862a, 2939, 3266, 3507, 3549, 3555, 3655b, 3973, 3973, 3974a, 3974b, 4249, 5079, 5381, 5811b	1360, 1375a, 2387, 3393, 3401, 3404
261.	50-21-5 598-82-3 [246]	Propanoic acid, 2-hydroxy- {lactic acid} $H_3C\text{-}CHOH\text{-}COOH$	126b, 172, 237, 568b, 1099, 1235, 1364, 1445, 1674, 1744, 1842, 1882, 2133, 2493, 2582, 2767, 2939, 3053, 3059, 3060, 3061, 3255, 3266, 3302, 3308, 3384, 3394, 3496, 3553, 3557, 3559, 4249, 5512, 5811b	120, 172a, 174b, 722, 568b, 1053, 1279, 2079, 2917a, 2939, 3052, 3053, 3060, 3266, 3486, 3797, 3973, 3974a, 4131, 4249, 5079, 5447, 5811b	3393, 3402, 3405
262.	97-64-3 [137]	Propanoic acid, 2-hydroxy-, ethyl ester {ethyl lactate} $H_3C\text{-}CHOH\text{-}COO\text{-}C_2H_5$	568b, 1371, 1884, 2761, 2762, 2765, 2766, 2777, 3266, 3553, 4249, 5811b	172a, 174b, 568b, 1053, 3266, 3370	
263.	79-31-2 [241]	Propanoic acid, 2-methyl- {isobutyric acid} $(H_3C)_2{=}CH\text{-}COOH$	563, 565, 568b, 775, 960, 1063–1066, 1068–1074, 1132, 1140, 1360, 1371, 1375a, 1388–1390, 1668, 1886, 2079, 2088, 2529, 2543, 2570, 2619, 2623, 2761, 2762, 2765, 2766, 2777, 2939, 3224, 3266, 3302, 3308, 3410, 3452, 3553, 3799, 3800, 4249, 4319, 5811b	120, 172a, 174b, 404, 563, 565, 568b, 908, 981a, 1053, 1085, 1087, 1999, 2014, 2079, 2270, 2283, 2338, 2339a, 2389, 2544, 2570, 2862a, 2917a, 2939, 3266, 3370, 3507, 3547, 3549, 3560, 3561, 3973, 3974a, 3974b, 4249, 5708, 5811b, 5846	1360, 1375a, 3393

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
264.	103-28-6 [7A]	Propanoic acid, 2-methyl-, phenylmethyl ester {benzyl isobutyrate}	172a	174b, 1248, 2339a, 3266, 4249	
265.	105-37-3 [149]	Propanoic acid, ethyl ester {ethyl propionate} H_3C-CH_2-COO-C_2H_5	625, 1140, 1903, 1904, 2088, 2858, 2939, 3266, 3302, 3308, 3797, 4249	172a, 174b, 1053, 2339a, 2939, 3266, 3370, 3797, 3974a, 4249	
266.	127-17-3 [394]	Propanoic acid, 2-oxo- {pyruvic acid} H_3C-CO-COOH	563, 568b, 1310, 2088, 2939, 3059, 3224, 3302, 3308, 3553, 4249, 5811b	69, 120, 172a, 174b, 563, 568b, 1053, 1305a, 1310, 1312, 1923, 2389, 2544, 2939, 3266, 3370, 3797, 3973, 3974a, 4249, 5811b, 5896	
267.	78-83-1 [234]	1-Propanol, 2-methyl- {isobutyl alcohol} $(H_3C)_2$═CH-CH_2OH	1140, 1416, 3266, 3302, 3797, 4249, 5811b	172a, 174b, 174b, 1053, 2282, 2339a, 3266, 3370, 4249	
268.	104-55-2 [74]	2-Propenal, 3-phenyl- {cinnamaldehyde}	568b, 1039, 1238, 3193, 3266, 3302, 4249, 5811b	568b, 1053, 2389, 2544, 2611, 3193, 3266, 3370, 3975, 4249	
269.	621-82-9 [75]	2-Propenoic acid, 3-phenyl- {cinnamic acid} C_6H_5-CH═CH-COOH	2767, 3265, 3266, 3557, 4159, 4249, 5811b	172a, 174b, 722, 1053, 1102, 1983, 2389, 2544, 2914, 3266, 3370, 3973, 4249, 5811b	
270.	140-10-3 [75]	2-Propenoic acid, 3-phenyl-, (*E*)- {*trans*-cinnamic acid}	568b, 3266, 3553, 4249	568b, 1053, 2092, 2389, 2544, 3266, 4249	
271.	102-94-3	2-Propenoic acid, 3-phenyl-, (*Z*)- {*cis*-cinnamic acid}	3266, 3553, 3557, 4249	1053, 2092, 2389, 2544, 3266, 4249	
272.	47018-25-7 [75]	2-Propenoic acid, 3-phenyl-, 2-phenylethenyl ester	3219, 3308, 3485, 4249		
273.	122-69-0 [78]	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester {cinnamyl cinnamate}	3219, 3224, 3308, 3485, 4249	172a, 174b, 1053, 3266, 3370	
274.	103-36-6 [130]	2-Propenoic acid, 3-phenyl-, ethyl ester {ethyl cinnamate}	2478, 3266, 3308, 4249	172a, 174b, 1053, 3266, 3370	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

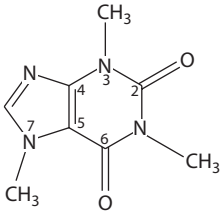
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
275.	103-26-4 [277]	2-Propenoic acid, 3-phenyl-, methyl ester {methyl cinnamate}	1379, 2487, 5811b	172a, 174b, 1053, 1379, 3266, 3370	
276.	7779-65-9 [226]	2-Propenoic acid, 3-phenyl-, 3-methylbutyl ester	2487	172a, 174b, 1053, 3266, 3370	
277.	103-41-3 [43]	2-Propenoic acid, 3-phenyl-, phenylmethyl ester {benzyl cinnamate}	2552, 2553, 3263, 3266, 3308, 3506, 3797, 4249, 5811b	172a, 174b, 1053, 3266, 3370	
278.	104-54-1 [77]	2-Propen-1-ol, 3-phenyl- {cinnamyl alcohol}	336, 568b, 4249	172a, 174b, 336, 568b, 1053, 1254, 1256, 3266, 3370, 3547, 4249	
279.	58-08-2 [63]	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine} 	568b, 1365, 1842, 3255, 3257, 3265, 3266, 3553, 4249, 5811b	568b, 1053, 3266, 4249	
280.	698-76-0 [338]	2*H*-Pyran-2-one, tetrahydro-6-propyl- {δ-octalactone}		172a, 174d, 404, 1053, 1254, 1256, 2389, 2544, 2917a, 3266, 3370, 3561, 4098a, 4249	
281.	4940-11-8 [140]	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy- {ethylmaltol}	90b, 568b, 3266, 4249, 5811b	172a, 174b, 568b, 1053, 3219, 3266, 3370, 4249	
282.	118-71-8 [256]	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}	568b, 1131, 1351, 1352, 1375, 1375a, 1375b, 1377, 1378, 1586, 1881, 1884, 2570, 2767, 2777, 3266, 3397, 3553, 3555, 3557, 4249, 5811b	172a, 174d, 568b, 965, 1053, 1590a, 2337, 2339b, 2386, 2389, 2544, 2917a, 3266, 3430, 3543, 3555, 3560, 3561, 5811b	1375a, 1377, 1378, 3401, 3402, 3404, 3405
283.	15707-24-1 [99]	Pyrazine, 2,3-diethyl-	1369, 1371, 1884, 2724, 2727, 2732, 2767, 3204, 3261, 3266, 3386, 4249	172a, 174b, 937, 1053, 1369, 3204, 3266, 3370, 3905, 4249	
284.	13238-84-1 [99]	Pyrazine, 2,5-diethyl-	1351, 1587a, 1884, 2570, 2727, 2731, 2732, 2735, 2767, 3204, 3266, 3386, 3491, 4249, 5811b	1053, 1369, 2338, 3204, 3266, 3905, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

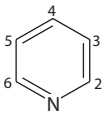
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
285.	13067-27-1 [99]	Pyrazine, 2,6-diethyl-	1351, 1587a, 1590, 1884, 2724, 2727, 2731, 2732, 2735, 2767, 3204, 3266, 3386, 3491, 4249	937, 1053, 1369, 2389, 2544, 2724, 3204, 3266, 3491, 3905, 4249	
286.	5910-89-4 [116]	Pyrazine, 2,3-dimethyl-	568b, 775, 1063– 1066, 1068–1074, 1348, 1349, 1351, 1360, 1364, 1369, 1371, 1375a, 1586, 1587a, 1884, 2142, 2337, 2439, 2470, 2543, 2545, 2724, 2727, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3261, 3266, 3491,4249, 4407, 4570a, 5811b	172a, 174b, 404, 568b, 937, 1053, 1369, 2337, 2339a, 2339b, 2359, 2724, 3204, 3266, 3491, 4249, 5811b	1360, 1375a
287.	123-32-0 [117]	Pyrazine, 2,5-dimethyl-	299, 480, 568b, 1063–1066, 1068–1075, 1348, 1349, 1351, 1364, 1365, 1369, 1371, 1587a, 1884, 2337, 2439, 2470, 2493, 2543, 2545, 2570, 2724, 2727, 2731, 2732, 2735, 2767, 2773, 2775, 3190, 3255, 3261, 3266, 3398, 3491, 3559, 3992, 4249, 4407, 4570a, 5811b	172a, 174b, 568b, 1053, 1369, 2337, 2339a, 2339b, 2359, 2386, 2724, 2917a, 3186, 3188, 3266, 3370, 3491, 4249	
288.	108-50-9 [118]	Pyrazine, 2,6-dimethyl-	299, 568b, 775, 1063–1066, 1068–1074, 1348, 1349, 1351, 1364, 1365, 1369, 1371, 1587a, 1884, 2337, 2387, 2439, 2470, 2543, 2545, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3255, 3261, 3266, 3491, 3555, 3559, 3888, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 937, 965, 1053, 1369, 2337, 2339a, 2339b, 2386, 2389, 2544, 2611, 2724, 2917a, 3266, 3491, 3555, 4249, 5811b	2387

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
289.	13360-65-1 [163]	Pyrazine,2-ethyl-3, 6-dimethyl- = Pyrazine,6-ethyl-2,5-dimethyl-	568b, 775, 1351, 1369, 1587a, 1884, 2337, 2439, 2727, 2731, 2735, 2767, 3261, 3266, 4249, 4570a	172a, 174b, 568b, 937, 1053, 2337, 3266, 3370, 3491, 4249, 5811b	
290.	13925-07-0 [162]	Pyrazine,2-ethyl-3, 5-dimethyl- = Pyrazine,3-ethyl-2,6-dimethyl-	568b, 775, 1351, 1369, 1587, 1587a, 1884, 2439, 2732, 2737, 2775, 3266, 4249, 4570a	172a, 174b, 431, 568b, 1053, 2836, 3266, 3370, 3491, 4249	
291.	15707-23-0 [165]	Pyrazine, 2-ethyl-3-methyl-	568b, 1075, 1351, 1364, 1587, 1587a, 2387, 2439, 2545, 2724, 2731, 2735, 2767, 3266, 4249, 4570a, 5811b	172a, 174b, 568b, 937, 1053, 2359, 2386, 2724, 3266, 3905, 4249	2387
292.	109-08-0 [315]	Pyrazine, methyl- = Pyrazine, 2-methyl- =	143, 157, 159, 167, 172, 299, 431, 480, 568b, 775, 1063–1066, 1068–1075, 1348, 1349, 1351, 1360, 1364, 1365, 1369, 1371, 1375a, 1427, 1428, 1587a, 1842, 1881, 1884, 1949, 2142, 2337, 2439, 2493, 2543, 2545, 2724, 2727, 2731, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3190, 3255, 3266, 3386, 3397, 3398, 3491, 3992, 4249, 4407, 4570a, 4733, 5811b	172a, 174b, 568b, 937, 965, 984, 1053, 1369, 1852, 1949, 2337, 2339a, 2359, 2544, 2611, 2724, 2917a, 3266, 3491, 4249, 5811b	1360, 1375a
293.	1124-11-4 [419]	Pyrazine, tetramethyl-	568b, 775, 1075, 1351, 1360, 1375a, 1587a, 1590, 1884, 2337, 2543, 2724, 2727, 2732, 2735, 2761, 2762, 2765, 2766, 2773, 2775, 3204, 3266, 3491, 3553, 3555, 4249, 4570a, 5811b	172a, 174b, 404, 568b, 937, 965, 1053, 1590, 2337, 2339b, 2386, 2389, 2544, 2724, 3204, 3266, 3370, 3491, 3555, 3905, 4249, 5811b, 17B01, 17B10	1360, 1375a

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

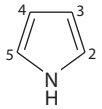
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
294.	14667-55-1 [444]	Pyrazine, trimethyl-	299, 568b, 775, 1063–1066, 1068–1075, 1348, 1349, 1351, 1360, 1369, 1371, 1375a, 1587a, 1881, 1884, 1949, 2337, 2387, 2470, 2506, 2507, 2543, 2545, 2570, 2724, 2727, 2732, 2735, 2761, 2762, 2765–2767, 2773, 2775, 2777, 3204, 3255, 3261, 3266, 3386, 3491, 3555, 3559, 4249, 4407, 4570a, 5811b	172a, 174b, 404, 568b, 937, 965, 1053, 1369, 1949, 2337, 2339a, 2339b, 2359, 2386, 2389, 2544, 2611, 2724, 2917a, 3204, 3266, 3370, 3491, 3555, 3905, 3974a, 4249, 5811b	1360, 1375a, 2387, 2506, 2507
295.	110-86-1 [391]	Pyridine 	38, 107, 126b, 156, 167, 172, 173a, 174b, 195, 237, 239, 299, 376, 395, 424, 462, 480, 512, 568b, 688, 775, 920, 985–988, 1063–1075, 1078, 1084, 1099, 1100, 1137, 1140, 1225, 1263, 1314, 1338, 1348, 1349, 1360, 1364, 1365, 1369, 1371, 1375a, 1386, 1426, 1427, 1437, 1445, 1580, 1587a, 1590, 1634, 1644, 1645, 1647–1649, 1659, 1673, 1674, 1699, 1741, 1744, 1803, 1812, 1842, 1857, 1884, 1890, 1891, 1903, 1911, 1966, 2001, 2006, 2088, 2133, 2142, 2170, 2191, 2224, 2226, 2228, 2230, 2233, 2234, 2267, 2270, 2313a, 2313c, 2326, 2337, 2342, 2342a, 2343, 2349, 2382, 2470, 2493, 2506, 2507, 2524, 2543, 2545, 2628, 2629, 2634, 2636, 2710, 2724,	120, 568b, 984, 1020, 1053, 1263, 1580, 1590, 1852, 2001, 2079, 2337, 2339a, 2359, 2389, 2544, 2724, 2917a, 2939, 2987, 3022, 3044, 3204, 3266, 3444, 3499, 3797, 3973, 3974a, 4064, 4249, 5079, 5390a, 5173, 5382, 5720, 5811b, 17B56	1360, 1375a, 2506 (0), 2507 (0), 3393

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine (cont.)	2734, 2761, 2762, 2765, 2766, 2773, 2775, 2777, 2799a, 2857, 2858, 2869, 2912, 2936–2938, 2939, 2973, 2986–2988, 3007, 3008, 3022, 3025, 3029, 3044, 3059, 3204, 3140, 3255, 3257, 3261, 3266, 3300, 3302, 3308, 3324, 3386, 3397, 3398, 3410, 3444, 3463, 3482, 3499, 3505, 3692, 3761, 3797, 3803, 3909, 3910, 3912, 3924, 3934, 3967, 3976, 3992, 3999, 4005–4007, 4064, 4065, 4120–4122, 4127, 4132, 4202, 4228, 4249, 4407, 5034, 5079, 5124, 5138, 5140, 5189, 5263, 5359, 5512, 5770, 5811b, 5836, 5869a		
296.	2294-76-0 [355]	Pyridine, 2-pentyl-	568b, 3255, 4249, 4570a	568b, 1053, 3266, 4249	
297.	536-78-7 [169]	Pyridine, 3-ethyl-	107, 568b, 775, 1063–1066, 1068–1075, 1078, 1084, 1099, 1140, 1316, 1348, 1349, 1360, 1364, 1369, 1371, 1375a, 1587a, 1634, 2142, 2228, 2233, 2234, 2387, 2470, 2493, 2543, 2545, 2724, 2761, 2762, 2765, 2766, 2773, 2775, 2869, 2912, 3255, 3261, 3266, 3302, 3308, 3386, 3397, 3398, 3410, 3463, 3491, 3499, 3505, 3797, 3976, 4249, 4407, 4570a, 4921, 5811b	568b, 984, 1053, 1078, 1157, 1316, 3266, 3430, 3973, 3974a, 4093, 4249, 5811b	1360, 1375a, 2387

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
298.	93-60-7 [283]	3-Pyridinecarboxylic acid, methyl ester {methyl nicotinate}	278, 1568, 3266, 4249, 5811b	1053, 1254, 1256, 1568, 2338, 2339a, 2611, 3266, 3491, 4249	
299.	109-97-7 [393]	1*H*-Pyrrole {azole} 	38, 157, 172, 241, 299, 480, 568b, 722, 884, 920, 1078, 1083, 1084, 1099, 1140, 1215, 1244, 1245, 1263, 1339, 1348–1350, 1354, 1361, 1375a, 1416, 1418, 1416–1418, 1426–1428, 1445, 1580, 1586, 1589, 1590, 1634, 1639, 1744, 1842, 1857, 2088, 2170, 2270, 2343, 2382, 2493, 2543, 2545, 2570, 2628, 2629, 2636, 2724, 2765–2767, 2775, 2799a, 2857, 2912, 2939, 3255, 3266, 3324, 3308, 3397, 3398, 3499, 3505, 3530, 3553, 3559, 3797, 3854, 3887, 4159, 4249, 5034, 5079, 5359, 5512, 5811b	568b, 722, 984, 1053, 1063–1066, 1068–1074, 1086, 1244, 1580, 1590a, 2359, 2386, 2724, 2767, 2903, 2908, 2917a, 2939, 3224, 3266, 3797, 3973, 4249, 5079, 5811b	1354, 1375a
300.	1401-55-4 [410]	Tannins {tannic acid}		120, 1053, 2270, 2154, 2939, 2947c, 3266, 3708, 3973, 4249, 5079, 5126, 5381	
301.	124-25-4 [322]	Tetradecanal {myristaldehyde} $H_3C\text{-}(CH_2)_{12}\text{-}CHO$	568b, 1366, 3266, 4249	404, 568b, 1053, 2093, 2094, 3266, 4249, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

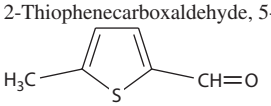
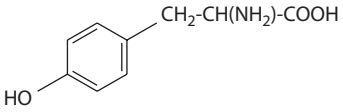
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
302.	544-63-8 [323]	Tetradecanoic acid {myristic acid} $H_3C\text{-}(CH_2)_{12}\text{-}COOH$	60, 101, 172, 257, 258, 568b, 765, 809, 1132, 1348, 1360, 1364, 1375, 1375a, 1375b, 1586, 1646, 1651, 1785, 1884, 2389, 2418, 2529, 2544, 2570, 2601a, 2761, 2762, 2765–2767, 2777, 2876, 2939, 3219, 3266, 3293, 3302, 3308, 3547, 3557, 3797, 4030, 4249, 4280, 4319, 4993, 5552, 5811b	60, 101, 120, 404, 568b, 634, 647, 835, 836, 838, 891, 908, 1053, 1330, 1651, 1785, 1893a, 1893b, 2079, 2270, 2283, 2338, 2339a, 2356, 2389, 2529, 2544, 2570, 2862, 2917a, 2939, 3194, 3219, 3266, 3328, 3332, 3547, 3549, 3797, 3842, 3973, 3974a, 4042c, 4249, 4280, 4397, 4993, 5079, 5695, 5811b	1360, 1375a
303.	124-06-1 [142]	Tetradecanoic acid, ethyl ester {ethyl myristate} $H_3C\text{-}(CH_2)_{12}\text{-}COO\text{-}C_2H_5$		172a, 174b, 568b, 908, 1053, 2093, 2389, 2544, 3266, 4249, 5811b	
304.	288-47-1 [421]	Thiazole 	568b, 1371, 1590, 3266, 4248, 4249	568b, 1053, 2359, 3266	
305.	13679-70-4 [290]	2-Thiophenecarboxaldehyde, 5-methyl- 	568b, 1590, 2761, 2762, 2765, 2766, 2777, 3266, 4249, 4570a	568b, 937, 1053, 1590, 3266, 4249	
306.	72-19-5 [422]	*L*-Threonine $H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	1351, 1910, 1914, 2724, 3266, 3302, 3491, 3555, 3797, 4249, 5811b	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1305a, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3555, 3705, 3780, 3797, 3973, 3974a, 3978, 4159, 4224, 4226, 4244, 4249, 4359, 4398c, 5079, 5811b, 5827, 5831, 5881	
307.	593-08-8 [434]	2-Tridecanone $H_3C\text{-}(CH_2)_{10}\text{-}CO\text{-}CH_3$		947, 1053, 3266, 4098a, 4249	

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
308.	60-18-4 [445]	*L*-Tyrosine 		120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1223, 1305a, 1329, 1330, 1332, 1351, 1493, 1918, 1965, 2270, 2337, 2338, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2939, 3266, 3491, 3499, 3705, 3780, 3797, 3973, 3974a, 3975, 3978, 4224, 4226, 4244, 4249, 4398c, 5079, 5785, 5811b, 5827, 5905, 5907	
309.	3796-70-1 [110]	5, 9-Undecadien-2-one, 6,10-dimethyl-, (*E*)- {geranylacetone} $H(CH_2\text{-}C(CH_3)=CH\text{-}CH_2)_2\text{-}CH_2\text{-}CO\text{-}CH_3$	568b, 1360, 1375a, 1586, 1949, 2570, 2761, 2762, 2765, 2766, 2777, 3266, 4249, 5811b	172a, 174b, 404, 568b, 1053, 1256, 1590a, 1949, 2015, 2338, 2339a, 2386, 2389, 2544, 2611, 2917a, 3188, 3215, 3217, 3219, 3266, 3329, 3354, 3370, 3545, 3547, 3549, 3550, 3560, 3561, 3905, 3973, 4098a, 4249, 5811b	1360, 1375a
310.	112-12-9 [449]	2-Undecanone {methyl nonyl ketone} $H_3C\text{-}(CH_2)_8\text{-}CO\text{-}CH_3$	1238, 3266, 4249	172a, 174b, 297, 404, 937, 1053, 2282, 3266, 4249	
311.	57-13-6 [451]	Urea $H_2N\text{-}CO\text{-}NH_2$	568b, 3266, 4249	172a, 174b, 568b, 622, 1053, 3266, 3370, 3973, 5079, 5811b	

(*continued*)

TABLE 24.3 (continued)
Tobacco and/or Tobacco Smoke Components Used as Tobacco Ingredients

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
312.	7004-03-7 [456]	Valine $(H_3C)_2$═CH-CH(NH_2)-COOH	1083, 1351, 1910, 1914, 2724, 2858, 2939, 3266, 3302, 3491, 3555, 3797, 4159, 4249	120, 158, 622, 749, 752–754, 826a, 927, 1053, 1063–1066, 1068–1074, 1086, 1223, 1329, 1330, 1332, 1351, 1493, 1918, 1919, 1965, 2270, 2337, 2338, 2339b, 2359, 2394a, 2453, 2532, 2597a, 2795, 2911c, 2914, 2939, 3266, 3491, 3499, 3555, 3705, 3726, 3780, 3797, 3973, 3974a, 3975, 3978, 4159, 4224, 4226, 4249, 4359, 4398c, 5079, 5493, 5785, 5827, 5831, 5881, 5905, 5907	
313.	7732-18-5 [459]	Water	50, 167, 172, 174, 194a, 211, 238, 239, 375, 403, 409, 427, 428, 445, 446, 480, 560, 568b, 603, 739b, 770, 825, 826, 846, 853, 916, 988a, 1063–1074, 1093, 1140, 1170, 1201, 1263, 1269, 1284, 1301, 1329, 1330, 1332–1334, 1346, 1354, 1375a, 1377, 1378, 1437, 1477, 1478, 1510, 1542, 1664, 1744, 1818, 1820, 1842, 1860, 1921, 1925, 1963, 1966, 2030, 2050, 2059, 2065, 2068, 2133, 2142, 2144, 2298, 2310, 2313b, 2274, 2398a, 2524, 2628, 2629, 2683, 2691–2695, 2721, 2741, 2744, 2843, 2854, 2855, 2920–2925, 2939, 3004, 3148a, 3187, 3190, 3224, 3228, 3258, 3266, 3302, 3308, 3370, 3531, 3548, 3569, 3572, 3575, 3583, 3584, 3696, 3876, 3900, 3917, 3976, 3992, 4060, 4078, 4120–4122, 4125, 4148, 4162, 4249, 4268, 5041, 5079, 5207, 5512, 5532, 5811b, 5836	69, 194a, 212, 480, 506, 541, 557, 568b, 918a, 954–956, 1053, 1115, 1164, 1206a, 1318, 1329, 1330, 1332, 1333, 1860, 1916a, 2151, 2153, 2603, 2739, 2740, 2744, 2765, 2766, 2914, 2939, 3029, 3266, 3370, 3569, 3575, 3576, 3797, 3819, 3941, 3962, 3973, 4043, 4249, 4272, 5018, 5031, 5053, 5079, 5165, 5419, 5585, 5609, 5612, 5656, 5723, 5774, 5803, 5811b, 5887	1330, 1332, 1354, 1375a, 1377, 1378, 3192, 4249

Note: The number in square brackets [] is that previously assigned (3266) to the tobacco ingredient component listed by Doull et al. (1053). The number with an A in square brackets [] is that previously assigned (3266) to the tobacco ingredient component listed by Baker et al. (174b, 174c, 24A01).
The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke.

Despite their criticism of the possible increased use of flavorants in the filler of low-"tar," low-nicotine cigarettes, the authors' admitted that prior to 1980, the U.S. cigarette manufacturers had apparently achieved a "reduction of toxic and tumorigenic effects in the smoke of low-'tar,' low-nicotine cigarettes."

In the U.S. Surgeon General's 1979 report [see pp. 63–64 in (4005)], the following was written:

> The trend toward low-tar, low-nicotine cigarettes and toward a reduction of undesirable volatile smoke compounds has brought about major changes in the smoke flavor of cigarettes. The use of rolled stems and reconstituted tobacco sheet admixed with leaf lamina and the use of effective filter tips are major factors inducing changes in smoke flavor. All of these developments have led to increased use of flavor additives, especially for low-tar, low-nicotine cigarettes. In fact, these new cigarettes require flavor corrections by additives in order to be acceptable to the consumer. Tobacco extracts as well as nontobacco flavors, such as licorice, cocoa, fruit, spices, and floral compositions, are used… At present, the selection of tobacco flavor additives from the GRAS (Generally Regarded As Safe) List or from natural extract and the screening of their smoke decomposition products for toxicity or other biological activity are not required by law and are done voluntarily by manufacturers.

Temperatures to which flavorants added to tobacco are exposed and the duration of the exposure during the smoking process range from 500°C to 700°C and the few seconds of the puff duration, respectively. Many of the flavor additives listed by the Surgeon General are used in cooking and/or baking where the exposure temperatures are lower than in the smoked cigarette, but the exposure time to the elevated temperature is much longer. This raises the question: Will more toxic compounds be formed from a given flavorant during foodstuff preparation or during cigarette smoking? When questioned about the need to determine the generation of toxic substances from a GRAS list additive used in cooking and/or baking, the FDA stated such studies were not required of the foodstuff manufacturer nor could they be done by the FDA since it had neither the staff, facilities, nor funds to undertake such studies.

In the U.S. Surgeon General's 1981 report [see pp. 51–52 in (4009)], it was noted

> Humectants and flavoring agents have long been used as additives in cigarette manufacture…In recent years, cigarette manufacturers' advertisements have focused on the flavor of new lower "tar" and nicotine cigarettes, enhanced presumably by the addition of tobacco constituents or by the addition of new flavoring materials, such as natural and synthetic chemicals. The identities and amounts of the additives actually used in the manufacture of U.S. cigarettes are not known. Systematic information has not been published or made available on the influence of these additives on the composition or biological activity of cigarette smoke.

A similar comment was made in the 1982 Surgeon General's report [see pp. 217–218 in (4010)]:

> The development of the low-tar cigarette required enrichment of smoke flavors in order to make the product acceptable to the consumer. The flavor is enhanced by addition of undescribed materials that may include concentrates of flavor precursors obtained from tobacco, licorice, extracts from other plants, or semisynthetic or fully synthetic flavor components. Because these additives have not been identified, no judgment can be made as to whether they result in new compounds or higher concentrations of hazardous components in the smoke. The practice of flavor enrichment requires detailed toxicological studies that are not available at present for scientific evaluation of their impact [LaVoie et al. (2314c); USPHS (4005)].

In the 1994 report by Doull et al. (1053) and the 2000 report by Paschke et al. (2895) on their analysis of reports on the effects of added cigarette tobacco ingredients on the chemical and biological properties of its MSS, both groups essentially reached the same conclusion: the added ingredients under the conditions of use contributed no adverse chemical or biological properties to the MSS.

In their 1997 review of the "changing cigarette," Hoffmann et al. (1716) did not discuss low-"tar" cigarettes or the presumed use of additional flavoring materials, identity unknown. In a second 1997 article on cigarette design changes implemented between 1950 and 1995, Hoffmann and Hoffmann [see pp. 345–346 in (1740)] discussed the casing additives sugars and humectants (glycerol, propylene glycol, diethylene glycol) but did not mention that some cigarette manufacturers do not use diethylene glycol. The transfer of humectants to cigarette MSS and their significant contribution to FTC "tar" yield were ignored. On flavor additives, they wrote

> In April 1994, the major U.S. cigarette companies released a list of 599 additives used at that time for the manufacture of cigarette [Doull et al. (1053)]. However, in the past, additional reactive flavor additives have been used (such as angelica lactone and linalool oxide; Leffingwell (2336)). An exception is menthol, which amounts to less than 2.5 mg in U.S. mentholated cigarette [Perfetti and Gordin (2923)]. Menthol is not carcinogenic in rodents [National Cancer Institute (24A10)], nor does this readily volatilized compound give rise to measurable amounts of carcinogenic hydrocarbons during smoking of cigarettes [Jenkins et al. (1936)]. Yet it is possible that the spraying of tobacco with menthol affects the burning characteristics of a cigarette and thus changes the concentration of toxic and/or tumorigenic agents in the smoke.

The Hoffmanns obviously ignored what Wynder and Hoffmann [see p. 527 in (4332)] wrote about the findings of Bock et al. (355) on the specific tumorigenicity of the MSS from menthol cigarettes:

> The results of Bock et al. [355] suggest no difference in tumorigenic activity of heptane-soluble "tar" from a mentholated cigarette compared with a plain cigarette when tested on a gram-to-gram basis.

Over the years, it has been repeatedly asserted that cigarette ingredients added at normal levels to pre-1980 cigarettes or at slightly increased levels to more recent lower-"tar" cigarettes might adversely modify the chemistry and biology of the MSSs from such cigarettes. However, despite these repeated assertions, no chemical or biological evidence has been presented by those authorities making such assertions in support of their assertions.

Table 24.4 summarizes many of the chemical and biological studies conducted since 1994 on the effect of tobacco ingredients on the chemical and biological properties of the MSS from cigarette containing a particular added ingredient or ingredient mixture. Many of the scientific criteria suggested by the Life Sciences Research Office (LSRO) personnel (24A08) are incorporated in the tabulated investigations. It is interesting that the LSRO in its 2004 monograph [see p. 50 in (24A08)] wrote about the Doull et al. list of 460 individual compounds: "However, the fate of very few of these chemicals has been studied in cigarettes."

This statement was made about the "very few" chemicals despite the listing by LSRO [see pp. 45–46 in (24A08)] of the studies by Baker et al. (174b, 174c), Massey et al. (24A09), and Baker and Smith (24A01) on 482 ingredients; the studies by Gaworski et al. (24A03, 24A04, 24A05) and Heck et al. (24A06) on over 170 ingredients; and the studies by Carmines (603), Roemer et al. (24A11), Rustemeier et al. (3370), and Vanscheeuwijck et al. (24A12) on 333 ingredients. In the latter studies (603, 3370, 24A11, 24A12), over 210 of the 333 ingredients (63%) were listed by Doull et al. as individual tobacco ingredients. Can more than 210 *vs*. 333 be considered "very few" agents in the smoke? LSRO is probably correct in its assessment of the number of individual components with a precise fate study, but examination and understanding of the pyrolysis data and effect of many of them on MSS chemical and biological properties provide much significant data on their behavior in a smoked cigarette. To date, there is much more known on the effect of added tobacco ingredients on MSS properties than there is on the effect of foodstuff additives on the properties of cooked foodstuffs.

Despite the wealth of information now available from the studies outlined in Table 24.4 that indicate that the ingredients—whether tobacco compounds or nontobacco compounds—added to cigarette tobacco do not significantly alter the MSS chemical or biological properties, none of the critics of tobacco ingredients has challenged the scientific findings presented in the publications listed, provided any contradictory scientific data, or suggested any additional definitive studies. This raises the question: Is this oft-repeated assertion about the deleterious effect of added tobacco ingredients like the many other antitobacco smoking assertions that have no supporting data or for which contradictory data or equivocal data have been generated [see Table 1 in Rodgman et al. (3307)]?

ACKNOWLEDGMENT

The authors are extremely grateful to the late Richard R. Baker for his meaningful contributions to several sections of this chapter that were included in part in previous ingredient publications.

TABLE 24.4
Summary of Tobacco Ingredient Studies Conducted from 1997 to Date

Analysis	Date	Number of Ingredients Studied	Reported Findings/Conclusions	Reference
Detailed literature survey of ingredients added to U.S. tobacco products	1994	599	It was concluded that there was no evidence that any ingredient added to commercial cigarette tobacco produces harmful effects under the conditions of use in cigarettes	Doull et al. (1053)
Effect of added tobacco ingredients on cigarette MSS chemistry	2002	333	The smoke chemistry data revealed changes toward both higher and lower amounts of various smoke constituents…. This suggests that the addition of 333 commonly used ingredients to cigarettes in three groups did not add to the toxicity of the smoke, even at the exaggerated levels tested… An overall assessment of our data suggests that these ingredients, when added to the tobacco, do not add to the toxicity of smoke, even at the elevated levels used in this series of studies	Carmines (603); Rustemeier et al. (3370)
	2002	482	In most cases, the flavor mixtures had no statistically significant effect on the smoke yields relative to the control cigarette. In a few cases, the small increases or decreases were observed for some analytes relative to the control cigarette. The smoke yields of the experimental cigarettes were well within the ranges observed in the three reference cigarettes	Baker and Smith (24A01)
	2004	450	The significances of differences between the test and control cigarettes were determined using both the variability of the data on the specific occasion of the measurement, and also taking into account the long-term variability of the analytical measurements over the 1-year period in which analyses were determined in the present study. This long-term variability was determined by measuring the levels of the 44 "Hoffmann analytes" in a reference cigarette MSS on many occasions over the 1-year period of this study The effects of 450 tobacco ingredients (many were individual compounds listed in Tables 24.1 and 24.2) added to tobacco as seven different mixtures on the yields of 44 "Hoffmann analytes" in cigarette MSS were determined. In most cases, the flavoring ingredient mixtures had no significantly statistical effect on the MSS "Hoffmann analyte" yields *vs*. those from the control cigarette. Occasionally, with some mixtures, differences would be observed in some "Hoffmann analyte" yields	Baker et al. (174b)
	2004	32	The effects of 29 casing ingredients and three humectants added to tobacco as 8 different mixtures on the yields of 44 "Hoffmann analytes" were determined. Many of the ingredient mixtures had no statistically significant effect on the MSS "Hoffmann analyte" yields *vs*. those from the control cigarette. An increase in one "Hoffmann analyte," formaldehyde, was reported when the ingredient mixture contained sugar	Baker et al. (174c)
Effect of added tobacco ingredients on cigarette MSS biology: (a) in vitro genotoxicity and cytotoxicity	1997, 2002	≈152	Although the mutagenic activities appeared to be similar, there were statistically significant differences in mutagenic activities among the samples (The differences were primarily due to the increase in mutagenicity of the CSC when the humectants [glycerol, propylene glycol] were not added to the cigarette tobacco and thus were not present as diluents in the CSC)	Bioresearch [for RJRT] (24A02); Rodgman (3263, 3264)
	2002	333	Within the sensitivity and specificity of the test systems, the in vitro mutagenicity and cytotoxicity of the cigarette smoke were not increased by the addition of the ingredients	Carmines (603); Roemer et al. (24A11)

(*continued*)

TABLE 24.4 (continued)
Summary of Tobacco Ingredient Studies Conducted from 1997 to Date

Analysis	Date	Number of Ingredients Studied	Reported Findings/Conclusions	Reference
	2002	482	The data have been analyzed and demonstrate no additional activity from the flavored cigarettes above that of the control products	Massey et al. (24A09)
(b) MSS smoke inhalation	1997, 2002	2 (Glycerol, propylene glycol)	It was concluded that addition of the tested humectants singly or in combination had no meaningful effect on the site, extent or frequency of respiratory tract changes associated with smoke exposure in rats	Heck et al. (24A06)
	1997	1 (Menthol)	The results of this 13-week inhalation study indicated that the addition of 5000 ppm menthol to tobacco had no substantial effect on the character or extent of the biological responses normally associated with inhalation of mainstream cigarette smoke in rats	Gaworski et al. (24A03)
	1998	170	The results indicate that the addition of flavoring ingredients to cigarette tobacco had no discernible effect on the character or extent of the biologic responses normally associated with inhalation of mainstream cigarette smoke in rats	Gaworski et al. (24A04)
	2002	333	The data indicate that the addition of these 333 commonly used ingredients, added to cigarette in three groups, did not increase the inhalation toxicity of the smoke, even at the exaggerated levels used	Carmines (603); Vanscheeuwijck et al. (24A12)
(c) MSS CSC and skin painting	1999	150	While tumor incidence, latency and multiplicity data occasionally differed between test and comparative reference CSC groups, all effects appeared to be within normal variation for the model system. Furthermore, none of the changes appeared to be substantial enough to conclude that the tumor promotion capacity of CSC obtained from cigarettes containing ingredients was discernibly different from the CSC obtained from reference cigarettes containing tobacco processed without ingredients	Gaworski et al. (24A05)
Pyrolysis of tobacco ingredients under conditions simulating those in the cigarette burning zone	2002/2004	291	The results are compatible with parallel studies in which the ingredients are added to tobacco and the effect on cigarette smoke constituents are measured. In general, the number of "Hoffmann analytes" detected among the pyrolysis products of the ingredients, and their levels, are low…. Of the 291 tobacco ingredients pyrolyzed, almost a third transfer out of the pyrolysis zone intact, and almost two thirds transfer at least 95% intact	Baker and Bishop (172a)
	2003		A review of the pre-2003 studies on the effect of added ingredients on the chemical and biological properties of cigarette MSS with emphasis on the yields of the "Hoffmann analytes." Their discussion included various published (603, 1053, 3263, 3264, 3266, 24A03, 24A04, 24A05, 24A06) and pre-published (172a, 174a, 174b, 3314a, 3370, 24A09, 24A11, 24A12) manuscripts on tobacco ingredients	Baker and Smith (174e)
	2004	482	This publication summarized the reported findings on the 482 tobacco ingredients studied by Baker et al. (174b, 174c). The major conclusion: Many of the added tobacco ingredient mixtures produced no significant effect on the yields of many of the "Hoffmann analytes" in the cigarette MSS. In a series of three biological studies on genotoxicity and cytotoxicity, the response due to MSS exposure was not distinguishable between the ingredient-treated cigarette and the control	Baker et al. (174a)

TABLE 24.4 (continued)
Summary of Tobacco Ingredient Studies Conducted from 1997 to Date

Analysis	Date	Number of Ingredients Studied	Reported Findings/Conclusions	Reference
	2004	1 (Glycerol)	A study to determine the effect of different levels of added glycerol on cigarette MSS yields: The glycerol transfer was proportional to that added to the tobacco blend.	Liu (2380)
	2005	159 Nonvolatile and complex ingredients (these ingredients were not individual compounds)	With a system simulating cigarette combustion conditions, pyrolysis of many of the nonvolatile ingredients gave no "Hoffmann analytes." When occasionally formed, the "Hoffmann analytes" included phenols, benzene, toluene, and styrene. Biologically active furfural, never listed as a significant biologically active smoke component by Hoffmann and his colleagues (1727, 1740, 1741, 1743, 1744, 1773, 1808), was occasionally formed	Baker and Bishop (172b)
	2006	1 (Sugar)	This study was an extension of the previously reported effect (174c) of sugar ingredients on the MSS yield of formaldehyde	Baker et al. (172c)

25 Pyrolysis

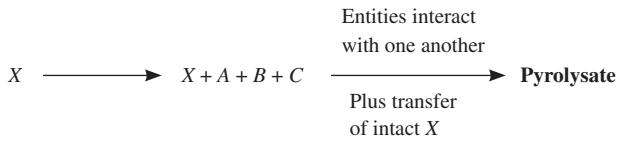
For many years, the fate during smoking of a compound added to cigarette tobacco was defined by its fate during pyrolysis as an individually pyrolyzed compound. The stimulus for this assertion was twofold: (1) Many publications were available that indicated the pyrolysis of many compounds—from relatively low-molecular-weight ones such as acetylene to much higher-molecular-weight ones such as the sterols—yielded tumorigenic polycyclic aromatic hydrocarbons (PAHs); (2) the ingredients to improve the smoking quality of a cigarette were added at such a low level that analytical data on their effect on smoke composition were almost impossible to generate. Because of this analytical problem with additives to the cigarette filler, many investigators utilized pyrolysis of individual tobacco components or additives in an attempt to define the spectrum of products and their influence on tobacco smoke composition and properties.

The assertion of the equivalence of the fate of a compound on pyrolysis *vs.* its fate in a cigarette tobacco filler during smoking persisted for over 20 years after the mid-1950s. As proponents of this equivalence, Wynder and Hoffmann [see pp. 346–347 in (4332)] wrote:

> Most pyrolysis studies with tobacco, tobacco extracts, extract fractions, individual components, and tobacco additives are performed in a nitrogen atmosphere. This procedure has often been criticized on the grounds that many of the toxic constituents formed during smoking of tobacco products occur as a result of combustion in air rather than in a nitrogen atmosphere. This criticism, however, cannot be maintained in view of studies by Newsome and Keith (2780) which demonstrated that a reducing rather than an oxidizing atmosphere exists at the cone region of a burning cigarette.

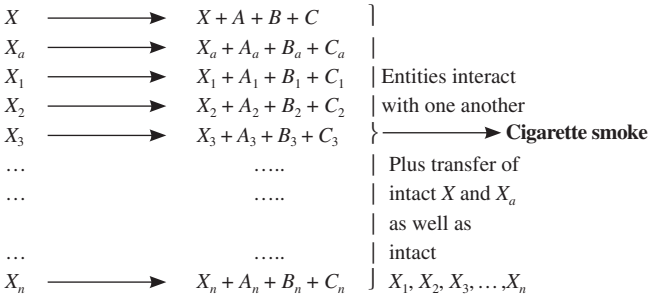
Consideration of the effect of pyrolysis and the cigarette smoking process reveals the following: In both cases, a given compound may undergo a variety of reactions. In the pyrolysis case, fragments produced from the compound during pyrolysis only have the opportunity to react with the unchanged compound itself or with each other. In the smoked cigarette case, the added compound, either inherent in tobacco or added, generates fragments during the smoking process which have the opportunity not only to react with intact volatilized tobacco components (over 6000 of which have been identified) but also to react with the reaction fragments produced from them.

If it is assumed that a given compound, compound X, during pyrolysis is not only transferred in part to the pyrolysate but also yields three pyrosynthetic fragments (A, B, and C), then these four entities (X, A, B, and C) may transfer to the pyrolysate intact or interact in a variety of ways to form a mixture of pyrolysate components.



If it is assumed not only that the same type of reaction occurs in a cigarette during the smoking process in the case of compound X, either added (X_a) to or inherent (X) in the tobacco blend, but also that similar degradation reactions occur with the other tobacco components ($X_1, X_2, X_3, \ldots, X_n$), the situation described in the following equations could exist, where n could be as high as or higher than 6000, the approximate number of identified tobacco components.

In the study of the addition of compound X to a cigarette tobacco filler, the added compound is designated as X_a. The inherent tobacco compound X and its fragments A, B, and C plus the added compound X_a and its fragments A_a, B_a, and C_a have the opportunity not only to react with each other but also to interact with $X_1, X_2, X_3, \ldots, X_n$, $A_1, A_2, A_3, \ldots, A_n$, $B_1, B_2, B_3, \ldots, B_n$, and $C_1, C_2, C_3, \ldots, C_n$, the fragments from hundreds of other tobacco components. In both the pyrolysis case and the cigarette smoke formation case, the number of fragments may, of course, be many more than the three designated as A, B, and C.



Obviously, pyrolysis of an individual compound (compound X) at a specific temperature and during the smoking process in a machine-smoked cigarette whose blend contains inherent compound X and added compound X_a are entirely different situations and will yield qualitative and quantitative differences between the compositions of the pyrolysates and the cigarette smoke. Qualitatively, there may be some similarities in the two compositions. Quantitatively, the probability of any similarity is extremely low. It should be noted that during the pyrolysis of compound X, a specific temperature such as 700°C or 600°C is usually maintained. During the smoking process occurring in the compound X- and $(X + X_a)$-containing cigarette, compounds X and X_a and their pyrogenetically generated fragments are exposed to a range of temperatures varying from nearly 1000°C at the fire cone

to 50°C–60°C near the butt. In addition, Britt et al. (435) noted that the residence time during most pyrolysis studies of tobacco components was much longer than that encountered by the tobacco components during the smoking process.

The reactions depicted earlier in pyrolysis of a component *vs*. those in the cigarette smoking process with a component added to the tobacco exist despite the assertion that the pyrolysis procedure has been specifically designed to simulate the smoking process (172b, 1648, 3616).

In 1979, Schmeltz et al. (3512) reported on the fate of radiolabeled nicotine during pyrolysis, and its fate during actual smoking of a cigarette containing the radiolabeled nicotine reveals at least two of the coauthors (Hoffmann, Schmeltz) had changed their long-held view on the supposed equivalence of compound behavior during pyrolysis and actual smoking. Schmeltz et al. wrote:

> Products obtained from the thermal degradation of [^{14}C] nicotine in a combustion tube (under pyrolytic conditions) and in a cigarette (undergoing machine smoking) were examined by gas-liquid chromatography (GLC), by GLC-mass spectrometry, and by radiochromatography. Under pyrolytic conditions in a combustion tube, nicotine underwent extensive degradation to pyridines, quinoline, arylnitriles, and aromatic hydrocarbons. In contrast, in a burning cigarette, a substantial portion of nicotine remained intact (≈41%), 12.5% underwent oxidation to CO_2, up to 11% was degraded to volatile pyridine bases, and negligible amounts were converted to neutral or acidic particulate components. A major portion of nicotine and its degradation products was also diverted to sidestream smoke. These results suggest to us that pyrolysis experiments may be limited for establishing the fate of nicotine and possibly other tobacco components in a burning cigarette.

On the basis of numerous pyrolysis studies, it has been postulated that a number of tobacco leaf components are the major precursors of components in tobacco smoke. Throughout this chapter, smoke components alleged by some investigators to play a role in the smoking–health issue have been emphasized, particularly those smoke components supposedly involved in the causation of lung cancer or other respiratory tract disorders. Carbon monoxide and nicotine have been proposed as cigarette mainstream smoke (MSS) components involved in cardiovascular problems. Nicotine occurs in cigarette smoke as a result of its transfer from the cut tobacco leaf where it is considered to be present in the so-called bound form as a variety of nicotine salts with organic acids (citric, malic, oxalic, palmitic, stearic, etc.). As noted by Perfetti (2918a, 25A47), these nicotine salts may have various structures, depending on the nature of the acid, e.g., the molar ratio of acid to nicotine may be 3:1, 2:1, or 1:1. During the cigarette smoking process, these salts, depending on their composition, are considered to decompose to yield products ranging from mainly nicotine plus the acid in the salt to traces of nicotine plus various nicotine reaction and degradation products plus the acid. It has been proposed that the nicotine in the smoke again "binds" with acidic components of the smoke and is considered to be present primarily in the mainstream particulate phase as "bound" nicotine, but the binding in cigarette MSS is different from that in the tobacco. In cigarette smoke, the "binding" or salt formation is considered to be primarily with the stronger aliphatic organic acids such as formic, acetic, etc., whose levels in smoke are substantial compared to those of palmitic acid, stearic acid, etc.

Table 25.1, modified and updated from similar tables by Chortyk and Schlotzhauer (722) and Baker (171a), summarizes the major precursor relationships proposed and/or demonstrated for tobacco leaf components and tobacco smoke components. These proposals are based in part on the results of a numerous pyrolysis studies. In some cases, the validation of the proposals is based on results obtained by addition of leaf components to tobacco and assessing the effect on the yields of specific MSS components when the "spiked" tobacco is smoked as a cigarette.

As noted previously, equivalence of the reaction mechanisms involved in pyrolysis and those involved in the tobacco smoking process was debated for many years, with the current consensus being that these processes are not equivalent. Also included are the results of research in the mid-1950s on the major tobacco and cigarette paper component, cellulose, either smoked in cigarette configuration [Fredrickson (1228), Fredrickson et al. (1238)] or burned or pyrolyzed in bulk. When the primary focus of the early research was on the pyrogenesis of PAHs, Wright (4281) demonstrated that the amount of benzo[*a*]pyrene (B[*a*]P) generated during bulk burning or bulk pyrolysis of cellulose was much greater than that generated during the burning of the cellulose (cigarette paper) in a cylindrical form, simulating its configuration in the cigarette.

25.1 INDIVIDUAL TOBACCO TYPES

In the early 1930s, Roffo (3320, 25A50, 25A51, 25A52) reported the production of skin tumors in laboratory animals by the repeated application of a "tar" obtained by the "destructive distillation" of tobacco. This "destructive distillate" from tobacco, as noted by Wynder and Hoffmann (4319, 4332), is in no way comparable to the smoke condensate generated from cigarettes during a smoking procedure simulating that used by the human smoker in terms of puff duration, puff frequency, and puff volume. Despite the fact that the puff volume, puff duration, and puff frequency were usually set at 35 mL, 2 s, and 1 puff/min, respectively, after the 1937 publication by Bradford et al. (424) on human smoking parameters, Wynder et al. (4306a) elected to use a puff frequency of 3 puff/min for the generation of cigarette smoke condensate (CSC) for their mouse-skin-painting studies, despite their assertion that the smoking regime simulated that of the human smoker.

In addition, the destructive distillation procedure used by Roffo is not comparable to the pyrolysis procedures used several decades later by other investigators, e.g., Lam (2255, 2257) and Wynder et al. (4355). Roffo's work is presented here for the sake of historical completeness. In later reports,

TABLE 25.1
Precursor Relationships between Tobacco Leaf Components and Tobacco Smoke Components

Smoke Component	Leaf Component	References
Monocyclic Aromatic Hydrocarbons		
Benzene, toluene, xylenes, etc.	Tobacco extracts	Schlotzhauer and Schmeltz (3465, 3466), Schlotzhauer et al. (3456)
	Paraffin hydrocarbons	Schlotzhauer and Schmeltz (3466)
	Aliphatic acids	Schlotzhauer and Schmeltz (3466)
	Sugars	Schlotzhauer and Schmeltz (3466)
	Amino acids	Patterson et al. (2902); Schlotzhauer and Schmeltz (3466), Higman et al. (1647)
PAHs		
Naphthalenes, anthracenes, phenanthrenes, pyrenes, chrysenes, fluoranthenes, benzopyrenes, etc.	Solanesol	Severson et al. (3616), Rodgman and Cook (3269, 3291)
	Terpenes	Schlotzhauer and Schmeltz (3466), Severson et al. (3616)
	Tobacco extracts	Rodgman and Cook (3269, 3291), Rodgman (3246), Schlotzhauer and Schmeltz (3465), Schlotzhauer et al. (3466), Severson et al. (3615, 3616)
	Paraffin hydrocarbons	Rodgman and Cook (3269, 3291), Rodgman (3246), Lam (2255, 2257), Schlotzhauer and Schmeltz (3466), Severson et al. (3616)
	Polysaccharides (pectin, cellulose, starch)	Wright (4281), Gilbert and Lindsey (1289), Higman et al. (1647)
	Phytosterols	Rodgman and Cook (3269, 3291), Wynder et al. (4355), Rodgman (3246), Severson et al. (3616), Schlotzhauer and Schmeltz (3466)
	Long-chained esters	Severson et al. (3616)
	Amino acids	Patterson et al. (2902); Higman et al. (1647)
	Sugars	Gilbert and Lindsey (1289), Higman et al. (1647)
	Triglycerides	Rodgman and Cook (3269)
Phenols	Lignin	Rodgman and Mims (3305), Schlotzhauer et al. (3468), Higman et al. (1647), Schlotzhauer et al. (3466)
Phenol, cresols, xylenols, dihydroxybenzenes, etc.	Sugars	Bell et al. (246), Spears et al. (3767),
	Polysaccharides (cellulose, pectin, starch)	Higman et al. (1647), Schlotzhauer et al. (3466)
	Protein	Higman et al. (1647)
	Amino acids	Higman et al. (1647)
	Tobacco extracts	Schlotzhauer et al. (3466)
	Extracted tobacco	Rodgman and Cook (3277), Rodgman and Mims (3305), Severson et al. (3616)
	Chlorogenic acid	Schlotzhauer et al. (3462)

(*continued*)

TABLE 25.1 (continued)
Precursor Relationships between Tobacco Leaf Components and Tobacco Smoke Components

Smoke Component	Leaf Component	References
Aldehydes and Ketones		
Formaldehyde, acetaldehyde, acrolein, acetone, α,β-dicarbonyls, quinolines, carbolines, etc.	Sugars	Gager et al. (1264, 1265), Houminer and Patai (1835d), Johnson et al. (1960), Higman et al. (1647)
	Polysaccharides (cellulose, pectin)	Zamorani et al. (4398d); Fredrickson (1228), Fredrickson et al. (1238)
	Triglycerides	Kitamura (2111a)
	Glycerol	Doihara et al. (1023, 1024), Kröller (2192, 2196)
Hydrogen Cyanide	Amino acids	Patterson et al. (2902, 2905), Higman et al. (1647), Johnson et al. (1967)
Aliphatic Nitrogen Compounds		
Aliphatic amines, volatile	Amino acids	Smith et al. (3729)
N-nitrosamines	Protein	Higman et al. (1647)
	Nicotine	Kaburaki et al. (2006), Schmeltz et al. (3512)
	Nicotine + nitrate	Tso et al. (3985), Hecht et al. (1564), Hoffmann et al. (1696)
Monocyclic Nitrogen compounds		
	Amino acids	Patterson et al. (2902), Higman et al. (1647)
Anilines, pyrazines, pyridines,	Amino acids + sugars	Green et al. (1369)
PYRs, TSNAs, etc.	Protein	Higman et al. (1647), Schmeltz et al. (3499)
	Nicotine	Schmeltz et al. (3512)
Polycyclic Nitrogen Compounds		
Indoles, carbazoles, acridines, quinolines, carbolines, etc.	Nicotine	Van Duuren et al. (4027), Kaburaki et al. (2006), Schmeltz et al. (3512)
	Amino acids	Patterson et al. (2902), Higman et al. (1647), Yamamoto et al. (4365a), Sugimura (3828c)
	Protein	Higman et al. (1647)
N-Heterocyclic Amines		
Trp-P-1, Trp-P-2, Glu-P-1, Glu-P-2, IQ, A*a*C, MeA*a*C, etc.	Amino acids	Chortyk et al. (726); Patterson et al. (2902), Akimoto (25A01), Dong et al. (1041), Sugimura et al.(3829a), Kosuga et al. (2178a); Sugimura (3828a, 3828b), Takeda et al. (3863a, 25A73), Yasuda et al. (4382a), Yoshida and Matsumoto (4387a, 4387b, 4388), Yamazoe et al. (4370a), Conner and Dominguez (25A17); Coleman and Perfetti (25A14), Coleman et al. (25A15)
	Protein	Yoshida et al. (4389A, 4390)

TABLE 25.1 (continued)
Precursor Relationships between Tobacco Leaf Components and Tobacco Smoke Components

Smoke Component	Leaf Component	References
Sulfur-Containing Compounds		
	Sulfur-containing amino acids	Fujimaki et al. (25A23), Kato et al. (2048, 2049) Smith et al. (3729)
Acids, Aliphatic		
Formic to nonanoic	Esters of mono- and disaccharides and aliphatic and terpenoid alcohols	Wynder and Hoffmann (4332)
Acids, Aliphatic		
Decanoic and higher	Esters of phytosterols, aliphatic alcohols, and terpenoid alcohols	Wynder and Hoffmann (4332), Severson et al. (3616)
Acids, Aromatic		
	Lignin	Wynder and Hoffmann (4332)

Roffo (3323, 3325) and his son (3316, 3318) claimed the identification of B[*a*]P in the destructive distillate of tobacco, but these claims were subsequently challenged by Wynder et al. (4306a) who noted:

> Roffo …claimed to have identified benzpyrene in tobacco tar, but this could not be confirmed by Hirst and his coworkers (813), and more recently that substance could not be detected by Waller (25A81). An examination by Eby (25A21) of the tobacco tar used in this study [the mouse skin-painting study by Wynder, Graham, and Croninger (4306a)] did not reveal any spectroscopic evidence of the known carcinogenic hydrocarbons.

Roffo (25A60) also claimed that the biological results in his painting results with the effect on the levels of "destructive distillate" from tobacco were the same no matter which type of tobacco was subjected to his destructive distillation process. That his destructive distillation was not comparable to the actual cigarette smoking process was demonstrated in later studies by Wynder and Hoffmann (4317, 4332) who reported that the different types of tobacco types (flue-cured, burley, Maryland, and Oriental) generated CSCs whose specific tumorigenicities were different as were their contents of B[*a*]P and phenol. The specific tumorigenicities and phenol levels per milligram of CSC were found to be in the sequence

Flue-cured = Oriental > Maryland > burley,

whereas the B[*a*]P levels per milligram of condensate were found to be in the sequence

Flue-cured > Oriental > Maryland > burley.

More recent confirmation of the differences among tobacco types in another bioassay has been obtained with regard to the specific mutagenicities (as measured in the Ames test with *Salmonella typhimurium*) of their smoke condensates generated under standard conditions. Results of both in-house studies [Smeeton et al. (3707)] and external studies [Mizusaki et al. (2568), Yoshida and Matsumoto (4388), Demarini (933)] indicate the response of different strains of *S. typhimurium* in the Ames test to smoke condensates from cigarettes fabricated with different tobacco types not only are dissimilar but also are in a sequence opposite that found for specific tumorigenicities determined in mouse-skin-painting studies, i.e., the mutagenicities based on an equivalent weight of smoke condensate were found to be in the sequence

Flue-cured < Oriental < Maryland < burley.

Critical reviews of the Roffo work have been published by Wynder et al. (4306a), Wynder and Hoffmann (4332), and Larson et al. (2264). All three groups asserted that the "destructive distillate" from tobacco, as prepared by Roffo, is not comparable to CSC generated under conditions more closely approximating those in the human smoking of a cigarette. Larson et al. also noted that the number of malignant tumors produced in all of the Roffo skin-painting studies with the destructive distillate from tobacco was so few (three malignant tumors [two carcinoma, one sarcoma] in nearly 1000 treated animals) as to be almost within experimental error.

Over the years, pyrolysis studies with tobaccos under a variety of conditions have provided diverse results with regard to the level of B[*a*]P found in the pyrolysate, e.g., Kröller (2196), Green and Best (1357), and Severson et al. (3616). The phenol/B[*a*]P ratios were also much compared in pyrolysates and MSSs, and they too provided diverse results, e.g., Wynder and Hoffmann (4319, 4332), R.J. Reynolds Tobacco Company (3190). Adams et al. (31) used catechol rather than phenol as an "indicator" for phenols, provided

MSS and SSS B[*a*]P and catechol data on four different types of commercial cigarettes. From these data, the calculated catechol/B[*a*]P ratios for the combined MSS and SSS were widespread, ranging from 1074:1 to 2680:1. The data reported by Severson et al. on the yields of phenol and benzopyrenes in the pyrolysates (and the ratios derivable from their data) demonstrated that the process involved in the generation of a tobacco pyrolysate is not comparable to the process involved in the generation of CSC from cigarettes made with the same tobacco and smoked under conditions simulating the human smoking process.

25.2 EXTRACTS FROM TOBACCO

The 1953 report of the successful production of carcinomas in mice repeatedly painted for their life span with daily doses of CSC generated by a smoking process supposedly simulating that used by human cigarette smokers [Wynder et al. (4306a)] led to a search for the smoke component(s) responsible for the biological response. No carcinogenic, cocarcinogenic, or promoting compound identified in CSC, when considered at its concentration in CSC, can explain the biological response obtained in mouse-skin-painting studies nor can it be explained when the carcinogenic, cocarcinogenic, and promoting components at their CSC concentrations are considered to be acting in concert.

The finding in 1913 by Staudinger et al. (25A68) that pyrolysis of isoprene yielded a "tar" was utilized a decade later by Kennaway (2073–2076). He reported that heating organic compounds (acetylene, isoprene, cholesterol, foodstuffs) at high temperatures (in air or an inert atmosphere) yielded "tars" or "pyrolysates" which were tumorigenic to the skin of laboratory animals. After the discoveries of the tumorigenicity of dibenz[*a,h*]anthracene (DB[*a,h*]A) and B[*a*]P, many such generated pyrolysates were shown to contain various tumorigenic PAHs [Rodgman (3233, 25A48)]. In the early 1950s, a controversy arose about the presence of such PAHs in CSC, a material generated by the exposure of tobacco—a mixture of many organic compounds—to temperatures ranging from slightly above ambient to over 900°C. By the late 1950s, this controversy was resolved by the identification in CSC of a variety of PAHs, including several [B[*a*]P, chrysene, benz[*a*]anthracene (B[*a*]A), 7,12-dimethylbenz[*a*] anthracene (DMB[*a*]A), DB[*a,h*]A] reported to give positive responses in skin-painted laboratory animals, albeit at dose levels far in excess of the their levels in CSC. Wynder and Hoffmann (4332) reviewed much of the early research on the identification of PAHs in CSC.

Demonstration that PAHs were present in CSC then led to research on their source(s). Cigarette paper [Wright (4281)], the lighting source (matches, flammable organic solvent-charged cigarette lighters), and PAHs in environmental pollutants to which tobacco might be exposed during growth, harvesting, and transportation [Campbell and Lindsey (583), Lyons (2426), Bentley and Burgan (285)] were eliminated as sources or precursors of PAHs in cigarette smoke. Extensive research subsequently determined that tobacco itself and/or its components were precursors of the PAHs in CSC.

As noted previously, in the 1930s, Roffo (3320, 25A50) claimed the production of malignant tumors in laboratory animals skin painted with a "destructive distillate" from tobacco. Roffo (3323, 3325) and his son [Roffo (3316, 3318)] also claimed identification of a benzopyrene or a "benzopyrene-like" substance in the distillate. Subsequently, Roffo reported that organic solvent extraction of tobacco yielded an organic solvent-insoluble tobacco residue whose "destructive distillate" was less tumorigenic in skin-painting studies than the "destructive distillate" prepared from the unextracted (control) tobacco (3327). Roffo postulated that the major tobacco precursor of the "distillate" component responsible for the tumorigenicity observed in laboratory animals was the phytosterols.

Coincident with general acceptance of biologically active PAHs in CSC were extensive pyrolysis studies not only on organic solvent-extractable materials from tobacco but also individual components and classes of components in the solvent-extracted materials. The organic solvent (pentane, hexane, heptane, petroleum ether) used as extractant removed waxlike organic components from the tobacco. These waxy materials comprised several series of long-chained saturated (1308, 3807) and unsaturated aliphatic hydrocarbons (3247, 3345) and alcohols (812, 3276), phytosterols and their long-chained fatty acid esters (3247), terpenoid alcohols such as solanesol (3344, 3359) and the duvanediols (3195, 3220, 3221, 3283, 3351, 3361), solanesyl esters with long-chained fatty acids (3296, 3358; 3616), and a series of esters of long-chained alcohols and long-chained fatty acids (3294).

Contradictory results were obtained on the yields of the allegedly tumorigenic PAHs and the biological properties of the CSCs from cigarettes fabricated from organic solvent-extracted tobaccos. With relatively nonpolar solvents such as pentane, hexane, and heptane, from 5% to 10% of the tobacco weight was removed by extraction with these solvents. Reductions in per cigarette PAH yields were reported for the MSSs from solvent-extracted tobaccos by numerous investigators, e.g., Campbell and Lindsey (583), Neukomm and Bonnet (2716), Rodgman (3241–3243, 3246, 3251), and Wynder et al. [Wynder (4294), Wright (4282), Wynder et al. (4355), Wynder and Hoffmann (4307, 4309)] on solvent extractions of tobaccos and their effect on the PAH yields in the CSC. Initially, the reductions in the MSS yields of the PAHs, particularly those with four or more fused rings, were reported as being significant when considered on a per cigarette yield basis. Subsequently, the same investigators (Wynder et al.) claimed that the reductions in PAH yields should be viewed as only marginal when the PAH yields were considered on a per gram of CSC basis. The % reduction in tumorigenicity [expressed as % tumor-bearing animals (TBA) in skin-painting experiments] of the mainstream CSCs from cigarettes fabricated with solvent-extracted

TABLE 25.2
Pyrolysis Studies on *n*-Hexane Extract from Tobacco

Pyrolysis Conditions		Pyrolysate, % of	Tumorigenic	Tumorigenicity Studies, TBA[a] Painted with Pyrolysate	
Temp., °C	Medium	Extract	PAHs	1% Solution	5% Solution
560	N2	50		0	0
640	N2	35		0	17
720	N2	32	Present	0	60
800	N2	28		60	97
880	N2	28	Present	77	
880	Air	30	Present	67	67

[a] % TBA (mice) with carcinoma at skin-painted site; similar percentages were found with skin-painted rabbits.

tobaccos was usually less than the % reduction in the levels of PAHs (with B[*a*]P, expressed in µg/g or ng/g of CSC, used as an "indicator" or for the levels of PAHs with four or more fused rings). It was obvious from data already in the literature describing tobacco smoke and tobacco pyrolysate compositions that B[*a*]P was not a valid "indicator" for the tetracyclic and higher PAHs demonstrated to be tumorigenic to mouse skin.

American investigators [Rayburn and Wartman (3091), Rayburn et al. (3092)] as well as French investigators [Cuzin et al. (885)] reported slight to no reductions in the levels of mainstream CSC PAHs, particularly B[*a*]P, as a result of organic solvent extraction of tobacco. Much of the early research on organic solvent extraction of tobacco to reduce the yields of PAHs in mainstream CSCs was reviewed by Wynder and Hoffmann (4319, 4332) and Hoffmann and Wynder (1798).

Organic solvent extraction of tobacco to control PAH levels in MSS fell from grace around 1960 when it was described by its early proponents, Wynder and Hoffmann (4309), as a process "impractical both technically and economically" and later was classified as "only of academic interest" by Wynder and Hecht (4306d), a view reported by the U.S. Surgeon General [see Table 26, p. 14: 114 in (4005)]. Pyrolysis studies have been conducted not only on the material extracted from the tobacco but also on the unextracted (control) tobaccos and the residual extracted tobaccos in attempts to define the precursor(s) of PAHs (and phenols) in cigarette MSS. In some respects, the differences between the compositions of the pyrolysates from solvent-extracted tobacco and from unextracted tobacco paralleled the differences between the compositions of the MSSs from cigarettes fabricated with solvent-extracted tobacco and with unextracted tobacco.

In 1958, Wynder et al. (4355) described the effect of varying the pyrolysis temperature on the yield of pyrolysate from an *n*-hexane extract from tobacco. The extracted material constituted 5.4% of the original tobacco weight and consisted of long-chained saturated and unsaturated aliphatic hydrocarbons, glycerides and other esters, solanesol and phytosterols and their esters, long-chained aliphatic esters, and α-tocopherol. Major findings from their study included the following (see also Table 25.2):

> The pyrolysate yields varied inversely as the pyrolysis temperature, i.e., the pyrolysate yield decreased as the temperature of pyrolysis was increased. Presumably, this is due to less decomposition of the extracted components to vapor-phase components (water, carbon monoxide, carbon dioxide, methane, etc.) at the lower pyrolysis temperatures.
>
> The percent conversion of the extracted components to PAHs decreased as the pyrolysis temperature decreased.
>
> The specific tumorigenicities of the pyrolysates, applied as 1% and 5% solutions in acetone in skin-painting studies involving both mice and rabbits, decreased as the pyrolysis temperature was lowered.
>
> Pyrolysis of the extract in either an inert atmosphere (nitrogen) or an oxygenated atmosphere (air) at 880°C did not markedly affect the findings with respect to the yield of pyrolysate, the generation of PAHs, or the specific tumorigenicity (mouse skin-painting bioassay) obtained with a solution of 1% pyrolysate in acetone.

Studies on organic solvent extraction of tobacco conducted from the mid- to late 1950s by Rodgman (3241, 3242, 3246, 3251), Ashburn (116, 117), and Ashburn and Rodgman (121) provided analytical data on the PAHs in mainstream CSC that in some ways paralleled the findings reported by Wynder (4294). Rodgman (3251) summarized the RJRT R&D findings as follows:

> Organic-solvent extraction of various tobacco types (flue-cured, burley, Oriental) and blends reduced the yields of both total and individual PAHs, e.g., B[*a*]P in mainstream CSC both on a per cigarette basis and on a weight of tobacco consumed basis. The per cigarette "tar" yields were also reduced in every instance.

Partition of the organic solvent extractables between a solvent system consisting of a polar solvent (aqueous ethanol) and

a nonpolar solvent (hexane or pentane) and returning each partition fraction separately to the organic solvent-extracted tobacco residue indicated:

> Addition of the nonpolar solvent-soluble material (which contained the bulk of the tobacco waxes) to the extracted tobacco residue returned the CSC PAH yield almost to that of the CSC from the unextracted (control) tobacco, and
>
> Addition of the polar solvent-soluble material (which consisted primarily of oxygen- and/or nitrogen-containing flavor-contributing tobacco components) to the extracted tobacco produced very little change in the PAH (both total and individual) level of the CSC.

These results were interpreted as an indication that the relatively high-molecular-weight, nonvolatile tobacco wax components were the major precursors in tobacco of the PAHs in smoke, whereas the moderate to low molecular weight and volatile flavorful components in tobacco did not contribute significantly to the PAH levels in smoke.

Addition of the organic solvent-soluble tobacco components, e.g., long-chained aliphatic hydrocarbon fraction, solanesol, or β-sitosterol, to unextracted (control) tobacco increased the levels of the total and some individual PAHs in the CSC. Thus, removal of tobacco wax components reduced the levels of both the total and individual PAHs in CSC, whereas addition of tobacco wax components increased the levels of both the total and individual PAHs in CSC (3251, 3269).

Examination of the relationship of the level of B[*a*]P to that of other individual PAHs in the various CSCs from the solvent-extracted tobaccos or from the component-"spiked" tobaccos confirmed what was already obvious from other literature data: B[*a*]P is not a valid "indicator" for either total PAHs or other individual PAHs with fewer than four fused rings, with four fused rings, or with more than four fused rings.

From the mid-1960s to the early 1970s, the USDA group described the pyrolysis of organic solvent extractables from tobacco. In the earlier studies, the pertinence of the pyrolysis results in defining the precursors in tobacco of the PAHs in the CSC was emphasized (3465, 3455), but subsequent research dealt with the precursors in tobacco of the simple phenols in cigarette smoke (3456, 3468).

In 1968, Schlotzhauer and Schmeltz (3465) noted that hexane extractables from tobacco constituted about 6% of the original tobacco weight, whereas the extracted tobacco residue constituted about 94% of the original tobacco weight. Pyrolysis of the hexane extractables and the extracted tobacco residue indicated that, of the total B[*a*]P determined in these two pyrolysates, about 60% was found in the hexane extractables pyrolysate (6% of the original tobacco) and 40% in the pyrolysate of the extracted tobacco residue (94% of the original tobacco). Schlotzhauer and Schmeltz (3466) also demonstrated by pyrolysis of individual components isolated from the hexane extract that the following were precursors of the PAHs in the pyrolysates: *n*-dotriacontane, stearic acid and linoleic acid, phytol, squalene, and β-sitosterol.

In 1973, Chortyk and Schlotzhauer (722) reviewed the pyrogenesis of tobacco smoke components. They discussed the extraction/pyrolysis results described earlier plus results of their studies on the pyrolysis (800°C) of fractions sequentially extracted from tobacco with a series of increasingly polar solvents (hexane, acetone, ethanol, water) (3458). Chortyk and Schlotzhauer (722) noted:

> The sources of about 70% of the aromatic hydrocarbons ranging from benzene to BaP, in the pyrolysates, were due to leaf components extractable with hexane and acetone: these extracts amounted to less than 25% of dry leaf weight. The hexane extractables (7.2% of leaf weight) accounted for 33% of the neutral products. The hexane-soluble material of cured leaf tobacco is known to include aliphatic and cyclic paraffins, fatty acids, phytosterols, steryl esters, and terpenes, all preferred precursors of aromatic hydrocarbons. The acetone extract (17.5% of leaf weight) contributed another 35% of aromatic hydrocarbons to the pyrolysate, indicating a further extraction of similar polycyclic aromatic hydrocarbons precursors. Together, these two extracts contributed 86% of the BaP content of the tobacco pyrolysate. The disproportionate contribution of these fractions to BaP formation becomes apparent from the following data: the hexane and acetone fractions, containing hydrocarbons and lipids, yielded about 700 mg [sic]* BaP per gram of material pyrolyzed, while the residual tobacco, consisting mostly of cellulose materials, yielded less than 34 mg [sic]* of BaP per gram pyrolyzed.

They also demonstrated that the major volatile phenols (phenol, cresols) were produced primarily by pyrolysis of the alcohol extractable and the final tobacco residue. These fractions accounted for 38% and 44%, respectively, of the total phenols yield. The alcohol extractables included polyphenolic tobacco pigment and low-molecular-weight sugars, whereas the final tobacco residue contained the polysaccharides celluloses, starch, pectins, and lignin. All these yield the simple phenols on pyrolysis or during tobacco smoking (248, 2043, 3277, 3305, 3453, 3468, 3767).

In 1978, Severson et al. (3616) revisited the organic solvent extraction of tobacco. They noted [see p. 277 in (3616)]:

> Numerous pyrolytic studies have shown that the hexane or petroleum ether…extract of tobacco contains the major precursors of smoke polycyclic aromatic hydrocarbons [Wynder et al. (4355), Schlotzhauer et al. (3468), Schlotzhauer and Chortyk (3451)]. However, many of these studies were made under conditions which produced optimum PAH yields [Schmeltz and Hoffmann (3489)]; thus, the PAH distributions were not comparable to those in [CSC] and the data obtained could not be exactly correlated with PAH production during the smoking process.

Severson et al. (3616) determined the pyrolytic conditions that gave the PAH profiles of tobacco pyrolysates that they claimed "could be correlated with [CSC] PAH profiles." Examination of their data indicates that this claim is not

* Obviously the reports of 700 mg of BaP and 34 mg of BaP formed from a gram of material pyrolyzed are in error.

valid. Severson et al. conducted two major experiments. They examined:

1. The effect of petroleum ether extraction on the PAH levels in the pyrolysates from the petroleum ether extractables PEE (8% of the original tobacco weight), the extracted tobacco residue (92% of the original tobacco weight), and the original tobacco.
2. The effect of chromatography of the petroleum ether extractables PEE with eight increasingly polar solvent systems, ranging from petroleum ether to an acetone:methanol solution, on the composition of each of the eight chromatographic fractions and on the PAH levels in the pyrolysates from each of the eight fractions.

Table 25.3, adapted from (3616), indicates that, at the optimum pyrolysis conditions specified (700°C, N_2), the totals of the PAH groups (except for the benzopyrene group) in the pyrolysates from the petroleum ether extractables (PEE) and the extracted tobacco residue (RES) are substantially higher (42%–89%) than the levels of the same PAH groups in the pyrolysate from unextracted tobacco. Table 25.3 also shows that the sum of the total PAHs in the pyrolysates from the two fractions [PEE and extracted tobacco residue (RES)] was 61% greater than the total PAHs in the control tobacco pyrolysate. Similar studies on individual and total acids and individual and total phenols in the same pyrolysates reveal that the sum of the total phenols in the pyrolysate of the PEE and the total phenols in the extracted tobacco residue (RES) was 21% less than the total phenols in the control tobacco pyrolysate; for acids, the sum of total acids in the pyrolysates from the two fractions (PEE plus residue) was 13% greater than the total acids in the control tobacco pyrolysate.

If this situation prevails in the relatively simple situation (PEE, extracted tobacco residue, and unextracted control tobacco) described earlier, then it is highly likely that the discrepancy will be enhanced when individual compounds are considered, i.e., there will be substantial uncertainty in any attempt to extrapolate from pyrolysis data on a specific compound, either present in or proposed to be added to tobacco, to what will actually happen to that compound during the smoking of a cigarette.

Since Severson et al. (3616) defined the composition of the eight chromatographic fractions, the remainder of their research findings will be discussed in the following section.

25.3 INDIVIDUAL TOBACCO COMPONENTS

The research conducted from the early 1950s to the mid-1960s on the organic solvent-soluble precursors in tobacco of the PAHs in cigarette MSS has been described in detail

TABLE 25.3
Comparison of PAH Fraction Levels, Phenol Yields, and Acid Yields in 700°C Pyrolysates from Tobacco, PEE, and the Tobacco Residue (RES) after Extraction

	Amount from				
Pyrolysate Components	Tobacco µg/1000 mg	PEE µg/80 mg	Residue µg/920 mg	Total PEE + Residue µg/1000 mg	% Diff., Total *vs.* Tobacco
PAH Group					
Naphthalene	3200	3900	1300	5200	63
Fluorene	1100	1100	860	1960	78
Phenanthrene	1600	1500	780	2280	43
Pyrene	630	820	350	1170	86
Chrysene	180	260	80	340	89
Benzopyrene	190	140	50	190	0
Totals	6900	7720	3420	11140	61
Phenol Group					
Phenol	3610	50	2620	2670	26
o-Cresol	750	50	630	680	20
m- + *p*-Cresol	1620	50	1180	1230	24
Ethyl-/dimethylphenols	910	130	700	830	–9
1-Naphthol	160	30	110	140	–13
2-Naphthol	140	20	110	130	–7
Totals	7190	330	5350	5680	–21
Acids					
Volatile acids (C_1–C_7)	330	140	230	370	12
Nonvolatile acids (C_{11}–C_{34})	12	11	4	15	25
Totals	342	151	234	385	13

by Wynder and Hoffmann [see pp. 345–351, 518 in (4332)] and Hoffmann and Wynder (1798). Despite the fact that the tumorigenic PAHs at their levels in cigarette smoke and acting in concert with promoting and/or cocarcinogenic but nontumorigenic PAHs, phenols, acids, etc., at their levels in cigarette smoke explain only a small fraction (less than 2%) of the biological response (measured as % TBA) observed in skin-painted laboratory animals, efforts to define the major precursors in tobacco of the tumorigenic PAHs in cigarette smoke were continued into the late 1970s, particularly by the USDA group at Athens, GA (3616). Despite the advances during this period in the laboratory techniques for (1) successful fractionation of complex mixtures such as those found in cigarette MSS and in the pyrolysates from various tobaccos, tobacco fractions, and tobacco components and (2) the quantitation of the levels of individual identified PAHs, phenols, aldehydes, ketones, etc., no revolutionary new precursor in tobacco of PAHs in tobacco smoke was discovered: The organic solvent-soluble tobacco components that yielded PAHs on pyrolysis were essentially those or structurally similar to those that had been proposed several decades earlier in the 1950s. Several tobacco components, structurally similar to those proposed earlier had not been identified as tobacco components in the 1950s, but once they were identified, logic dictated they would yield PAHs either on pyrolysis or during the tobacco smoking process. For example, in the late 1950s, Wright [(4282), cf. Rodgman (3243)] theorized that the high-molecular-weight terpenes (other than the phytosterols) and the phytosterols themselves were major precursors in tobacco of the PAHs in tobacco smoke. These proposals were subsequently confirmed: In 1958, Rodgman and Cook (3269, 3291) demonstrated in a "spiking" experiment with solanesol that it was an effective precursor of total and individual PAHs in cigarette MSS as indicated by the increased levels in the PAHs in the MSS from solanesol-"spiked" tobacco cigarettes *vs*. those in the MSS from control tobacco cigarettes. Similarly, Rodgman and Cook reported that results from phytosterol-"spiked" tobacco cigarettes indicated the phytosterol was a major precursor of PAHs in MSS. In 1979, Severson et al. (3616) demonstrated that solanesol pyrolysis generated substantial amounts of PAHs *vs*. other organic solvent-soluble tobacco components.

In subsequent sections, pyrolysis studies on various tobacco components categorized as follows will be discussed:

Nicotine
Organic solvent-soluble components: long-chained aliphatic saturated and unsaturated hydrocarbons; terpenoid alcohols such as the duvanediols, phytosterols, phytol, and solanesol; normal long-chained aliphatic alcohols; esters of these groups of alcohols with long-chained aliphatic acids (palmitic, stearic, oleic, etc.)
Structural components of tobacco (the biopolymers such as lignin and the polysaccharides cellulose, starch, and pectins and their constituent monosaccharides such as glucose and fructose)
Acids
Proteins and amino acids

Nicotine (as well as the other nicotine-related alkaloids in tobacco, usually present in trace amounts) is the one tobacco component whose level in tobacco is sometimes controlled by removal in a denicotinization process. In contrast to the removal or reduction of its level in the case of nicotine, materials such as simple sugars, glycerol, and some flavorants are added to the tobacco blend to augment their existing levels in the tobacco and to enhance certain consumer acceptable organoleptic properties of the MSS. Materials such as licorice, cocoa, and other flavorants are added to impart other consumer acceptable organoleptic properties to the smoke (2341).

25.3.1 Nicotine

Over the years, the results of numerous studies on the pyrolysis of nicotine have been published. Many of them, e.g., those of Frank et al. (25A22) and Woodward et al. (4275a, 25A84, 25A85) in the early 1940s, preceded the escalation in the 1950s of the interest in the cigarette smoke–health issue. Other early studies of nicotine pyrolysis in air or nitrogen included those in the early 1960s by Jarboe and Rosene (1923a) and Kobashi et al. (25A37, 25A38). In 1964, pyrolysis products generated from nicotine during the tobacco smoking process were summarized by Kuhn (2228).

In 1960, Van Duuren et al. (4027) extended their studies on tumorigenic PAHs in mainstream CSC to identify three tumorigenic *N*-heterocyclic compounds: the aza-arenes dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]-carbazole. Their yields were 0.1, 2.7, and 0.7 ng/cig, respectively, substantially less than that of the ng/cig yield reported for B[*a*]P in the early 1960s. These three *N*-heterocyclics had also been reported as mouse-skin tumorigens [see tabulation in Hartwell (1544)]. Dibenz[*a,h*]acridine and dibenz[*a,j*]acridine were also identified by Van Duuren et al. in pyrolysates from nicotine and pyridine (750°C, N_2).

However, the presence of these aza-arenes in tobacco smoke or nicotine pyrolysate has been questioned. Of the numerous reports on this class of compound in tobacco smoke, only one report describes the identification of one of the three, dibenz[*a,j*]acridine: Wynder and Hoffmann (4319, 4332) reported that their group, Candeli et al. (587), was able to confirm the presence of dibenz[*a,j*]acridine but not dibenz[*a,h*]acridine in mainstream CSC. The per cigarette yield for dibenz[*a,j*]acridine reported by Candeli et al. (587) was almost four times that reported by Van Duuren et al. Since 1963, no other investigator has reported these three compounds in tobacco smoke or a nicotine pyrolysate.

In 1970, Kaburaki et al. (2006) reported the results of their pyrolysis of nicotine at various temperatures in air and

in N_2. The two tumorigenic benzacridines reported in a nicotine pyrolysate by Van Duuren et al. as components of their nicotine pyrolysate were not found by Kaburaki et al.

Schmeltz et al. (3499) described the results of their pyrolysis of several nitrogenous tobacco components, including nicotine:

> We could not detect benzo(a)pyrene in nicotine pyrolyzates, nor could we confirm the presence of the physiologically active dibenzacridines and dibenzcarbazole reported in tobacco smoke and in nicotine and pyridine pyrolyzates by Van Duuren [4027].

In their review of the pyrogenesis of tobacco smoke components, Chortyk and Schlotzhauer (722) emphasized the failures of several investigators to confirm the two dibenzacridines and 7*H*-dibenzo[*c,g*]carbazole in nicotine pyrolysates:

> Since nicotine is the most abundant and best known tobacco alkaloid, its pyrolysis has been thoroughly studied [Woodward et al. (4275a), Jarboe and Rosene (1923a)]. More recent work [Kaburaki et al. (2006)] on the pyrolysis of nicotine and various alkylpyridines has resulted in a proposed mechanism for the thermal degradation of nicotine… Schmeltz [Schmeltz et al., (3499)] also studied nicotine and identified a number of previously unreported compounds in the nicotine pyrolysates… These included pyrrole, acenaphthene, indole, skatole, and anthracene and/or phenanthrene. However, the presence of dibenzacridines and dibenzcarbazole, previously reported in nicotine and pyridine pyrolysates, could not be confirmed [Van Duuren et al. (4027)].

In 1977, Schmeltz and Hoffmann (3491) in their review of *N*-containing components of tobacco and tobacco smoke discussed the generation of various pyridines from nicotine during both the actual smoking process and pyrolysis. Schmeltz and Hoffmann (3491) did report the identification by Van Duuren et al. (4027) of the two dibenzacridines in cigarette smoke and nicotine pyrolysate. They did not, however, comment on the inability of other investigators (587, 2006, 3499) to confirm the findings of Van Duuren et al.

In 1979, Schmeltz et al. (3512) reported their major findings from a study of the fate of radiolabeled nicotine during pyrolysis and during the actual smoking of a radiolabeled nicotine-treated cigarette:

> Under combustion tube pyrolysis conditions, nicotine in either silica gel matrix (pyrolysis temperature = 600°C, 750°C, or 900°C) or tobacco matrix (600°C) underwent extensive degradation to pyridines, quinolines, arylnitriles, and aromatic hydrocarbons.
>
> In a burning cigarette during actual smoking, a substantial portion of the nicotine (about 41%) remains intact, 12.5% is oxidized to carbon dioxide, as much as 11% is degraded to volatile alkylpyridines, and negligible amounts are converted to neutral or acidic components of the particulate phase.
>
> Dibenz[*a,h*]acridine and dibenz[*a,j*]acridine reported nearly two decades earlier by Van Duuren et al. (4027) were not identified in this study.

Schmeltz et al. (3512) noted:

> In ongoing studies we are now identifying those compounds that are formed from nicotine only as minor compounds (<0.1%) which nevertheless can contribute to the toxicity of the smoke. To this group of minor smoke constituents having nicotine as a precursor belong the dibenzacridines.

From their experimental results, Schmeltz et al. (3512) concluded that pyrolysis experiments may be of limited value for establishing the fate of nicotine and possibly other tobacco components in a burning cigarette.

The pyrolysis system in this study [cf. Higman et al. (1648)] was designed to be the optimum simulation of the smoking process. Obviously, nicotine did not behave in this pyrolysis system as it did in the burning cigarette during actual smoking. Examination of the 1979 Schmeltz et al. publication on the fate of nicotine during pyrolysis *vs*. actual smoking reveals at least two of the authors (Hoffmann, Schmeltz) definitely changed their opinion on their long-held view on the equivalence of compound behavior during pyrolysis and actual smoking, e.g., Wynder and Hoffmann (4332) earlier wrote:

> Most pyrolysis studies with tobacco, tobacco extracts, extract fractions, individual components, and tobacco additives are performed in a nitrogen atmosphere. This procedure has often been criticized on the grounds that many of the toxic constituents formed during smoking of tobacco products occur as a result of combustion in air rather than in a nitrogen atmosphere. This criticism, however, cannot be maintained in view of studies by Newsome and Keith [2780] which demonstrated that a reducing rather than an oxidizing atmosphere exists at the cone region of a burning cigarette.

With regard to the dibenzacridines and dibenzocarbazole from nicotine during pyrolysis and the smoking process, Table 25.4 summarizes the state of knowledge: None of the investigations conducted from 1963 through 2000 on the levels of these three aza-arenes in mainstream CSC confirmed the 1960 findings of Van Duuren et al. (4027).

Another aspect of the involvement of nicotine (and related tobacco alkaloids) in the generation of allegedly harmful tobacco and/or smoke components is the formation of tobacco-specific *N*-nitrosamines (TSNAs).* It is claimed by Hoffmann et al. that TSNAs such as *N′*-nitrosonornicotine (NNN) and 4-(*N*-methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) are formed from nicotine and other minor nicotine-related alkaloids during various stages of tobacco development and treatment (growing, curing, aging) [Hecht et al. (1563, 1564), Adams et al. (22)]. TSNAs appear in cigarette MSS as a result of two mechanisms: (1) direct transfer of the TSNAs from the tobacco to the smoke, (2) pyrogenesis during the smoking process. For example, Hoffmann et al. (1734) and Adams et al. (29) estimated that 40%–46% of the

* TSNAs include NNN from nicotine and nornicotine, NNK from nicotine, *N′*-nitrosoanatabine (NAT) from nicotine and anatabine, and *N′*-nitrosoanabasine (NAB) from anabasine.

TABLE 25.4
Dibenz[*a,h*]acridine, Dibenz[*a,j*]acridine, and 7*H*-Dibenzo[*c,g*]carbazole in Nicotine Pyrolysates (Pyr) and Mainstream CSC

	Dibenz[*a,h*]acridine		Dibenz[*a,j*]acridine		7*H*-Dibenzo[*c,g*]carbazole	
Investigators	**Pyr**	**CSC**	**Pyr**	**CSC**	**Pyr**	**CSC**
Van Duuren et al. (4027)	Yes	Yes	Yes	Yes	No	Yes
Candeli et al. (587); Wynder and Hoffmann (4319,4332)	NE	No	NE	Yes	NE	NE
Kaburaki et al. (2006)	No	NE	No	NE	NE	NE
Schmeltz et al. (3499)	No	NE	No	NE	No	NE
Schmeltz et al. (3512)	No	No	No	No	No	No
Snook (3733)	NE	No	NE	No	NE	No
Snook et al. (3750)	NE	No	NE	No	NE	No
Grimmer et al. (1409)	NE	No	NE	No	NE	No
Kamata et al. (2021)	NE	No	NE	No	NE	NE
Sasaki and Moldoveanu (3414)	NE	No	NE	No	NE	NE
Rustemeier et al. (3370)	NE	No	NE	Yes	NE	NE

Yes, Compound identified; No, compound not found or identified; NE, substrate not examined for compound in question.

NNN in MSS was a result of its transfer from the tobacco blend. The remainder—54%–60%—in MSS was due to pyrogenesis of NNN from nicotine and nornicotine during the smoking process. Similar data were generated for NNK: 26%–37% by direct transfer, 63%–74% by pyrogenesis.

The levels in MSS of TSNAs such as NNN can presumably be reduced by reduction in the level of nicotine and/or nitrate in the tobacco blend (499). However, Brunnemann et al. (511) have presented contradictory data on the significance of the correlations among the levels of nitrate, nicotine, and TSNAs in tobacco.

Since the TSNAs are components of the MSS particulate phase, control of their levels in smoke is also possible by any means that controls the yield of the MSS particulate matter. These include the following:

- Use of reconstituted tobacco sheet
- Expanded tobacco
- High filtration efficiency
- Air dilution by increased paper porosity and/or ventilated filter tips [Hoffmann et al. (1719)]

Unlike the volatile *N*-nitrosamines such as dimethylnitrosamine (DMNA), the TSNAs are not amenable to selective filtration by use of plasticized filter tips.

25.3.2 Organic Solvent-Soluble Components (Long-Chained Aliphatic Hydrocarbons, Phytosterols, Solanesol, High-Molecular-Weight Esters, etc.)

The tobacco smoke components "known" in 1954 numbered fewer than 100 (2170). At that time, the chemical composition of tobacco was as equally ill defined as that of its smoke. Pyrolyses conducted throughout the 1950s involved the organic solvent-soluble material from tobacco and were limited either to the total extractables or to a few classes of known tobacco components, e.g., phytosterols, long-chained saturated aliphatic hydrocarbons. These relatively high-molecular-weight compounds were present in tobacco at levels usually exceeding 0.5% and presented little problem in collecting sufficient material for study. Subsequent research on tobacco (and tobacco smoke) composition resulted in the isolation and elucidation of the structures of numerous classes of organic solvent-soluble compounds, including those listed in Table 25.5.

The early work of Roffo (3327) on the reduction of tumorigenicity of a "destructive distillate" from a solvent-extracted tobacco (ethyl alcohol), his claim that alcohol extraction removed the tumorigen precursor from the tobacco, and his proposal of the phytosterols as the tumorigen precursor(s) were described previously. Despite the fact that the "destructive distillate" from tobacco was not equivalent to cigarette smoke particulate matter, the proposal of the phytosterols as precursors in tobacco of PAHs was based on sound reasoning and previous experimental findings. Nearly two decades earlier, Kennaway (2073–2075) had demonstrated that pyrolysis of isoprene, acetylene, and cholesterol, yielded pyrolysates tumorigenic to mouse skin. Cholesterol was once considered unique to animal tissue, but subsequently, trace amounts were found in plant tissue, including tobacco [Stedman (3797), Grunwald et al. (1434)]. Of the tobacco and tobacco smoke sterols, the two present at the highest level are stigmasterol and β-sitosterol. These differ from each other and cholesterol in the structure and configuration of the side chain on the cyclopentane ring. They occur in tobacco as free phytosterols and phytosteryl derivatives (esters, glycosides). Pyrolysis of sterols generates high levels of chrysene. Its four rings are configurationally similar to that of the sterol ring system.

In the mid-1920s, Kennaway and others were concerned about the fate of cholesterol when animal tissue was heated during roasting and broiling. Cholesterol pyrolysis experiments were crude attempts to duplicate what happened to it

TABLE 25.5
Organic Solvent-Soluble Components of Tobacco Identified Post-1955

Compound	Reported in Tobacco by	Reported in Tobacco Smoke by
Solanesol	Rowland et al. (3359)	Mold and Booth (2590), Wynder and Wright (4354)[a], Rodgman and Cook (3270)
Neophytadiene	Rowland (3345)	Rodgman (3247)
α-Tocopherol	Rowland (3347)	Rodgman and Cook (3271)
Squalene	Fredrickson (1229)	Van Duuren and Schmitt (4033), Rodgman et al. (3297)
Solanesenes	—	Rodgman et al. (3297)
Solanesyl esters	Rowland and Latimer (3358)	Rodgman and Cook (3270), Rodgman et al. (3296)
Phytosteryl esters	Rowland and Latimer (3358)	Rodgman et al. (3296)
Long-chained aliphatic alcohols	Cook et al. (812)	Cook et al. (812)
Long-chained aliphatic esters	Rodgman et al. (3294), Arrendale et al. (103)	Rodgman et al. (3294)
Duvanediols	Roberts (3195), Roberts and Rowland (3220, 3221), Rowland and Roberts (3360), Rowland et al. (3361)	Rowland et al. (3361)
Phytyl esters	Severson et al. (3616)	Rodgman and Cook (3287)

[a] Wynder and Wright (4354) reported geraniol as a cigarette smoke constituent. However, the infrared spectrum of the isolate was identical with that of solanesol, not geraniol (Wright, private communication to A.R.).

during the cooking process. Here again, the presence of other tissue components (amino acids, proteins, lipids, carbohydrates) with cholesterol during cooking would certainly have affected the results when compared to the results obtained from pyrolysis of cholesterol alone.

In 1928, Kennaway and Sampson (2080) also demonstrated that the specific tumorigenicities of pyrolysates from cholesterol and other organic compounds increased as the pyrolysis temperature was increased. This observation was later confirmed with saturated aliphatic hydrocarbons (2257) and phytosterols [Wynder et al. (4355, 4356)] isolated from tobacco. In the latter two studies, the yield of PAHs generated during pyrolysis of the compounds in question increased as the pyrolysis temperature increased. Wynder et al. (4355) and Wynder and Hoffmann (4332) reported that pyrolyses of a hexane extract of tobacco gave decreasing yields of pyrolysate "tar" as the pyrolysis temperature increased: 560°C, 50%; 640°C, 35%; 720°C, 32%; 800°C, 28%; and 880°C, 28%. They also reported that pyrolysis at 880°C of the hexane extractables in air *vs.* their pyrolysis in N_2 gave pyrolysates whose yields were essentially the same [30% (air) *vs.* 28% (N_2)] and whose specific tumorigenicities were comparable in skin-painting studies with the mouse and rabbit. Similar findings were reported for aliphatic tobacco hydrocarbons pyrolyzed either in air or in N_2 at 800°C with regard to PAH composition and specific tumorigenicity in skin-painting studies.

Table 25.6, adapted from Lam (2257), demonstrates the relationship between PAH generation and pyrolysis temperature for aliphatic tobacco hydrocarbons pyrolyzed in air at several temperatures. Calculation of the yield ratios [PAH, mg/g/B[*a*]P, mg/g] of the other PAHs *vs.* B[*a*]P reveals significant information: In this case of pyrolysis, there was no consistency between the change in ratios of PAH/B[*a*]P as the temperature was increased from 700°C to 800°C, e.g., in the case of the tetracyclic PAHs, the PAH/B[*a*]P ratio decreased for pyrene and chrysene but increased for fluoranthene; for the pentacyclic PAHs, the ratio decreased for both perylene and B[*e*]P; for the hexacyclic PAH dibenzo[*def,mno*]chrysene, the ratio increased. These same trends existed whether PAH/B[*a*]P ratios were calculated as molar yields or, as in Table 25.6, as absolute quantities (μg of PAHs generated per gram of aliphatic tobacco hydrocarbons pyrolyzed).

The significance of these data and calculations is their demonstration in 1956 that in even the simplest pyrolysis situation, B[*a*]P is not a valid "indicator" for the PAHs with four or more rings and their supposed relationship to tumorigenic activity [Wynder and Hoffmann (4317, 4319, 4332)]. In addition to these data by LAM, other contrary data which demonstrated the invalidity of the concept of B[*a*]P as an "indicator" for PAHs with four or more rings and the tumorigenicity of the substrate (CSC, pyrolysate) containing them were generated not only by Wynder et al. (4355, 4356) but also by Campbell and Lindsey (583), Rodgman and Cook (3286), Gori (1329, 1330, 1332, 1333), NCI (2685), and Severson et al. (3616).

The lack of correlation between CSC content of B[*a*]P and specific tumorigenicity was demonstrated by Lazar et al. (2320) who reported that a 30-fold increase in B[*a*]P content by its addition to CSC produced no increase in the specific tumorigenicity to mouse skin of the B[*a*]P-enhanced CSC *vs.* the control CSC applied at equal dose levels. This lack of correlation between the B[*a*]P concentration in CSC and

TABLE 25.6
PAHs from Aliphatic Tobacco Hydrocarbons Pyrolyzed in Air at Various Temperatures

	Quantity (μg) of PAH Formed on Pyrolysis (in Air) of Aliphatic Tobacco Hydrocarbons (1.0 g)				
	At 800°C		At 700°C		At 600°C
PAH	PAH, μg/g	PAH/B[*a*]P[a]	PAH, μg/g	PAH/B[*a*]P[a]	PAH, μg/g
Naphthalene	14,260	41.94 [2/5][b]	4760	158.7	0
Acenaphthene	0	0 [3/5][c]	0	0	0
Acenaphthylene	3,520	10.35 [3/5][c]	480	16.00	0
Phenanthrene	3,840	11.29 [3/5][c]	580	19.33	0
Anthracene	580	1.71 [3/5][c]	110	3.67	0
Pyrene	960	2.82 [4/5][d]	320	10.67	0
Fluoranthene	1,700	5.00 [4/5][d]	24	0.80	0
Chrysene	400	1.18 [4/5][d]	86	2.87	0
Perylene	34	0.10 [5/5][e]	4	0.13	0
Benzo[*a*]pyrene	**340**	**1.00**	**30**	**1.00**	0
Benzo[*e*]pyrene	400	1.18 [5/5][e]	80	2.67	0
Dibenzo[*def,mno*]chrysene	42	0.12 [6/5][f]	<1	<0.03	0
Totals	26,076	86.87	6474	21.47	0

[a] B[*a*]P = B[*a*]P.
[b] [2/5] = bicyclic/pentacyclic B[*a*]P.
[c] [3/5] = tricyclic/pentacyclic B[*a*]P.
[d] [4/5] = tetracyclic/pentacyclic B[*a*]P.
[e] [5/5] = pentacyclic/pentacyclic B[*a*]P.
[f] [6/5] = hexacyclic/pentacyclic B[*a*]P.

its specific tumorigenicity was also recognized by the U.S. Surgeon General who wrote 1981 [see p. 36 in (4009)]:

> The contribution of BaP or PAH in general to mouse skin carcinogenesis by cigarette smoke condensate cannot be fully measured at this time. Wynder and Hoffmann [4332] found a correlation between BaP levels and carcinogenic activity of smoke condensates from several types of cigarettes. A much larger series of experimental cigarettes was studied in the smoking and health program of the National Cancer Institute. No significant dependence of carcinogenic potency on BaP content was observed [Gori (1329, 1330, 1332, 1333), NCI (2683)].

The post-1930 stimulus for PAH research was provided by the following events: the independent syntheses of DB[*a,h*]A in 1929 by CLAR (760) and Fieser and Dietz (1184); the demonstration of its mouse-skin tumorigenicity by Kennaway and Hieger (2078); the early 1930s reports by Cook et al. (726, 727) on several PAH isolates from coal tar, known to be tumorigenic to the skin of mice and rabbits; identification of two coal tar isolates as B[*a*]P and B[*a*]A; and the demonstration of the tumorigenicity to mouse skin of B[*a*]P (194, 726).

In addition to Kennaway and Sampson (2080), numerous investigators after 1932/1933 examined the pyrolysates from sterols in conjunction not only with the alleged tumorigenicity and PAH content of "destructive distillates" from tobacco, CSCs, and pyrolysates of tobacco, tobacco extractables, and individual tobacco components but also with the alleged tumorigenicity and PAH content of heated foodstuffs and their role in digestive tract cancer. For example, Roffo, in addition to his tumorigenicity studies with "destructive distillates" from various tobaccos types (3320, 3324, 25A51) and organic solvent-extracted tobaccos (3327), investigated the tumorigenicity of heated or oxidized fats (25A53, 25A55, 25A59) and the "tars" and phenanthrene derivatives from cholesterol pyrolyzed (25A56, 25A57, 25A58) or irradiated in air (25A54).

Other investigators who examined the chemical and biological properties of cholesterol pyrolysates included Steiner et al. (25A69), Falk et al. (1171), and Bischoff and Rupp (25A10). Previously, Veldstra (4042a) had demonstrated that 3,5-cholestadiene, produced pyrolytically from cholesterol, was tumorigenic to skin-painted laboratory animals. Subsequently, cholesten-4-one was found to be both tumorigenic to mouse skin and a component of the pyrolysate from cholesterol and/or its derivatives. These and other pyrolysate findings on composition (PAHs in the pyrolysate) and properties (tumorigenicity of pyrolysate and/or the components of pyrolysates generated from cholesterol or its naturally occurring derivatives) were summarized by Rodgman (3233, 3242). Although the pentacyclic PAH 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (previously known as 3-methylcholanthrene or 20-methylcholanthrene), a potent mouse-skin tumorigen, may be prepared by a series of chemical reactions from a sterol-derived compound structurally related to cholesterol, it has never been identified in a sterol pyrolysate. Although Kröller (2191) claimed the identification of 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) in mainstream CSC, his identification of it was questioned by Wynder

and Hoffmann (4332) who asserted that it and other alkylated PAHs had never been reported as a combustion or pyrolysis product. Wynder and Hoffmann (4332) also questioned the reports by Pietzsch (2962) and Kröller (2191) of the presence in CSC of the methylated PAH DMB[*a*]A. It and other methylated PAHs in mainstream CSC were reported in 1960 by Rodgman and Cook (3273). In addition, in 1963, Grossman et al. (1431, 1432) reported alkylated naphthalenes in the pyrolysate from solanesol, a major tobacco component. In the 1970s, Snook et al. reported not only several dimethylbenz[*a*]anthracenes in CSC (3756) but also a great number of alkylated PAHs in CSC (3757). Thus, the Wynder–Hoffmann assertion about the presence of alkylated PAHs in MSS was incorrect.

Campesterol, stigmasterol, β-sitosterol, and cholesterol have been identified both free and/or bound (as esters, etc.) in tobacco and CSC [see Grunwald et al. (1434) for a summary of the early research on tobacco sterols and their derivatives]. In their study, Grunwald et al. found that these four sterols constituted about 0.16% of the tobacco weight, and about 15% of them were transferred to MSS. According to Grunwald et al., the remainder of the sterols were "Lost in the smoke sidestream, pyrolyzed during the smoking process and/or deposited in the butt." Thus, a cigarette containing 1.0 g of the tobacco studied by Grunwald et al. would contain 1600 µg of these sterols and deliver about 240 µg to MSS. About 82 µg of the 240 µg would be β-sitosterol, a compound reported to be anticarcinogenic to several *N*-nitrosamines [Grunwald et al. (1434)]. This indicates the relative proportions of these four sterols in tobacco: Cholesterol is the least plentiful of the four tobacco sterols in Table 25.7.

Except for minor differences in the side-chain structure, the cholesteryl oleate studied by Veldstra (4042a) is structurally similar to the phytosteryl ester fraction isolated from tobacco by Rowland and Latimer (3358) and from CSC by Rodgman et al. (3296). It was subsequently identified as a mixture of esters of stigmasterol and β-sitosterol with long-chained saturated (palmitic, stearic) and unsaturated (oleic, linoleic) acids. In the late 1950s to early 1960s, Rodgman and Cook were unsuccessful in their CSC study to identify the stigmasterol- or β-sitosterol-derived dienes or ketones corresponding to the tumorigenic 3,5-cholestadiene and cholesten-4-one generated during pyrolysis of cholesterol or its esters. However, Benner et al. (273) subsequently identified 3,5-campestadiene (VIb) and 3,5-stigmastadiene (VId) in tobacco smoke [cf. Eatough et al. (1099, 1100)]. The following paragraphs summarize the relationships, both known and proposed, between a sterol such as cholesterol and its various pyrolysis products:

TABLE 25.7
Total, Free, and Bound Sterols in Cigarette Tobacco

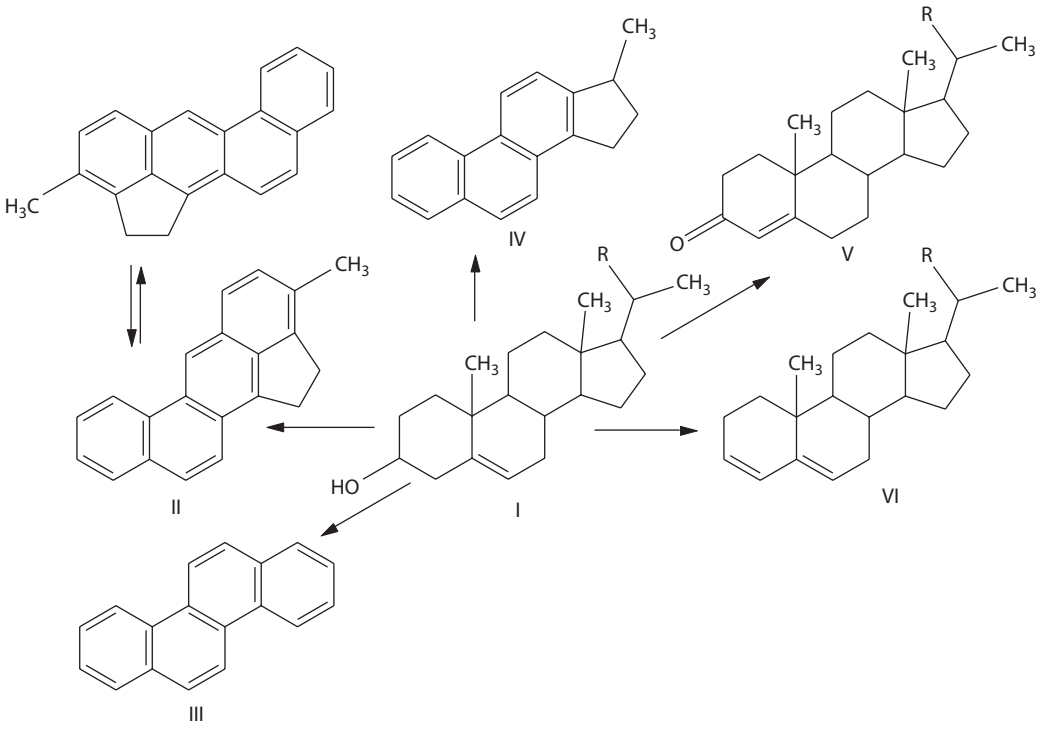
			Total	
Sterol	Free, µg/g Tobacco	Bound, µg/g Tobacco	µg/g Tobacco	%
Stigmasterol	326	262	588	37
β-Sitosterol	185	366	551	34
Campesterol	129	173	302	19
Cholesterol	79	86	165	10
Total	719	887	1606	100

Because of the results of the studies by Kennaway (2073–2076), Kennaway and Sampson (2080), and Roffo (25A56, 25A57, 25A58) on the generation of tumorigenic pyrolysates from cholesterol or cholesterol-containing foodstuffs, the question was raised: What is the relationship between these observations on tumorigenic cholesterol pyrolysates and the incidence of stomach and digestive tract cancers? When many studies, beginning in 1934 [see summary in Hartwell (1544)], revealed that 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) was a potent tumorigen equivalent in potency in mouse-skin-painting bioassays to B[*a*]P and DB[*a,h*]A, extensive research was conducted in attempts to determine whether it was generated from cholesterol during various cooking processes. Examination of the entries in the catalogs by Hartwell (1544) and Shubik and Hartwell (3664) for the four PAHs considered to be potent tumorigens revealed 474 studies involving 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methyl-cholanthrene) between 1934 and 1953, 410 studies involving B[*a*]P between 1932 and 1953, 275 studies involving DB[*a,h*]A between 1930 and 1953, and 91 studies involving DMB[*a*]A between 1938 and 1953.

One of the most potent PAHs in mouse-skin-tumor induction is 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) which theoretically could be formed pyrogenetically from sterols such as cholesterol {Ia}. In addition to the trace level of cholesterol present in tobacco, tobacco usually contains substantial levels of several phytosterols [campesterol {Ib}, β-sitosterol {Ic}, stigmasterol {Id}, ergosterol {Ie}] structurally similar to cholesterol. These phytosterols differ from cholesterol {Ia} in the structure of the long side chain. Stigmasterol {Id} is structurally similar to β-sitosterol {Ic} except for a double bond at the C_{22} carbon. The legend to Figure 25.1 indicates the differences among cholesterol, campesterol, β-sitosterol, ergosterol, and stigmasterol. These sterols, present in tobacco in both the free and bound form (as glycosides, esters), are transferred intact to MSS.

These sterols constitute about 0.2% of the tobacco weight. Table 25.7, adapted from Grunwald et al. (1971), illustrates the relative proportions of these sterols in tobacco. These data indicate that cholesterol and cholesteryl derivatives are the least plentiful of the free and bound sterols in tobacco. These levels are similar to those of the standard and reference cigarettes in the National Cancer Institute (NCI) "Less Hazardous" Program (1329, 1330, 1332 1333, 2683).

As shown in Figure 25.1, pyrolysis of cholesterol {Ia} yields chrysene {III} and a Diels hydrocarbon {IV}, a methylcyclopentaphenanthrene. Both PAHs have also been isolated from pyrolysates of the major tobacco phytosterols. While cholesterol {Ia} and the tobacco phytosterols [campesterol {Ib}, β-sitosterol {Ic}, stigmasterol {Id}] have not been shown to generate 3-methylcholanthrene {II} on pyrolysis, cholesterol {Ia} and its esters with long-chained acids do generate the mouse-skin tumorigens 4-cholesten-3-one {Va} and 3,5-cholestadiene {VIa} (1171). Veldstra (4042a)



Legend

	Sterol,	R =
Ia	Cholesterol	-$(CH_2)_3$-$CH(CH_3)_2$
Ib	Campesterol	-$(CH_2)_2$-$CH(CH_3)$-$CH(CH_3)_2$
Ic	β-Sitosterol	-$(CH_2)_2$-$CH(C_2H_5)$-$CH(CH_3)_2$
Id	Stigmasterol	-CH═CH-$CH(C_2H_5)$-$CH(CH_3)_2$
Ie	Ergosterol[a]	-CH═CH-$CH(CH_3)$-$CH(CH_3)_2$

II	1,2-Dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene)		
III	Chrysene	IV	Diels hydrocarbon
Va	4-Cholesten-3-one	VIa	3,5-Cholestadiene
Vb	4-Campesten-3-one	VIb	3,5-Campestadiene
Vc	β-4-Sitosten-3-one	VIc	β-3,5-Sitostadiene
Vd	Stigmasten-3-one	VId	3,5-Stigmastadiene
Ve	Ergostadien-3-one	VIe	3,5,7-Ergostatriene

[a] Ergosterol has a double bond at the seven position

FIGURE 25.1 Possible sterol degradation products.

reported that the pyrolysis of cholesteryl oleate also yielded 3,5-cholestadiene {VIa}. Cholesteryl oleate was probably a component of the mixture of steryl esters described in flue-cured tobacco by Rowland and Latimer (3358) and in tobacco smoke by Rodgman et al. (3296). The steryl esters included sterols esterified with a series of saturated (palmitic, stearic, etc.) and unsaturated (oleic, linoleic, etc.) acids.

In the late 1950s, Rodgman proposed that on thermal degradation during the smoking process, campesterol, stigmasterol, and β-sitosterol and their esters might generate the ketones {Vb, Vc, Vd} and dienes {VIb, VIc, VId} analogous to 4-cholesten-3-one {Va} and 5-cholestadiene {VIa}, and they might also be mouse-skin tumorigens like their cholesterol counterparts.

Several PAHs other than chrysene and Diels hydrocarbon (Figure 25.1) were subsequently identified in sterol pyrolysates. In 1959, Wynder et al. (4355, 4356) reported that PAHs were generated at both temperatures when tobacco sterols were pyrolyzed in air at 720°C and 850°C. At these temperatures, the pyrolysates constituted 28% and 22%, respectively, of the phytosterols pyrolyzed; B[*a*]P constituted 0.1% and 1.0%, respectively, of the pyrolysates. These results with phytosterols pyrolyzed at two different temperatures are similar to those reported for the pyrolyses of aliphatic tobacco hydrocarbons (2255–2258).

In 1962, Van Duuren (4022) described the identification of pyrene and B[*a*]P in a stigmasterol pyrolysate. Badger et al. (142) in their pyrolysis study of tobacco phytosterols reported the identification of some 30 PAHs, all previously reported as CSC components. They also noted the accentuated production of chrysene *vs.* its generation by pyrolysis of aliphatic tobacco hydrocarbons. Chrysene, reported to be tumorigenic to mouse skin, is a sterol pyrolysis product characteristically generated at a high level compared to that for other PAHs in the pyrolysate. The four-ring arrangement in chrysene is similar to that of the sterol rings. The International Agency for Research on Cancer (IARC) eventually removed chrysene from the tumorigen list.

From a precursor "spiking" experiment involving addition to tobacco of aliphatic tobacco hydrocarbons, a phytosterol (β-sitosterol), or solanesol, it was noted that the increase in the chrysene yield in the CSC was much more pronounced with phytosterol-treated tobacco than with aliphatic hydrocarbon- or solanesol-treated tobacco (3251, 3269, 3291). Doubling the levels of solanesol, aliphatic tobacco hydrocarbons, and phytosterols by addition of each to a control tobacco blend resulted in increases in the B[*a*]P yields in the mainstream CSCs of 13%, 13%, and 16%, respectively. However, the chrysene yields were increased by 16%, 28%, and 183%, respectively. Tripling the addition levels increased the B[*a*]P levels in the mainstream CSCs by 18%, 20%, and 28%, respectively, and the chrysene levels by 22%, 50%, and 239%, respectively.

In their study of the petroleum-ether-extractable material (8% of tobacco weight) from tobacco which was chromatographically separated into eight fractions (see Table 25.8), Severson et al. (3616) identified PAHs in the pyrolysates from Fractions F-2 and F-3 (containing phytosterol derivatives) and from Fractions F-5 and F-6 (containing unbound phytosterols). Their PAH data for these four pyrolysates from phytosterol-rich tobacco fractions showed high yields of chrysene *vs.* those in the pyrolysates from the essentially phytosterol-free fractions (F-1, F-2, F-7, and F-8).

TABLE 25.8
Component Distribution in Eight Subfractions from a Petroleum Ether Extract of Tobacco (8% of Tobacco Weight) (3616)

Chromatographic Fraction		
No.	**%**	**Major Component(s)**
F-1	5.3	Long-chained saturated hydrocarbons, neophytadiene
F-2	4.3	Esters of sterols and terpenoid alcohols
F-3	8.9	Esters of sterols and solanesol
F-4	29.2	Solanesol
F-5	6.6	Solanesol, sterols, and long-chained fatty acids
F-6	20.3	Sterols and long-chained fatty acids
F-7	15.8	Polar esters of fatty acids
F-8	9.6	Polar esters of fatty acids

TABLE 25.9
Conversion of Tobacco Leaf Constituents to Total MSS PAHs

Leaf Constituent	% Conversion to Mainstream PAHs
Phytosterols	<1.0
Palmitic acid	<1.0
Neophytadiene	0.10
Polar fraction	0.15
Alkaloids	0.10

Although their study dealt with pyrolysis of tobacco phytosterols, Schmeltz et al. (3511) did determine the percent conversion of phytosterols (and other components) to MSS PAHs by use of radiolabeled phytosterols generated by growing tobacco in an atmosphere containing radiolabeled CO_2, isolating radiolabeled tobacco components, and adding them individually to cigarettes which were then smoked and the MSS analyzed. Their data are summarized in Table 25.9. Their 1978 finding with radiolabel techniques (<1% conversion to PAHs) for the tobacco phytosterols is comparable to the 1958 data of Rodgman and COOK (3269, 3291) who, using classical chemical techniques in a "spiking" experiment, reported the conversion of β-sitosterol to PAHs to be about 0.6%,

As noted by Wynder and Hoffmann (4319, 4332), the first group of tobacco components studied by pyrolysis was the "tobacco paraffins." Subsequently, these were shown to consist of a mixture of *n*- (normal), *iso*- (2-methyl-), and *anteiso*- (3-methyl-) saturated hydrocarbons C_nH_{2n+2}, the bulk of which comprised hydrocarbons ranging from 10 or 12 to more than 40 carbon atoms. These hydrocarbons were also extractable from tobacco by pentane, hexane, or petroleum ether. Pyrolysis studies in air or an inert atmosphere (N_2, He) with either the tobacco-derived saturated aliphatic hydrocarbon fraction or individual components of the fraction [see Lam (2255, 2256, 25A39), Wynder et al. (4356)] or individual hydrocarbons [see Lam et al. (2260) for *n*-pentacosane, Haefele and Giles (1480) for *n*-hentriacontane, Badger and Novotny (151) for *n*-decane, Badger et al. (142) and Lam (2256) for *n*-dotriacontane (dicetyl)] indicated that these tobacco components yielded pyrolysates reported to be tumorigenic in mouse-skin-painting bioassays and to contain many PAHs, several of which were tumorigenic in long-term mouse-skin-painting bioassays.

The PAHs identified in the various pyrolysates ranged in complexity from bicyclic (naphthalenes), tricyclic (acenaphthenes, anthracenes, phenanthrenes), tetracyclic (pyrenes, fluoranthenes, chrysenes, benzanthracenes), pentacyclic (perylenes, benzopyrenes, dibenzanthracenes, benzofluoranthenes), hexacyclic (dibenzochrysenes), and heptacyclic (coronene). Eventually, all the PAHs identified in the various pyrolysates were identified in mainstream CSC. In every case where the pyrolysis temperature was lowered, the yields of the PAHs in the pyrolysate also decreased (see Table 25.6).

From data they generated, Rayburn and Wartman (3091) and Rayburn et al. (3092) challenged the concept that the saturated aliphatic hydrocarbons in tobacco were precursors of the PAHs in mainstream CSC. Wynder and Hoffmann (4319, 4332), in turn, criticized the experimental procedures which provided the data upon which Rayburn et al. based their argument:

> The experimental findings [of Rayburn et al.] are partially based on total polycyclic hydrocarbons of similar ultraviolet spectra and not on analytical data. The report did not mention counting techniques for C^{14}-labeled paraffins nor their quenching effects. These, as well as other factors, appear to weaken considerable the challenge of a concept based on extensive experimental data.

In 1979, Severson et al. (3616), in their study of the PEE (8% of tobacco weight) chromatographically separated into eight fractions (see Table 25.8), reported the identification of PAHs in the pyrolysate from Fraction F-1, the fraction containing the saturated aliphatic hydrocarbons extracted from the tobacco.

As recently as 1985, Lam et al. (2260) identified numerous PAHs in the pyrolysate from *n*-pentacosane, a known component of the saturated aliphatic hydrocarbon fraction present in tobaccos.

In 1958, Rodgman and Cook (3269, 3291) added tobacco-derived saturated aliphatic hydrocarbons to a tobacco blend in a "spiking" experiment and determined the effect of the addition on the PAH levels in mainstream CSC. They reported the added saturated hydrocarbons increased the yield of PAHs in cigarette MSS and thus were precursors of the smoke PAHs.

The structure of the unsaturated C_{45} polyisoprenoid alcohol, solanesol, was established in 1956 by Rowland et al. (3359). Despite the fact that solanesol was one of the major individual components of the extractable waxes from tobacco, its pyrolysis was not reported until 1962. While Lam (2255) favored the saturated hydrocarbons as the major precursors in tobacco of PAHs in smoke, Wynder (4294) considered both the saturated hydrocarbons and the phytosterols to be the major precursors. Wright (4282) proposed that the phytosterols and other terpenoids such as solanesol were the major precursors in tobacco of PAHs in smoke. In spite of their differences of opinion on the relative importance of these tobacco components in their contribution to smoke PAHs, they collaborated on several studies in the late 1950s (4355, 4356). Subsequently, the saturated hydrocarbons, the phytosterols, and other terpenoids such as solanesol were shown to be important in the formation of PAHs in tobacco smoke (3251, 3269, 3291, 3616).

In the early 1960s, Grossman et al. (1431, 1432) examined the pyrolysate from solanesol and reported the identification of monocyclic hydrocarbons (benzene and cyclopentene derivatives) (1431) and bicyclic aromatic hydrocarbons (naphthalenes) (1432). No tricyclic PAHs were reported. In 1963, Gil-Av and Shabtai (1286) postulated that solanesol in tobacco was a source of tobacco smoke PAHs and proposed a mechanism for their generation from solanesol: Solanesol and other similarly configured terpenoid compounds, e.g., neophytadiene, squalene, duvane derivatives, depolymerized during the smoking (or pyrolytic) process to produce isoprene which, in turn, reacted with itself and subsequent reaction products to generate a tumorigenic "tar" such as that described in the mid-1920s by Kennaway (2073–2075). This "tar" derived from solanesol via isoprene would contain the requisite tumorigenic PAHs such as B[*a*]P. Although Gil-Av and Shabtai (1286) demonstrated the presence of B[*a*]P in an isoprene pyrolysate, they did not study the pyrolysis of solanesol.

Severson et al. (3616) described the pyrogenesis of PAHs from solanesol in their study of the petroleum ether tobacco extractables (8% of tobacco weight) which they chromatographically separated into eight fractions (see Table 25.8). Fraction F-4 was primarily solanesol. Fraction F-3 contained solanesyl esters. Severson et al. (3616) summarized the contribution of solanesol to PAHs in its pyrolysate (and in CSC):

> The carotenoids and solanesol are most like responsible for the high levels of the multialkylated PAH found in the [petroleum ether]-extract pyrolyzate and, by analogy, in CSC. Because of its relative abundance in leaf, solanesol may contribute as much as 40% of the benzopyrenes produced on pyrolysis of the [petroleum ether] extract of tobacco.

As noted previously, 1958 precursor experiments (3251, 3269, 3291), in which solanesol was added at several levels in a "spiking" experiment and the effect of this addition on the levels of total and individual PAHs in cigarette MSS was determined, demonstrated that solanesol in tobacco was indeed a significant precursor of PAHs in cigarette MSS.

Phytol, a terpenoid alcohol, is a known component of tobacco leaf. It and its structurally similar dehydration product, neophytadiene, probably occur in tobacco leaf through the degradation of chlorophyll whose structure includes phytol (3345). Neophytadiene (3247), phytol (3285), and phytyl esters (3287) are present in tobacco smoke (see Table 25.5). Schmeltz et al. (3511), in their 1978 radiolabel study, determined the contribution of neophytadiene to PAHs in cigarette MSS. They estimated that about 0.1% of the tobacco neophytadiene is converted during the smoking process to PAHs in the MSS (see Table 25.9). The pyrolysis products of neophytadiene and phytol were examined in 1985 by Lam et al. (2260). Numerous PAHs were identified in the pyrolysates of both compounds. However, as a result of their study of the pyrolysis of phytol and a phytol derivative, Moldoveanu et al. (5539) considered in 2010 that phytol was not a significant contributor to PAHs in cigarette smoke, a view that disagreed with the findings of Lam (2260) and Schlotzhauer and Schmeltx (3466) and the earlier views and findings of Wright (4282), Rodgman (3251), Rodgman and Cook (3269, 3291), Schmeltz et al. (3511), and Severson et al. (3616) on the contribution of polyisoprenoid components in tobacco to the levels of PAHs in cigarette smoke.

Normal long-chained aliphatic alcohols, known minor components of tobacco (614, 615, 25A18, 25A80) and tobacco smoke (812), may not play a significant role as PAH precursors. In fact, Carruthers and Johnstone (614, 615), who

TABLE 25.10
PAHs from Tobacco Components Pyrolyzed in a N_2 Atmosphere at 650°C

	Quantity (ng) of PAH Formed on Pyrolysis of Tobacco Component[a] (1.0 mg) at 650°C (in N_2)									
PAH[b]	Cell	Lign	Pect	Star	Sucr	Gluc	Fruc	Mal	Citr	Oxal
Acenaphthylene	1.60	0.80	0.20	0.56	0.24	0.27	1.04	0.16	0.50	0.15
Fluorene	5.84	80.00	2.87	0.32	0.12	0.07	1.18	6.32	1.73	0.03
Anthracene	3.37	5.44	5.39	1.04	0.70	0.36	1.39	0.70	0.98	0.30
Pyrene	1.29	0.33	1.33	0.35	0.24	0.66	0.35	1.66	0.24	0.20
Pyrene, 3-methyl-	1.31	0	0.29	0.11	0.15	0.01	0.11	1.19	0.89	0.01
Fluoranthene	1.64	0.58	1.52	0.94	0.35	0.45	1.06	1.36	0.06	0
Benz[*a*]anthracene[c]	1.86	0.44	2.73	1.16	0.41	0.43	1.20	1.30	0.05	0
Benzo[*a*]pyrene[c]	0.78	0.47	0.45	0.17	0.10	0.29	0.33	0.35	0.17	0.01
Benzo[*e*]pyrene[c]	0.85	0.22	0.34	0.04	0.02	0.11	0.02	0.08	0.37	0
Dibenzo[*def,mno*]chrysene	0.10	0	0.09	0.01	0	0.05	0.05	0.01	0.02	0.003
Coronene	0.44	0	0.15	0.03	0.03	0.01	0.05	0.06	0.11	0.02

[a] Cell, cellulose; Lign, lignin; Pect, pectin; Star, starch; Sucr, sucrose; Gluc, glucose; Fruc, fructose; Mal, malic acid; Citr, citric acid; Oxal, oxalic acid.

[b] Several other PAHs were found in some, but not all, of the pyrolysates, namely, azulene, naphthalene, alkylnaphthalenes, acenaphthene, phenanthrene, and perylene.

[c] Tumorigenic to mouse skin in skin-painting studies.

identified 1-docosanol in tobacco, found little of its dehydration product, 1-docosene, in tobacco smoke. They postulated that long-chained primary alcohols such as 1-docosanol were little affected by pyrolysis. Severson et al. (3616) cataloged the major components in eight chromatographic fractions of the PEE from tobacco (see Table 25.8). Each fraction was subjected to pyrolysis. Surprisingly, Severson et al. did not list long-chained primary alcohols in any of the eight chromatographic fractions!

25.3.3 Structural Components of Tobacco (Cellulose, Lignin, Pectins, etc.)

Since cellulose, pectins, starch, lignin, and proteins—the so-called structural components of tobacco—are organic compounds, i.e., contain carbon, with one or more of the carbons linked to hydrogen,* they will generate PAHs during high-temperature pyrolysis much in the same manner as the compounds studied in the mid-1920s to early 1930s by Kennaway (2073–2076). In his studies, Kennaway demonstrated that pyrolysis of various organic compounds—from simple ones such as acetylene or isoprene to more complex ones—would generate pyrolysates tumorigenic to mouse skin. Subsequently, these and similar organic compound-derived pyrolysates were shown to contain a variety of PAHs (1286, 2264b), some of which were potent mouse-skin tumorigens. Obviously, PAHs should be generated from the structural components of tobacco during the reactions occurring when tobacco is smoked in a cigarette. Interest in the major precursors in tobacco of the PAHs in MSS eventually led to the conclusion that the major precursors in tobacco of cigarette MSS PAHs in cigarette MSS were the organic solvent-extractable, high-molecular-weight tobacco components such as the saturated aliphatic and unsaturated aliphatic hydrocarbons, the phytosterols, terpenoid alcohols such as solanesol (3251, 3269, 3291, 3616, 4332).

During the search for the major PAH precursors in tobacco, all of the previously mentioned organic solvent-soluble tobacco components [*cf.* Table 25.5] that were examined by pyrolysis were shown to yield PAHs. In 1957, Gilbert and Lindsey (1289) reported their results on the amounts of various PAHs in the pyrolysates (650°C, N_2) from the major structural components from flue-cured tobacco. These included cellulose, pectins, starch, and lignin; the simple sugars, sucrose, glucose, and fructose; and the acids, malic acid, citric acid, and oxalic. Their data, modified to indicate nanograms of individual PAHs generated per milligram of tobacco component pyrolyzed,† are summarized in Table 25.10.

Numerous pyrolysis experiments were conducted from the mid-1950s to the mid-1980s on tobacco components and tobacco fractions and residues obtained by solvent extraction of tobacco. However, meaningful comparison of the results has been difficult because of the lack of uniformity in the pyrolysis

* Examination of the data reported by Gilbert and Lindsey (1289) on the pyrogenesis of PAHs from various tobacco constituents would appear to contradict this statement. Gilbert and Lindsey reported the generation of a series of PAHs in the pyrolysate (see Table 25.10) from the dicarboxylic acid oxalic acid [$(COOH)_2$] which obviously has no carbon–hydrogen bond. However, it is known that a major product of the thermal decomposition of oxalic acid is formic acid [H-COOH] via decarboxylation. Formic acid does have the requisite carbon–hydrogen bond.

† Nanogram of PAH generated per milligram of tobacco component pyrolyzed = microgram of PAH generated per gram of tobacco component pyrolyzed = parts per million (ppm) of PAH from the tobacco component pyrolyzed.

conditions employed in the studies. Even when some similarity existed between experimental conditions used in two separate experiments, precise comparison was confounded by the fact that different tobaccos or blends were used in the experiments, e.g., Gilbert and Lindsey (1289) examined the PAH yields in the pyrolysates (650°C, N_2) from the structural components of a flue-cured tobacco grown a year or two prior to their 1957 study; Severson et al. (3616) examined the pyrolysates (produced at a variety of temperatures including 650°C, N_2) from a flue-cured tobacco probably grown a few years before their 1979 publication and from a tobacco blend.

In their detailed study, Severson et al. (3616) examined the following pyrolysates: a flue-cured tobacco; its PEE (8% of the tobacco weight); the tobacco residue after petroleum ether extraction; and eight chromatographic fractions (Fractions F-1 through F-8) derived from the PEE. Unfortunately, Severson et al. conducted several key pyrolysis experiments at 700°C only. It should also be noted that tobaccos, such as the flue-cured tobaccos, used by Gilbert and Lindsey and by Severson et al. would not be identical because of the differences in agronomic conditions and practices for the tobaccos grown in the mid-1950s *vs*. the mid-1970s.

Table 25.11 summarizes pyrolysis data from Lam (2257), Gilbert and Lindsey (1289), and Severson et al. (3616) with particular emphasis on the somewhat similar experimental conditions (pyrolysis temperature, atmosphere) and on the yields of B[*a*]P and B[*e*]P from the pyrolysis of different tobaccos, blend, components, and/or fractions. The data

TABLE 25.11
Conversion of Components in Tobacco to B[*a*]P during Pyrolysis

	Level in Tobacco		Pyrolysis		Theoretical Contribution to[a] Benzo[*a*]pyrene		Total Benzopyrene[b]	
Tobacco Component of Fraction	**%**	**mg/g**	**T,°C**	**Atmos**	**ng/mg**	**ng**	**ng/mg**	**ng**
Flue-Cured Tobacco Components (1289)								
Cellulose	9.0	90	650	N_2	0.78	70.2	1.43	128.7
Lignin	3.5	35	650	N_2	0.47	16.5	0.69	24.2
Pectin	10.7	107	650	N_2	0.45	48.2	0.79	84.5
Starch	4.0	40	650	N_2	0.17	6.8	0.21	8.4
Sucrose	4.2	42	650	N_2	0.10	4.2	0.12	5.0
Glucose	11.0	110	650	N_2	0.29	31.9	0.40	44.0
Fructose	7.8	78	650	N_2	0.33	25.7	0.35	27.3
Malic acid	10.1	101	650	N_2	0.35	35.4	0.43	43.4
Citric acid	0.6	6	650	N_2	0.17	1.0	0.54	3.2
Oxalic acid	1.0	10	650	N_2	0.01	0.1	0.01	0.1
Total	61.9	619				240.0		368.8
Fractions from Flue-Cured Tobacco (3616)								
F-1 Aliphatic hydrocarbons	0.42	42	650	N_2			29	122
F-4 Solanesol	2.34	234	650	N_2			930	2,1762
F-6 Phytosterols	1.62	162	650	N_2			670	10,854
Fractions from University of Kentucky 1R1 Tobacco Blend (3616)								
PEE	8.0	80	650	N_2			320	25,600
PEE	8.0	80	700	N_2			380	30,400
PEE	8.0	80	800	N_2			1140	91,200
1R1 Tobacco blend	100.0	1000	700	N_2	190	190,000		
PEE	8.0	80	700	N_2	1750	140,000		
PEE	92.0	920	700	N_2	54	50,000		
Other Studies with Tobacco Components (2257)								
Saturated aliphatic hydrocarbons[c]	0.5	5	600	Air	0	0	0	0
Saturated aliphatic hydrocarbons[c]	0.5	5	700	Air	30	30	110	550
Saturated aliphatic hydrocarbons[c]	0.5	5	800	Air	340	1700	740	700
Flue-Cured CSC (4317)					90[d]			

[a] It is assumed that 1 g of tobacco is consumed during the cigarette smoking.
[b] Total BP = B[*a*]P + B[*e*]P.
[c] Saturated aliphatic hydrocarbons isolated from flue-cured tobacco.
[d] Estimated total of B[*a*]P in MSS (4317) plus SSS from an all-flue-cured tobacco cigarette is 45 ng in MSS plus an estimated 45 ng in SSS.

in Table 25.11, plus additional data in the publications cited, indicated that the structural components as well as other components and fractions (organic solvent-soluble or -insoluble) from tobacco yielded a variety of PAHs on pyrolysis, but the structural components—the biopolymers—such as cellulose, pectins, starch, lignin, on a per unit weight pyrolyzed basis generated much lower yields of PAHs than did the organic solvent-soluble components and/or fractions. Even in the cases where tobacco components are not only soluble in organic solvents but also are relatively highly oxygenated, they show a low propensity to generate PAHs on pyrolysis. This fact was demonstrated by Severson et al. (3616) in their study of the pyrolysates from the eight chromatographic fractions (Fractions F-1 through F-8) from the PEE from flue-cured tobacco. They noted:

> Extraction fractions F-1 and F-8 yielded relatively low yields of PAH on pyrolysis, the former because of its thermally stable hydrocarbon content, and the latter because of its polar oxygenated constituent content. Such oxygenated compounds, having a relatively low carbon content yield low amounts of the alkyl residues essential for PAH formation [see Badger et al. (148), Schmeltz and Hoffmann (3489)]…

The Fraction F-8 components which Severson et al. in their pyrolysis studies demonstrated to have a low propensity to yield PAHs on pyrolysis are similar both structurally and property-wise (molecular weight, volatility) to some of the compounds used in "top dressing" formulations for tobacco smoking products [see tabulations in Doull et al. (1053), Leffingwell et al. (2341)]. Presumably, "top dressing" components applied to tobacco products on pyrolysis would behave similarly during pyrolysis to the Fraction F-8 oxygenated tobacco components described by Severson et al. [see pp. 284–285 in (3616)].

Even though the structural components of tobacco on pyrolysis did yield PAHs, albeit at a much lower level than other classes of tobacco components, their contribution to tobacco smoke composition became important from another point of view: When only a small portion (about 2%–3%) of the biological response observed in mice (or other rodents) skin painted with CSC could be explained by its content of the PAHs reported to be tumorigenic to mouse skin [see pp. 14–51/52 in (4005), Wynder et al. (4303)], additional explanations for the observed biological response were sought. The concepts of promotion and cocarcinogenesis were introduced into the theory of CSC tumorigenicity in an attempt to explain the observed biological response in the mouse-skin-painting studies.

In the 1950s, Boutwell et al. (414) and Boutwell and Bosch (414) reported that low-molecular-weight phenols such as phenol itself and the cresols, nontumorigenic per se in skin-painting experiments, enhanced the tumorigenicity in mouse-skin-painting studies of PAHs reported to be tumorigens. In 1959, Roe et al. (3314) reported the promoting effect of a phenolic fraction from cigarette MSS. Two years later, Wynder and Hoffmann (4313) examined phenol as a promoter of several PAHs (B[*a*]P, DMB[*a*]A) and concluded:

> Promoting substances present in tobacco smoke can increase and accelerate the tumor yield of carcinogenic polynuclear hydrocarbons that by themselves are not present in sufficient concentration to yield any tumors or yield them only after a prolonged latent period.

The low-molecular-weight phenols are extremely low-level components of tobacco but are present in cigarette MSS at levels many times those in tobacco. This led to the search in the late 1950s to early 1960s for precursors in tobacco of the alleged biologically active phenols in tobacco smoke.

Studies by Rodgman and Cook (3277), Rodgman and Mims (3305), and Rodgman (3251) on the effect of tobacco components (lignin, pectin) added to a cigarette tobacco blend on low-molecular-weight phenol levels in MSS and similar studies [Spears et al. (3767), Bell et al. (248)] on the effect of tobacco carbohydrates (glucose, sucrose, starch, cellulose, or pectin) added to cigarette tobacco filler on phenol levels in MSS demonstrated that these tobacco components were major precursors of the simple phenols in cigarette MSS.

From 1962 through 1971, Newell and Best conducted studies with radiolabeled components isolated from tobaccos grown in a radiolabeled CO_2 atmosphere. Among these radiolabeled components studied were the cell wall components or biopolymers [pectin (2764), starch (2764), α-cellulose (2764)] of the tobacco. Each component was added individually to cigarette tobacco, and their contributions to various classes of MSS components, particularly the PAHs and the phenols, were determined. Table 25.12 summarizes the

TABLE 25.12
Conversion of Pectins, Starch, and Cellulose to Specific PAHs and Phenols during Smoking

	Percent of Added Tobacco Component Converted during Smoking to Smoke Component		
Smoke Component	**Pectins**	**Starch**	**Cellulose**
PAHs			
Pyrene	ND	ND	0.0000546
Benzo[*a*]pyrene	0.0000014	0.0000136	0.0000021
Benz[*e*]acephenanthrylene[a]	0.0000018	0.0000017	0.0000060
Benzo[*k*]fluoranthene	0.0000032	ND	ND
Phenols			
Phenol	0.00125	0.0034	0.0036
o-Cresol	0.0010	0.0030	0.0046
m-Cresol + *p*-Cresol	0.00077	ND	0.0048
Guaiacol	0.00115	ND	0.0024
2,5-Xlenol	ND	ND	0.0022

ND, not determined.

[a] Benz[*e*]acephenanthrylene was formerly known as benzo[*b*]fluoranthene.

Newell–Best findings on the percent conversion during smoking of these three structural components to specific PAHs and phenols.

Examination of these data indicates that the percent conversion of these structural components to phenol ranges from one (0.0013%) to about four (0.0036%) one thousandths of a percent, whereas the conversion of these three components to B[*a*]P ranges from about 1 (0.0000014%) to about 14 (0.0000136%) one millionth of a percent. Such data may be used to estimate the conversion to PAHs and phenols of a flavorant (structurally similar to but of lower molecular weight and higher volatility than these biopolymers) added to the tobacco blend.

Numerous pyrolysis studies were conducted on these precursors of phenols. In each case, the generation of simple phenols [phenol, cresols, numerous xylenols] was observed. Kato et al. (2043) reported the pyrolysis of tobacco lignin yielded phenol, cresols, xylenols, and guaiacol—all known components of cigarette MSS. Examination of the structure of lignin reveals why it would readily yield these phenols as well as other substituted phenols such as vanillin [Ball (176a)].

From the mid-1960s to the early 1980s, the USDA tobacco research group—initially at Philadelphia, PA, subsequently at Athens, GA—described the pyrolysis of various tobacco components and the yield of phenols in the pyrolysates. Tobacco components examined for their propensity to generate the simple phenols during pyrolysis included the following:

- Cellulose, pectin, lignin, and the so-called tobacco pigment (3468).
- The major tobacco polycarboxylic acids—malic, citric, and fumaric plus the sodium salts of citric and lactic acids (3486). In the late 1950s, a mixture of sodium and potassium citrates was used as an additive on cigarette paper to control its combustion properties.*
- Tobacco and tobacco extracts [Kennedy and Riehl (25A35), Schlotzhauer et al. (3456), Severson et al. (3616)].
- Cellulose, glucose, and fructose [Higman et al. (1647)]. The latter two sugars† are used in casing materials applied to cigarettes during manufacture [Leffingwell et al. (2341)].

With regard to the generation of phenols by the tobacco acids, Schmeltz et al. (3486) noted:

> The data show that citric, malic and related acids give rise to phenols on pyrolysis. The yields, however, are lower than those from other phenol-forming materials present in tobacco leaf.

Despite the repeated assertions of the promoting potency for PAHs of the CSC phenolic fraction [Roe et al. (3314)] and the simple phenols, particularly phenol itself [Wynder and Hoffmann (4313, 4332)], contradictory evidence was reported. In 1962, Bock and Moore (25A11) challenged the concept that the weakly acidic portion of CSC was a tumor promoter. In fact, Wynder and Hoffmann (4319), strong proponents in 1964 of the promoting effect of the phenols in smoke, wrote:

> Definite tumor-promoting activity for a variety of phenols may be regarded as established.

However, this statement was omitted from their 1967 book in which Wynder and Hoffmann [see p. 626 in (4332)] wrote:

> Phenol and some of its derivatives have been shown to possess tumor-promoting activity…However, a reduction of phenols in tobacco smoke condensate has not led to a concomitant reduction of tumorigenicity in the corresponding 'tars'.

In 1971, Van Duuren et al. (4035), in a discussion of tumor promoters and the complexity of CSC and its potential role in carcinogenesis, reported that "Phenol, which is a weak tumor-promoting agent, is indeed an inhibitor of tumorigenesis when applied simultaneously with benzo[*a*]pyrene."

Two years later, Van Duuren et al. (4029) concluded from their cocarcinogenesis research that "Phenol has been regarded as an important 'tumor promoter' in [cigarette smoke condensate]…[but our] work indicates that it is inactive in cocarcinogenesis and, indeed, has a slight inhibitory effect on benzo[*a*]pyrene carcinogenesis."

Chortyk and Schlotzhauer (722) reviewed the studies reported during the preceding two decades on pyrolysis of tobacco components and the relationship of the pyrolysis results to the pyrogenesis of tobacco smoke components.

In 1979, Martin et al. (2468a) not only reported the results of their own research on the generation of a variety of phenols during the pyrolysis of lignin derived from several sources but also reviewed the results of their own and earlier studies by other investigators on lignin pyrolysis.

From their 1981 and 1982 studies on pyrolysis, Schlotzhauer and Chortyk (3453) and Schlotzhauer et al. (3452) reported the pyrogenesis of phenols not only from cellulose and lignin but also from chlorogenic acid and other polyphenols. Cellulose was defined as a major precursor of cresols and xylenols in smoke; lignin as a major precursor of guaiacol, eugenol, and catechol in smoke; the polyphenols, e.g., chlorogenic acid, as major precursors of the catechols in smoke.

* A mixture of sodium and potassium salts of citric acid was used as a cigarette paper additive, initially at RJRT and subsequently throughout the U.S. tobacco industry since the late 1950s. This additive ensured that the cigarette paper combustion char line slightly preceded the tobacco combustion char line. In the late 1950s, Rodgman (3246) demonstrated that inclusion of sodium and potassium citrates in the cigarette paper additive system reduced the levels of PAHs in the MSS.

† Glucose and fructose are naturally occurring components present at relatively high levels (10%–25%) in Oriental and flue-cured tobaccos but at relatively low levels (usually less than 2%) in burley and Maryland tobaccos [e.g., see Wynder and Hoffmann (4332)]. For many years, the two simple sugars glucose and fructose were added as such or in the form of "invert sugars" to the cigarette blend as part of the casing materials formulation. Low levels of the disaccharide sucrose, a known naturally occurring component of tobacco, were also added.

TABLE 25.13
Pyrolysis *vs.* Actual Smoking Conditions: Conversion of Glucose, Fructose, and Cellulose to B[*a*]P

Experimental Conditions	Conversion (ppm or µg/g) of Tobacco Component to B[*a*]P		
	Glucose	Fructose	Cellulose
Pyrolysis (650°C, N_2) [Gilbert and Lindsey (1289)]	0.29	0.33	0.78
Pyrolysis (840°C, N_2) [Higman et al. (1647)]	47.5	98.4	288.8
Actual smoking conditions (35 mL puff, 2 s duration, 1 puff/min) [Newell and Best (2764)]	ND	ND	0.21

ND, not determined.

In 1975, Schlotzhauer and Chortyk (3452), emphasizing the toxicants in tobacco smoke, reported that the yields of PAHs and phenols in the pyrolysate from reconstituted tobacco sheet (RTS) were significantly lower than those from flue-cured tobacco leaf when generated under the same experimental conditions. Extrapolating their pyrolysis results to the formation of specific components of tobacco smoke, Schlotzhauer and Chortyk noted that "…the continued use of reconstituted tobacco sheet in tobacco products appears warranted."

Comparison of data obtained under different pyrolysis conditions with cellulose, glucose, and fructose with data generated under actual smoking conditions reveals the problem of attempting such a comparison. In Table 25.13 are summarized data from Gilbert and Lindsey (1289), Higman et al. (1647), and Newell and Best (2764) on the conversion (ppm or µg/g) of such tobacco components to B[*a*]P during pyrolysis under two different conditions (650°C and 840°C, N_2) and when smoked in a cigarette under actual smoking conditions (35 mL puff, 2 s puff duration, 1 puff/min). The degree of conversion of tobacco components, such as cellulose, to B[*a*]P under different pyrolysis conditions parallels the degree of conversion of other tobacco components such as the saturated aliphatic hydrocarbons to B[*a*]P under different pyrolysis conditions, e.g., Lam (2257) and his findings summarized in Table 25.11. The conversion of cellulose to B[*a*]P increases several hundredfold as the pyrolysis temperature increased nearly 200°C (from 650°C to 840°C). Under actual smoking conditions, the cellulose-to-B[*a*]P conversion was less than 30%* of the conversion at 650°C. Similarly, under actual smoking conditions, the conversion of cellulose to B[*a*]P was only 0.073% of the conversion at 840°C. Thus, these data from several sources indicate that the fate of a tobacco component on pyrolysis is not equivalent to its fate under actual smoking conditions [cf. the conclusion of Schmeltz et al. (3512) on the fate of nicotine on pyrolysis *vs.* its fate during actual smoking].

As noted in reviews of the thermal degradation products from tobacco carbohydrates (cellulose, pectins, starch, sugars) by Roberts et al. (3225) and by Schumacher (3551), pyrolysis of the carbohydrate components of tobacco results in generation of several classes of compounds other than PAHs and phenols. Among these were aldehydes and ketones, considered significant in smoking–respiratory tract issues. It was asserted during the 1960s that aldehydes and ketones, shown to be ciliastatic in vitro to ciliated tissue, were important because of their significant impairment (by extrapolation) of the action of human respiratory tract cilia. Such impairment was considered part of the mechanism of lung cancer causation by cigarette smoke. However, their importance diminished after the reported findings of Dalhamn et al. (892) that these cigarette smoke-derived, water-soluble in vitro ciliastats were removed in large part by the "scrubbing action" of the fluids coating the surfaces of the oral cavity and laryngeal area, a phenomenon demonstrated several years earlier by Rodgman et al. (3306).

Early studies (1955–1959) on carbonyl components included those of Fredrickson (1228) who examined the volatile MSS components from all-cellulose cigarettes. Many were identified as aldehydes and ketones (1238, 1239). In 1959, Laurene et al. (2310) reported the unequivocal identification of acrolein in cigarette smoke, and cellulose in tobacco was a major precursor of it in smoke. Grob (1413) subsequently demonstrated in 1962 that, during smoking, cellulose generated high levels not only of acrolein but also the ketone 3-buten-2-one.

In 1966, Latimer (25A40) reported several aldehydes (acetaldehyde, acrolein) and ketones (acetone, 2-butanone) in the pyrolysate from tobacco-derived starch. At Philip Morris R&D, Gager et al. (1264, 1265) noted from their study with radiolabeled sugars added to cigarette tobacco that acetaldehyde and acetone were formed during the smoking process in the highest yields from added sugars but their levels were reduced because of the levels generated from other major tobacco components such as cellulose, pectins, and starch.

In their 1976 literature review of pyrolysis products from carbohydrates, Roberts et al. (3225) noted that, of the more than 140 compounds identified in the pyrolysates from glucose, fructose, sucrose, cellulose, and starch, 21 were aldehydes, 30 were ketones. Of these 51 pyrolysis products identified at that time, 40 had been identified as cigarette MSS components.

In 1977, Ohnishi and Kato (2850) described the identification of several carbonyl compounds in the pyrolysates from the tobacco cell wall polysaccharides cellulose, hemicellulose, and pectins. They noted that these biopolymeric polysaccharides constituted 30%–50% of the dry weight of the tobacco they were studying. Sakuma et al. pyrolyzed tobacco-derived cellulose (3401), chlorogenic acid, and rutin (3400) and reported various aldehydes and ketones plus numerous phenols in the pyrolysates. Many of the pyrolysate components identified have also been identified in cigarette MSS.

* Conversion of cellulose to B[*a*]P under actual smoking conditions = 0.21 mg/g; conversion of cellulose to B[*a*]P at 650°C = 0.78 mg/g. Percent ratio for 650°C pyrolysis = 100 × 0.21/0.778 = 27%; for 840°C pyrolysis = 100 × 0.21/288.8 = 0.073%.

25.3.4 Acids

The research findings of Gilbert and Lindsey (1289) on the generation of a variety of PAHs during the pyrolysis of major components of tobacco, including several polycarboxylic acids (oxalic, malic, and citric acids), were discussed previously (see Table 25.10). These acids may constitute from 3% to 12% of dry tobacco weight (1289, 1329, 1330, 1332, 1333). At RJRT R&D, the fate of these acids during smoking in a cigarette was determined by Newell and Best in studies with radiolabeled acids added individually to cigarette tobacco (2763). In 1967, Schmeltz et al. (3486), in their attempt to define precursors in tobacco of several classes of compounds in cigarette smoke, studied the nature and levels of phenols generated in the pyrolysates of malic, citric, aconitic, and fumaric acids or their sodium salts. Thus, pyrolysis of tobacco leaf acids yielded phenols (3486) and PAHs (1289). Although direct comparison is somewhat difficult because of the 50°C pyrolysis temperature difference in the Gilbert–Lindsey *vs.* Schmeltz et al. studies, the PAHs appeared to be generated in much lesser amounts per gram of tobacco leaf acid pyrolyzed than were the phenols. Table 25.14 summarizes data obtained from the studies.

Pyrolysate products obtained from several short-chained aliphatic acids or their sodium salts were examined. Schmeltz and Schlotzhauer (3498) pyrolyzed sodium acetate at 500°C and 800°C. The 800°C pyrolysate was much more complex than that produced at 500°C. This was true for the numbers of pyrolysate components generated and those with aromatic structures. Among the latter were several alkylbenzenes and phenols. Rudenko and Konsinska (25A61) reported similar findings from their pyrolysis of propionic acid, present in tobacco in bound form. At the USDA, Geisinger et al. (1279) demonstrated that pyrolysis of malic and lactic acids at temperatures from 500°C to 900°C (in 100°C increments) yielded both aromatic hydrocarbons and phenols. With malic acid, the aromatic hydrocarbon complexity increased (increased methylation) as the temperature increased. Bicyclic indene was the only PAH detected in the 500°C and 600°C pyrolysates. Indene and naphthalene were detected in the 700°C pyrolysate. Tricyclic acenaphthylene, anthracene, phenanthrene, and fluorene were detected in the 800°C pyrolysate, tetracyclic pyrene, and chrysene in the 900°C pyrolysate. Pyrolytic products from several aromatic acids present either free or bound in tobacco were investigated, e.g., Zane and Wender (4403) demonstrated in 1963 that pyrolysis of rutin, quercetin, and chlorogenic acid (tobacco polyphenols with bound caffeic acid) yielded catechol as the major product, alkylcatechols, resorcinol plus several furancarboxaldehydes. Similar results were reported by the USDA group (3462) at Athens, GA.

In 1969, Jones and Schmeltz reported catechol as the major pyrolysis product (32%) from free caffeic acid (1981) and stilbene as the major pyrolysis product from *trans*-cinnamic acid (1983). *trans*-Cinnamic acid pyrolysate also contained low yields of several bicyclic and tricyclic PAHs. The results of these and similar pyrolysis studies with tobacco acids were reviewed by Chortyk and Schlotzhauer (722).

Indirect evidence that major leaf acids such as malic, citric, and oxalic acids in tobacco contributed low PAH levels to pyrolysates from tobacco fractions was provided by Severson et al. (3616). When tobacco was extracted with hexane or petroleum ether, the bulk of these acids did not appear in the extract but remained in the insoluble tobacco residue. Severson et al. reported that the pyrolysate from the extractables (8% of tobacco weight) contained more than twice the amount of total PAHs than did the pyrolysate from residual tobacco (92% of tobacco weight). In the same study, Severson et al. (3616) examined the levels of a various PAHs (bicyclic to pentacyclic) in the pyrolysates of eight chromatographic fractions from the PEE. Several fractions consisted primarily of free fatty acid mixtures such as myristic, palmitic, stearic, oleic, and linoleic acids (Fractions F-5 and F-6) and esters of long-chained saturated and unsaturated alcohols with these acids (Fractions F-7 and F-8, see Table 25.8). As described previously, Schmeltz et al. (3511) demonstrated that less than 1% of radiolabeled palmitic acid, isolated from tobacco grown in a radiolabeled CO_2 atmosphere and added to cigarette tobacco filler, was converted to PAHs during the smoking process.

Pyrolysis products from esters such as ethyl acetate and isobutyl acetate, both possible flavorants for tobacco smoking products, have been reported [Leffingwell et al. (2341), Miyagawa (2563)]. The principal pyrolysis products from both acetates were CO, CO_2, methane, acetic acid, and acetone. Isobutyl acetate yielded isobutylene as a major product. Products from pyrolysis of the esters formed from long-chained fatty acids* and glycerol (triglycerides) were

TABLE 25.14
Pyrolysis of Leaf Acids: Generation of Selected Phenols and PAHs

Compound Generated, ng/mg of Acid Pyrolyzed	Pyrolysis Conditions		Acid Pyrolyzed		
	T,°C	Atm.	Malic	Citric	Oxalic
PAHs [Gilbert and Lindsey (1289)]					
Benz[*a*]anthracene	650	N_2	1.30	0.35	0
Benzo[*a*]pyrene	650	N_2	0.33	0.17	0.01
Phenols [Schmeltz et al. (3486)]					
Phenol	700	N_2	89	25	ND
o-Cresol	700	N_2	79	38	ND
m-Cresol + *p*-Cresol	700	N_2	79	51	ND

ND, not determined.

* The major long-chained fatty acids, either free or bound, in tobacco are lauric acid (C_{12}), myristic acid (C_{14}), palmitic acid (C_{16}), stearic acid (C_{18}), oleic acid (C_{18}, 1 carbon–carbon double bond), linoleic acid (C_{18}, 2 carbon–carbon double bonds), and linolenic acid (C_{18}, 3 carbon–carbon double bonds). However, bound and free acids in tobacco (and in tobacco smoke) are not limited to acids with even-numbered carbon chains [Bellin (258, 259), Rodgman et al. (3294), Swain and Stedman (3842, 25A72), Wynder and Hoffmann (4332)].

TABLE 25.15
Conversion of Trimyristin Added to Tobacco to PAHs during Actual Cigarette Smoking (3269)

	MSS Delivery of PAH, µg/cig, at Trimyristin Addition Level to Tobacco Blend, mg/g		PAH Increase	
PAH	0	4.0	In ng/4.0 mg of Trimyristin Added	In ng/mg[a] of Trimyristin Added
Naphthalenes[b]	15.8[c]	17.7[c]	1900	475
Anthracene	0.247	0.255	8[d]	2
Pyrene	0.051	0.045	6[d]	1.5
Fluoranthene	0.213	0.207	(6)[d]	0
Chrysene	0.018	0.018	0[d]	0
Benzo[*a*]pyrene	0.081	0.086	5[d]	1.25

[a] ng/mg = parts per million (ppm).
[b] Naphthalenes represent a mixture of naphthalene plus several methyl-, dimethyl-, and trimethylnaphthalenes.
[c] Micrograms produced per gram of tobacco burned.
[d] Within experimental error of analytical procedure.

described by Higman et al. (1646) (tripalmitin, tristearin) and Kitamura (2111a) (trilaurin, tripalmitin). In the early 1970s, Halaby and Fagerson (25A28) pyrolyzed palmitic, oleic, and linoleic acids plus their triglycerides. Numerous PAHs were identified in the pyrolysates. They reported that B[*a*]P was generated from each acid and from each triglyceride at about 100 ppm of the compound pyrolyzed. In their studies on precursors in tobacco of PAHs in tobacco smoke, Rodgman and Cook (3269) demonstrated that addition of 0.4% (4.0 mg/g of tobacco) of trimyristin to tobacco produced, under actual smoking conditions, a 6% increase in total PAHs in the MSS. The changes in individual PAH yields are shown in Table 25.15. These changes are also expressed in Table 25.15 in terms of the conversion (ng/mg or ppm) of the added trimyristin to individual PAHs. The changes observed in the levels of individual PAHs are well within the experimental error for PAH analyses in the late 1950s.

25.3.5 Proteins and Amino Acids

Amino acids, both as free acids and as acids bound within protein molecules, are present in all of the tobacco types (flue-cured, burley, Oriental, Maryland). The diversity and levels of amino acids in various tobaccos have been presented by Gori (1329, 1330) and Tso and Chaplin (3975). The amino acids occurring free and/or bound in tobaccos include alanine, α-aminobutyric acid, arginine, aspartic acid, cystine, glutamic acid, glycine, histidine, isoleucine, leucine, lysine, methionine, ornithine, phenylalanine (Phe), proline, serine, threonine, tryptophan (TRY), tyrosine, and valine.

The presence in cigarette MSS of numerous free amino acids and amino-acid-derived compounds was demonstrated in the mid-1950s. This occurred soon after the publication of the results of several cigarette-smoke-related epidemiological and biological studies led to a massive escalation in tobacco smoke composition studies; e.g., Buyske et al. (562) identified glutamic acid and its derivative glutamine (glutamic acid 5-amide) in tobacco smoke. Other amino acids identified in tobacco smoke [cf. Ishiguro and Sugawara (1884)] include alanine, aspartic acid (and asparagine), cysteine, glycine, leucine, ornithine, Phe, proline, serine, threonine, and valine.

In the early 1960s, pyrocoll (dipyrrolo[*a,d*]pyrazine-5,10-dione) was identified in cigarette MSS by Mold et al. (2592) who proposed that either free or bound proline was its precursor. During their study of the isolation and identification of *N*-heterocyclic components (the indoles and carbazoles) in cigarette MSS, Rodgman and Cook (3279) confirmed the presence of pyrocoll. Two decades earlier, Van Order and Linwall (25A78) had demonstrated that dry distillation of TRY yielded indole and 3-methylindole (skatole), both of which were subsequently identified in tobacco smoke (3279) and in burley tobacco by Roberts [see citation in Rodgman and Cook (3279)].

From their pyrolysis studies (850°C, N_2) with lysine, leucine, and TRY, Patterson et al. (2902) reported that each yielded the *N*-heterocyclic compounds indole, quinoline, isoquinoline, several nitriles, and PAHs ranging from bicyclic to tetracyclic (see Table 25.16). B[*a*]P was found only in the leucine pyrolysate. From their own findings and from a previous report by Jarboe and Rosene (1923a) that quinoline and isoquinoline were components of a nicotine pyrolysate Patterson et al. suggested that the precursors in tobacco of quinoline and isoquinoline in tobacco smoke might be nicotine and/or the amino acids. They also reported that TRY, per mole pyrolyzed, yielded a phenol fraction weighing about five times that generated from lysine and about 30 times that from leucine.

Patterson et al. (2903) reported the effect of temperature on the pyrolysate composition from Phe, with emphasis on PAHs yields, and the effect of TRY or pyrrole (PYR) on the pyrolysate composition when equimolar quantities of

TABLE 25.16
Components in Pyrolysates from Lysine, Leucine, and TRY (2902)

Pyrolysate Component	Yield, mg/mole of Amino Acid Pyrolyzed		
	Lysine[a]	Leucine	TRY
Nitrogen Compounds			
Hydrogen cyanide	+	+	+
Aniline	60	5	–
Quinoline	160	8	17.7
Isoquinoline	80	6	2.4
Benzonitrile	470	40	1370
o-Tolunitrile	30	+	610
m-Tolunitrile	30	30	+
p-Tolunitrile	20	+	+
Phenylacetonitrile	6	–	400
Indole	20	+	610
1-Naphthonitrile	10	30	350
2-Naphthonitrile	–	–	170
Cyclic Hydrocarbons			
Styrene	5	20	–
Biphenyl	10	30	+
Bibenzyl	2	–	+
Indene	40	70	–
Naphthalene	210	620	1100
Naphthalene, 1-methyl-	10	40	+
Naphthalene, 2-methyl-	10	50	–
Acenaphthene	20	–	–
Acenaphthylene	30	19	3
Fluorene	10	80	140
Anthracene/phenanthrene	30	250	7900
Fluoranthene	10	90	210
Pyrene	10	110	270
Pyrene, methyl-	2	20	–
Benzofluorene	10	30	150
Chrysene	10	50	110
Criphenylene	+	+	+
Benz[*a*]anthracene	+	+	+
Benzopyrene	–	30	–

+ Indicates the presence of compound; – indicates the absence of the compound.

[a] Pyrolyzed as lysine monohydrochloride.

Phe + TRY or Phe + PYR were pyrolyzed (see summary of results in Table 25.17). The difference between the pyrogenesis of PAHs from Phe and equimolar quantities of Phe + TRY mixture prompted Patterson et al. (2903) to propose amino acid addition to tobacco to control the PAH content of the CSC:

> These results suggest the possibility that aromatic hydrocarbon content of tobacco "tar" may be affected by the amino acid composition of the tobacco and that it might be possible to affect deliberately the amount of aromatics and bases formed by adding suitable additives, such as amino acids, to the tobacco.

In 1971, when Patterson et al. made this suggestion, the presence in amino acid pyrolysates of the *N*-heterocyclic amines and the inordinately high mutagenicity of several of them were unknown.

Higman et al. (1647) reported the generation of PAHs, phenols, pyridines, indole, quinoline, and other aromatic bases during pyrolysis of tobacco amino acids and proteins [cf. review on pyrogenesis of smoke components by Chortyk and Schlotzhauer (722)]. The results reported by Higman et al. are summarized in Table 25.18.

TRY was found to be the precursor in tobacco of harman (1-methyl-9*H*-pyrido[3,4-*b*]indole) and norharman (9*H*-pyrido[3,4-*b*]indole) in tobacco smoke, compounds originally identified in tobacco and tobacco smoke by Poindexter and Carpenter (2972). That TRY was indeed a precursor in tobacco of the harmans in smoke was demonstrated by addition of radiolabeled TRY to tobacco and identification of radiolabeled harman and norharman in the MSS.

More recent amino acid pyrolysis studies led to the isolation and identification of several *N*-heterocyclic amines reported not only to be tumorigenic to mouse skin but also to show inordinately high mutagenicity [Ames bioassay (*S. typhimurium*)]. Initial impetus for amino acid pyrolyses was not the definition of the relationship between tobacco precursors and smoke components but the observation that extracts of broiled, fried, or roasted foodstuffs were highly mutagenic (Ames bioassay). These *N*-heterocyclic amines, derived from amino acids and/or proteins in heated foodstuffs, were defined as "cooked food" mutagens. These studies in the 1970s on the tumorigenicity and mutagenicity of extracts of cooked foodstuffs are reminiscent of the studies in the 1920s by Kennaway (2073–2076) who reported the tumorigenicity of extracts of heated foodstuffs or pyrolysates from compounds such as cholesterol and by Roffo (25A56, 25A57, 25A58) who reported the tumorigenicity of pyrolyzed cholesterol. Subsequently, pyrolysates from many foodstuffs and cholesterol were shown to contain various PAHs, including B[*a*]P. Identification of highly mutagenic *N*-heterocyclic compounds in amino acid pyrolysates was followed by their identification not only in heated foodstuffs but also in mainstream CSC.

In 1977, Sugimura et al. (3829) reported the identification of the potent mutagens 3-amino-1-methyl-5*H*-pyrido[4,3-*b*] indole (Trp-P-2) and 3-amino-1,4-dimethyl-5*H*-pyrido [4,3-*b*]indole (Trp-P-1) in TRY pyrolysate. The next year, Yamamota et al. (4365a) identified two potent mutagens in glutamic acid pyrolysate: aminodipyrido[1,2-*a*:3′,2′-d]imidazole (Glu-P-2) and 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*] imidazole (Glu-P-1).

Table 25.19 lists several *N*-heterocyclic amines which exhibit high mutagenicity in the Ames bioassay, are amino acid pyrolysis products, and have been identified in heated foodstuffs and CSC (3828c). On a per μg basis, B[*a*]P in the Ames bioassay with *S. typhimurium* (TA 98 strain) shows about 200 revertants/μg. Several of the amino-acid-derived compounds in Table 25.19 exceed the B[*a*]P effect (TA 98 strain) by factors ranging from about 10 to over 2100.

TABLE 25.17
Pyrolysis of Phe: Effect of Pyrolysis Temperature and Effect of Equimolar Addition of TRY or PYR (2903)

	Phe Pyrolyzed at				Material Pyrolyzed		
Pyrolysate Component[c]	450°C	650°C	850°C	950°C	Phe 850°C	Phe + TRY[a] 850°C	Phe + PYR[b] 850°C
Monocyclic Aromatic Hydrocarbons							
Biphenyl	–	1270	10,300	4360	10,300	2980	2240
Bibenzyl	10,300	12,000	2550	+	2550	–	345
PAHs							
Indene	–	360	2730	–	2730	–	170
Naphthalene	120	1450	3500	1270	3500	3525	5600
Naphthalene, 1-methyl-	–	+	–	–	–	–	730
Naphthalene, 2-methyl-	–	–	–	–	–	2980	345
Acenaphthene	–	485	1940	<180	1940	54	86
Acenaphthylene	–	1700	2550	730	2550	400	990
Fluorene	425	1330	4500	850	4500	780	650
Phenanthrene/anthracene	4120	9700	20,000	7900	20,000	1440	2410
Benzofluorene	–	485	1940	2600	1940	220	390
Fluoranthene	–	485	1270	600	1270	160	40
Pyrene	–	3500	3200	1200	3200	300	390
Pyrene, methyl-	–	–	3200	<600	3200	220	+
Chrysenes	–	485	2550	1580	2550	160	300
N-Containing Compounds							
Benzonitrile	1270	850	7880	1270	7880	3800	1465
o-Tolunitrile	–	360	2850	60	2850	680	260
m-Tolunitrile	–	60	–	60	–	1380	260
p-Tolunitrile	–	180	180	–	180	380	260
Phenylacetonitrile	–	1400	–	–	–	220	130
1-Naphthonitrile	–	1400	–	–	–	1140	1000
Indole	–	2300	725	–	725	17,350	860
Quinoline	–	1800	12,000	300	12,000	25,750	1300
Isoquinoline	–	3000	10,900	180	10,900	1100	430

[a] Pyrolysis involved equimolar quantities of Phe and TRY (total mol. wt. = 369).
[b] Pyrolysis involved equimolar quantities of Phe and PYR (total mol. wt. = 232).
[c] Yield of pyrolysis component in µg/g of compound or mixture pyrolyzed.

Yoshida and Matsumoto (4387a) reported the identification of two α-carbolines in CSC: 2-amino-9*H*-pyrido[2,3- *b*] indole (AαC) and 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole (MeAαC). These and several other compounds were reported in CSC by Yamashita et al. (4367, 4368). The quantitative levels of the possibly amino-acid-derived, mutagenic *N*-heterocyclics in CSC are shown in Table 25.19. In their studies, they emphasized in particular the identification and quantitation of 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ) because of its inordinately high mutagenicity (433,000 and 490,000 revertant/µg in the Ames bioassay, *S. typhimurium* strain TA 98).

Demonstration of the mutagenicity of the compounds in Table 25.19 was followed by demonstration of their tumorigenicity in laboratory animals. Ohgaki et al. (2849a) demonstrated the tumorigenicity of IQ in mice. Takayama et al. (3862c) and Tanaka et al. (3865c) reported its tumorigenicity in rats. Trp-P-1 and Trp-P-2 were reported to be tumorigenic in mice by Matsukura et al. (2491a) and in rats by Hosaka et al. (1835a) and Takayama et al. (3862d). Ohgaki et al. (2849b) reported that Glu-P-1, Glu-P-2, AαC, and MeAαC were tumorigenic in mice, and Takayama et al. (3862b) reported Glu-P-1 and Glu-P-2 to be tumorigenic in rats.

Hoffmann and Hecht (1727) discussed the amino-acid-derived aromatic amines in cigarette smoke as follows:

> Of the known carcinogenic pyrolysis products of the amino acids, so far only 2-amino-3-methylimidazo(4,5-*f*)quinoline has been detected in trace amounts of 0.26 ng in the smoke of a Japanese filter cigarette [Yamashita et al. (4368)].

Apparently, Hoffmann and Hecht had overlooked not only the reports of the identification in CSC of several other known "carcinogenic" pyrolysis products of amino acids, e.g., A*a*C and MeA*a*C [Yoshida and Matsumoto (4387a)] or Trp-P-1 and

TABLE 25.18
Components in Pyrolysates from Amino Acids (Proline and Glycine) and Proteins (Casein and Collagen) (1647)

	Amino Acid or Protein			
Pyrolysate Component	**Casein**	**Collagen**	**Proline**	**Glycine**
Nitrogen Compounds				
Hydrogen cyanide	+	+	+	+
Pyridine	+	+	+	+
Pyridine, 2-methyl-	+	+	+	+
Pyridine, 3-methyl-	+	+	+	+
Pyridine, 4-methyl-	+	+	+	+
Pyridine, 3-vinyl-	+	+	–	–
Aniline	+	+	+	–
PYR	+	+	+	+
Quinoline	+	+	+	–
Isoquinoline	+	+	+	–
Indole	+	+	+	–
Benzonitrile	+	+	–	+
o-Tolunitrile			+	+
m-Tolunitrile	+	+	+	–
Cyclic Hydrocarbons				
Benzene	+	+	+	–
Toluene	+	+	+	+
Styrene	+	+	–	+
Xylenes	+	+	–	+
Indene	+	+	–	+
Naphthalene	+	+	–	–
Fluorene	+	+	–	–
Phenols				
Phenol	+	+	–	–
o-Cresol	+	–	–	–
m-Cresol	+	+	–	–
p-Cresol	+	+	–	–
Phenol, ethyl-	+	+	–	–
Xylenol	+	+	–	–

+ Indicates the presence of compound; – indicates the absence of the compound. In the publication by Higman et al. (1647), actual pyrolysis yield data are listed for each compound.

Trp-P-2 [Yamashita et al. (4367)], but also the reports on their tumorigenicity in several animals species [Matsukura et al. (2491a), Hosaka et al. (1835a), Ohgaki et al. (2849a, 2849b), Takayama et al. (3862c, 3862d), Tanaka et al. (3865c)].

Table 25.20 summarizes the MSS yields of *N*-heterocyclic amines considered to be significant tumorigens [Hoffman and Hoffmann (1740, 1741)] plus the assessment of the IARC (1870) on their tumorigenicity in laboratory animals and humans.

Table 25.21 illustrates precursor relationships, either demonstrated or proposed, between *N*-containing components such as the amino acids and proteins and tobacco smoke components. The tabulation of possible flavorants for tobacco smoking products by Leffingwell et al. (2341) included contributions to tobacco smoke taste and aroma of 23 amino acids added individually to the cigarette filler.

During tobacco growth, curing, aging, and/or the smoking process, tobacco sugars may react with ammonia and/or amino acids to yield Amadori compounds which, when heated during the smoking process, will generate a variety of pyrazines [Green et al. (1369)]. Many pyrazines identified in tobacco smoke are highly flavorful and contribute uniquely to the aroma and taste not only of tobacco smoke but also of a variety of consumer food products such as coffee, tea, cocoa, roasted peanuts, and roasted, broiled, or fried meats, poultry, and fish [Maga and Sizer (2439)].

25.4 TOBACCO ADDITIVES

25.4.1 Additives Used in Tobacco Production

Much information exists in the tobacco literature on the use and levels of use of various materials added to tobacco during growth, harvesting, and storage and on such materials that either remain unchanged on the tobacco as residual material or are chemically altered. These materials include insecticides, herbicides, fungicides, fumigants, and sucker growth inhibitors (see Chapter 21). Acceptable use levels of these are prescribed in the United States by appropriate government agencies. Comments, e.g., see Wynder and Hoffmann* (4332), Guthrie (1457), and Guthrie and Sheets (1460) on the use of pesticides, etc., were published in increasing numbers, after the mid-1960s when smoke components or classes of components allegedly responsible for the effects of cigarette smoke in smoke–disease association could not explain the observed effects at the levels in cigarette smoke.

Two types of materials have been examined in greater detail than most of the others. These are discussed in this section because there is substantial information on their pyrolysis products, their transfer per se from cigarette tobacco to its MSS, their degradation during the actual smoking process, and/or their effect as either transferred or degraded materials on the biological activity. Even in these two cases, no attempt has been made to include all the available references. These include the following classes of materials:

- *Sucker growth inhibitors*: Representative sucker growth inhibitors or suckering agents include maleic hydrazide, currently used as an alkali metal salt, and the *normal*, even-numbered carbon chain saturated alcohols, ranging in carbon chain length from (C_6) 1-hexanol through C_{12} (1-dodecanol) (4332).
- *Pesticides*: Particularly those pesticides that are chlorinated, e.g., DDT, Aldrin®, Dieldrin® (4332).

25.4.1.1 Sucker Growth Inhibitors

The pyrolysis of long-chained saturated alcohols such as 1-docosanol and long-chained unsaturated alcohols such as

* It should be noted that, in their earlier review, Wynder and Hoffmann (4319) discussed pesticide-derived arsenic in tobacco and tobacco smoke, but they did not discuss tobacco production additives such as sucker growth inhibitors, pesticides, etc., and their effects on tobacco and tobacco smoke properties.

TABLE 25.19
Amino-Acid-Derived *N*-Heterocyclic Amines

Compound		Mutagenicity[a], rev/μg		
Code	**Name**	**TA 98**	**TA 100**	**Level in CSC, ng/cig[b]**
IQ	Imidazo[4,5-*f*]quinoline, 2-amino-3-methyl-	433,000 490,000	7000	0.26
Trp-P-1	5*H*-Pyrido[4,3-*b*]indole, 3-amino-1,4-dimethyl-	39,000	1700	0.29–0.48
Trp-P-2	5*H*-Pyrido[4,3-*b*]indole, 3-amino-1-methyl-	104,200	1800	0.82–1.1
Glu-P-1	Dipyrido[1,2-*a*:3′,2′-*d*]imidazole,2-amino-6-methyl-	49,000	3200	0.37–0.89
Glu-P-2	Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-	1900	1200	0.25–0.88
A*a*C	9*H*-Pyrido[2,3-*b*]indole, 2-amino-	300	20	25–260
MeA*a*C	9*H*-Pyrido[2,3-*b*]indole, 2-amino-3-methyl-	200	120	2–37

[a] *S. typhimurium*, strain TA 98 or TA 100, with S-9 mix.
[b] See Hoffmann and Hoffmann (1997, 1998).

TABLE 25.20
Summary of Lists of Tumorigenic *N*-Heterocyclic Amines Identified in Tobacco Smoke

					IARC[a] Evaluation of Evidence of Tumorigenicity in	
Component	**Hoffmann and Hecht (1727)**	**OSHA (2825)**	**Hoffmann and Hoffmann (1740, 1741)**	**MSS Yield ng/cig[a]**	**Laboratory Animals**	**Humans**
Glu-P-1	–	–	+	0.37–0.89	Sufficient	–
Glu-P-2	–	–	+	0.25–0.88	Sufficient	–
Trp-P-1	–	–	+	0.29–0.48	Sufficient	–
Trp-P-2	–	–	+	0.82–1.1	Sufficient	–
A*a*C	–	–	+	25–260	Sufficient	–
MeA*a*C	–	–	+	2–37	Sufficient	–
IQ	–	–	+	0.26	Sufficient	Probable
PhIP	–	–	+	11–23	Sufficient	Possible
IQ	–	–	+	0.26	Sufficient	Probable

[a] Data from Hoffmann and Hoffmann (1740, 1741).

phytol and solanesol, known to be naturally occurring components of tobacco, was discussed previously.

One of the most widely used and effective commercial preparations used for inhibition of sucker growth is "Off-Shoot-T," a mixture consisting primarily of the even-numbered straight-chained alcohols 1-hexanol, 1-octanol, 1-decanol, and 1-dodecanol [Collins et al. (25A16)]. Pyrolysis studies by Higman et al. (1644, 1645) with individual alcohols of "Off-Shoot-T" revealed that much of the alcohol was transferred intact to the pyrolysate. Much of the remainder was converted to the corresponding alkene; e.g., 1-decanol yielded 1-decene. Because of their volatility and low molecular weight, conversion of the alcohols to PAHs was minimal.

Definitive evidence that the alcohol sucker growth inhibitors added to tobacco did not augment the tumorigenicity of cigarette MSS was provided in the second set of experimental cigarettes studied in the NCI "Less Hazardous" Cigarette Program (1330, 2683). The chemical and biological properties of the MSSs from three samples (hand-suckered tobacco, tobacco treated with the recommended level of alcohol sucker growth inhibitor, and tobacco treated with 100 times the recommended level) were compared among themselves and with the Standard Experimental Blend, SEB II. Data obtained are shown in Table 25.22. Examination of the data indicates that neither the normal use level of the alcohol nor a use level 100 times normal had any significant adverse effect on the mainstream CSC properties. The MSS phenol yields were increased from the hand-suckered and both alcohol-treated tobacco samples, but the increase elevation had no significant effect on the CSC biological properties. The results were described by Gori (1330) as follows:

> No statistically significant differences were observed among Hand-suckered, Fatty Alcohol-Normal and Fatty Alcohol *x* 100 Blends (variables 60, 61, and 62).

TABLE 25.21
Precursor Relationships between *N*-Containing Tobacco Leaf Components and Tobacco Smoke Components

Code	Component	Demonstrated or Proposed Precursor	Biological Activity			
			Tumorigen	Mutagen	Cocarcinogen	Anticarcinogen
	TRY	trp	—	—	—	—
Pyrocoll	Dipyrrolo[*a,d*]pyrazine-5,10-dione	prol	—	—	—	—
	9*H*-Pyrido[2,3-*b*]indole	trp	—	—	—	—
	9*H*-Pyrido[2,3-*b*]indole, 2-methyl-	trp	—	—	—	—
	9*H*-Pyrido[2,3-*b*]indole, 2-pentyl-	trp	—	—	—	—
	9*H*-Pyrido[2,3-*b*]indole,2-(2-methyl-propyl)-	trp	—	—	—	—
A*a*C	9*H*-Pyrido[2,3-*b*]indole, 2-amino-	trp	Yes	Yes	—	—
MeA*a*C	9*H*-Pyrido[2,3-*b*]indole,2-amino-3-methyl-	trp	Yes	Yes	—	—
Norharman	9*H*-Pyrido[3,4-*b*]indole	trp	—	Yes	—	—
Harman	9*H*-Pyrido[3,4-*b*]indole, 1-methyl-	trp	—	Yes	—	—
	9*H*-Pyrido[3,4-*b*]indole, 1-ethyl-	trp	—	?	—	—
	9*H*-Pyrido[3,4-*b*]indole, 1-propenyl-	trp	—	?	—	—
	9*H*-Pyrido[3,4-*b*]indole, 1-butyl-	trp	—	?	—	—
Trp-P-2	5*H*-Pyrido[4,3-*b*]indole,3-amino-1-methyl-	trp	Yes	Yes	—	—
Trp-P-1	5*H*-Pyrido[4,3-*b*]indole,3-amino-1,4-dimethyl-	trp	Yes	Yes	—	—
IQ	Imidazo[4,5-*f*]quinoline,2-amino-3-methyl-	creat (?)	Yes	Yes	—	—
Glu-P-1	Dipyrido[1,2-*a*:3′,2′-*d*]imidazole, 2-amino-6-methyl-	glut	Yes	Yes	—	—
Glu-P-2	Dipyrido[1,2-*a*:3′,2′-*d*]imidazole,2-amino-	glut	Yes	Yes	—	—
	Indole	trp; lys; leuc	—	—	—	—
	Indole, 3-acetonitrile	trp	—	[a]	—	Yes
	Indole, 2,3-dimethyl-	trp	—	Yes	—	—
	Indole, 1-methyl-	trp	—	—	Yes	—
	Indole, 3-methyl-	trp	—	—	—	—
	Quinoline	trp; lys; leuc	Yes	Yes	—	—
	Isoquinoline	trp; lys; leuc	—	—	—	—

trp, tryptophan; prol, proline; lys, lysine; leuc, leucine; creat, creatinine; Glut, glutamic acid.
[a] Acetonitrile has been designated as a mutagen precursor.

In the summary report (2683) on the four sets of NCI Tobacco Working Group (TWG) experimental cigarettes, this statement was expanded:

> The fatty alcohol, fatty alcohol x 100, and hand-suckered blends showed no significant differences among themselves or from the SEB II blend.

It is interesting to note that biological responses (% TBA), ranging from a high of the average of 48% for the four replicate SEB II CSCs to a low of 36% for the CSC from the sample treated with alcohol at the normal use level, were considered to show "no significant difference."

Maleic hydrazide, another growth inhibitor used as a suckering agent on tobacco, is used in the United States as its potassium salt. Prior to 1982, use on tobacco involved application of maleic hydrazide as its diethanolamine salt. Such use was banned in 1981 by the Environmental Protection Agency (EPA) (1147) soon after it was reported that tobacco treated with it generated *N*-nitrosodiethanolamine (NDELA) during smoking. NDELA was subsequently reported to be a potent, tissue-specific tumorigen in laboratory animals [see Hoffmann et al. (1696) and references therein].

Over the years, the pyrolysis of maleic hydrazide has been much studied, e.g., by Patterson et al. (2907), Smith et al. (3728), Harke et al. (1507), and Clough et al. (25A13). Also studied have been its transfer (estimated at ≤4%) as intact maleic hydrazide from tobacco to cigarette MSS [Haeberer (1470), Liu and Hoffmann (2383, 2384)] and its generation of hydrazine during smoking (2385).

TABLE 25.22
NCI Study (Second Set of Experimental Cigarettes): Effect of Long-Chained Alcohol Sucker Growth Inhibitors on Cigarette Smoke Properties (1330, 2683)

Code No.	Cigarette Filler	Phenol, µg/g of CSC	PAH, µg/g of CSC		% TBA at Daily CSC Dose of	
			B[*a*]A	B[*a*]P	25 mg	50 mg
42	SEB II	3.83	1.08	0.58	50	54
43	SEB II	3.66	0.89	0.82	52	40
44	SEB II	3.90	0.90	0.79	41	49
45	SEB II	3.81	0.86	0.65	47	50
	Avg. (Code Nos. 42–45)	3.80	0.93	0.71	47.5	48
60	Hand suckered	4.42	0.89	0.73	54	45
61	Alcohol[a] level: normal application rate	4.46	0.73	0.50	43	36
62	Alcohol level: 100 times normal application rate	4.83	0.79	0.51	49	41

CSC, cigarette smoke condensate; B[*a*]A, benz[*a*]anthracene; B[*a*]P, benzo[*a*]pyrene; TBA, tumor-bearing animals.
[a] Alcohol, long-chained alcohols in sucker inhibiting reagent.

However, in his 1979 report, the U.S. Surgeon General (4005) noted that maleic hydrazide was not a significant precursor of either hydrazine or 1,1-dimethylhydrazine in cigarette smoke. Smith et al. (3728) reported that the pyrolysis of maleic hydrazide at 600°C yielded CO_2 (24%), CO (2%), HCN (3%), NH_3 (9%), N_2 (3%), hydrazine (trace), and a black residue (50%), structure unknown, whose empirical formula was $C_{15}H_{15}N_5O_2$.

In the fourth set of experimental cigarettes in the NCI's "Less Hazardous" Cigarette Program, the chemical and biological (mouse-skin-painting bioassay) properties of mainstream CSC from a "pesticide"-treated tobacco cigarette were compared to those of the CSC from a control cigarette, SEB IV (1333, 2683). Gori (1333) listed the pesticides, sucker growth inhibitors, etc., used and described the chemical analyses and bioassays of the pesticide-treated and control tobaccos and their MSSs. Among the additives used in the treatment of the "pesticide"-treated tobacco were maleic hydrazide (MH-30), a 10-carbon alcohol ("Contak"), and DDT. Because both maleic hydrazide and DDT were on the tobacco, the chemical and biological results from the MSSs from these samples are discussed later.

25.4.1.2 Pesticides

As mentioned in earlier chapters, the biological response observed in mice skin painted with CSC or its fractions cannot be explained on the basis of the identified components and their levels in the CSC. In an attempt to define the biological response, Wynder and Hoffmann fractionated CSC and determined that the major part of the tumorigenicity that could be accounted for (only a few percent) arose from a PAH-rich fraction designated as Fraction B [Wynder and Hoffmann (4332, 4342), Hoffmann and Wynder (1798, 1800)]. In addition to 39 PAHs, totally or partially identified, among which were several known to be mouse-skin tumorigens, Fraction B contained 27 *N*-heterocyclic compounds (indoles, carbazoles, acridans), 5 *O*-heterocyclic compounds (dibenzofurans), and 6 chlorinated compounds that were either insecticides (DDD, DDT) or their chlorinated derivatives (*trans*-4,4′-dichlorostilbene) [Hoffmann and Wynder (1800)]. According to Hoffmann and Wynder (1800), *trans*-4,4′-dichlorostilbene (DCS) is one of the major pyrolysis products of the most important tobacco insecticides DDT and DDD. They also stated:

> DCS is neither a complete carcinogen nor a tumor initiator, nor a tumor promoter, but the DCS (0.3%) can accelerate significantly the tumorigenicity of a B*a*P solution (0.003%) when both agents are applied concurrently.

However, it should be noted that the use in tobacco culture of chlorinated insecticides such as DDD and DDT in the United States was discontinued in the late 1960s. For example, between 1968 and 1974, the residual DDT levels per gram of U.S. flue-cured tobacco decreased rapidly and substantially (over 200-fold) as follows: 1968, 52 µg/g; 1970, 6 µg/g; 1974, 0.23 µg/g [USPHS (4005), IARC (1870)].

From 1967 through 1973, the organochlorine-containing pesticides such as DDT and TDE were subjected to detailed examination not only for their contribution to cigarette MSS composition by direct transfer and/or degradation to simpler compounds during the smoking process but also to the composition of their pyrolysates. Investigators involved included Nesemann et al. (1968) from BAT (West Germany), Hoffmann et al. (1756, 1767) from the Sloan Kettering Institute and American Health Foundation, Carpenter and Frost (606) from Carreras Tobacco, Chopra et al. from North Carolina A&T [Chopra and Osborne (709, 25A12), Chopra and Domanski (707), Chopra et al. (708), Chopra and Thekkekandam (713, 714)], and Kennedy et al. (25A36) from Mississippi State.

Chopra and Osborne (709) initially studied the pyrolysis of *p,p′*-DDT to identify degradation products. They compared the pyrolysis data with those from actual smoking studies and commented on the differences observed:

> There are two differences in the pyrolysis of DDT reported earlier and the degradation of DDT in tobacco smokes: the concentration of DDT is much greater in the former and hydrogen in the latter. The DDT degradation products as we have found are as would be expected from the difference in the reaction conditions. It is thus possible to predict the fate of a pesticide in tobacco smoke by studying its pyrolysis pattern. Also these investigations show that at the combustion zone hydrogen plays a very important role in the reactions taking place.

Chopra et al. employed these pyrolysis data to identify the transfer and degradation products generated from pesticide-treated tobaccos during the smoking process [Chopra and Domanski (707), Chopra et al. (708), Chopra and Osborne (25A12), Chopra and Thekkekandam (713, 714)]. The results reported indicated the effect of added pesticides on MSS composition primarily in terms of the transfer of intact pesticides from tobacco to smoke or the products generated from them during the smoking process. In the NCI study of the fourth set of cigarettes (1333, 2683), the effect of added pesticides on chemical and biological properties (mouse-skin painting) was examined. As noted previously, the "pesticides" included the sucker growth inhibitors maleic hydrazide (MH-30) and "Contak®" (1-decanol) in addition to DDT (1333). Other compounds present in the mix used in the tobacco treatment according to government-approved procedures and treatment levels included Lorsban®, Dylox®, Enide®, Lannate®, and Carbaryl®. According to Smith et al. (3727), pyrolysis of Carbaryl® (methyl carbamic acid, 1-naphthyl ester) gave three major products in the pyrolysate: unchanged Carbaryl (»40%), 1-naphthol, and methyl isocyanate.

Some results from the NCI study of the MSS from the "pesticide"-treated tobacco are shown in Table 25.23. The conclusions were [see p. 29 in (1333)] as follows:

> Pesticide-Free and Pesticide-Treated Tobaccos: Two cigarettes tested in the fourth experiment were made from tobacco grown [in] Prince Edward Island (PEI) [Canada]. One of the tobaccos was pesticide-free and the other was pesticide-treated… There are no statistically significant differences among the [probability of survival] values at either dose level… Relative condensate yields from these cigarettes are presented… These yields confirm the [probability of survival] values, namely: there is no clear cut difference between the pesticide-free and pesticide-treated tobaccos.

It was also noted in the summary (2683) of the NCI 10-year "Less Hazardous" Cigarette Program:

> No significant differences were observed between cigarettes made from pesticide-treated tobacco leaves and pesticide-free tobacco leaves.

These findings, at least with respect to the maleic hydrazide added, are in agreement with the comments of Chopra (704) in his theoretical discussion of the relationships among pyrolysis, maleic hydrazide, the actual smoking of tobacco treated with maleic hydrazide, and B[*a*]P:

> Evidence and data so far available on maleic hydrazide are not sufficient to suggest the MH [maleic hydrazide] is a health hazard to the smoker… Thus far it is reasonable to assume that there is not enough data or justification to consider the use of MH as a health hazard to the smoker.

In the late 1970s, two excellent reviews on reagents used to treat tobacco and their effects on tobacco chemistry were authored by Steffens (3911a) and by Sheets and Leidy (3634). The latter review included considerable information on the effect of such compounds added to tobacco on MSS composition. Sheets and Leidy (3634) summarized the data which indicated the gradual decline in the levels on tobacco of insecticides such as DDT following the government's proscription of their use on tobacco (and other crops) in the United States. Their summary is similar to that

TABLE 25.23
NCI Study (Fourth Set of Experimental Cigarettes): Effect of Pesticides Addition on Cigarette Smoke Properties (1333, 2683)

			PAH, µg/g of CSC		% TBA at Daily CSC Dose of	
Code No.	Cigarette Filler	Phenol, µg/g of CSC	B[*a*]A	B[*a*]P	12.5 mg	25 mg
04	SEB IV	3.79	0.99	0.72	24	49
14	SEB IV	2.98	1.11	0.79	36	56
29	SEB IV	3.95	0.96	0.71	24	55
32	SEB IV	3.19	1.55	0.60	27	55
	Avge (04,14,29,32)	3.48	1.15	0.70	27.8	53.8
69	Pesticide-free control	5.33	1.05	0.83	34	54
39	Pesticide treated	6.21	1.21	0.79	27	43

CSC, cigarette smoke condensate; B[*a*]A, benz[*a*]anthracene; B[*a*]P, benzo[*a*]pyrene; TBA, tumor-bearing animals.

provided earlier by Guthrie (1457) on the gradual decline of the tobacco arsenic level following the discontinuance in 1952 of arsenate use on tobacco. By 1968, the arsenic level in U.S. tobacco had decreased from a 1951 level of ≈50 µg/g of tobacco (dry weight) to 0.5–1.0 µg/g [USPHS (4005) 1979d; IARC (1870)]. In 1975, Griffin et al. (1391) reported arsenic values of 0.5–0.9 µg/g for U.S. tobaccos.

A pesticide used to control cigarette beetles in stored tobaccos and tobacco products was methoprene (Altosid®) or in the formulation Kabat®. The use of the well-studied methoprene (5-isopropyl(2*E*,4*E*)-11-methoxy-3,7,11-trimethyl-2,4-dodecadienoate) escalated markedly in the 1990s. Methoprene is also acceptable for controlling pests on various foodstuffs as well as mosquito larvae in water supplies. Using radiolabeled methoprene in a cigarette, Frisch et al. (1242, 1243) reported that 38.2%–39.4% of the activity was found in the MSS, 52.3%–52.4% in the sidestream smoke (SSS), and 8.1%–8.4% in the 23 mm butt. Of the activity in the MSS, 96.8% was due to methoprene transferred from the treated tobacco. Of 1.3% total activity found in mainstream vapor phase, 86% consisted of radioactive CO plus CO_2; the remaining 14% of the activity was distributed among 10 vapor-phase components, all normally found as vapor-phase components of cigarette MSS.

25.4.2 Additives Used in Cigarette Manufacture

The pyrolysate compositions from various tobacco additives, including casing materials and humectants, and their effect on cigarette MSS composition and properties were described by Roberts et al. (3225, 3226) and by Schumacher (3551). In this section, additional data are discussed.

25.4.2.1 Casing Materials (Sugars, Cocoa, Licorice)

Casing materials used in cigarette products in the United States are licorice, cocoa, and the sugars—including the invert sugars (glucose plus levulose) and sucrose. While they did not discuss the topic in their 1964 review (4319), Wynder and Hoffmann (4332) did discuss the possible effects on cigarette MSS properties of inclusion of casing materials in the tobacco filler with particular emphasis on licorice because of its glycyrrhizin content. Glycyrrhizin, the potassium and calcium salt of glycyrrhizic acid, is polycyclic with five cyclohexane rings in the picene configuration. (Figure 25.2). Picene is a PAH identified in several pyrolysates by Badger et al. (142) and Kröller (2195) and in CSC by Snook et al. (3756).

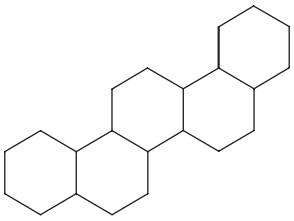


FIGURE 25.2 The picene configuration present in glycyrrhizic acid.

TABLE 25.24
Pyrolysis of Licorice *vs.* Flue-Cured Tobacco: B[*a*]P Generation

Material Pyrolyzed	Pyrolysate wt., mg/g Pyrolyzed	B[*a*]P	
		Total, ng	ng/mg of Pyrolysate
Licorice	117	24.8	0.21
Flue-cured tobacco	133	70.5	0.53

According to an assertion by Wynder and Hoffmann (4332), glycyrrhizin in licorice added to tobacco could be a precursor of PAHs in smoke. In an ill-defined experiment, Hoffmann et al. (1766) compared the B[*a*]P yield in the MSS from pipe tobacco (containing 30% casing materials, including licorice [level unspecified]) smoked in a pipe (2 puff/min) with the B[*a*]P level in the MSS from cigarette tobacco (no licorice added) smoked identically, i.e., in a pipe. The B[*a*]P levels were 27 and 10.5 µg/100 g of tobacco smoked, respectively. Later, Hoffmann and Rathkamp (1754) stated that the pyrolysis of licorice yielded PAHs. This finding was subsequently confirmed by Green and Best (1356, 1357) whose data on B[*a*]P generated during identical pyrolyses of licorice and flue-cured tobacco are summarized in Table 25.24. They also identified 35 other compounds in the licorice pyrolysate [Green and Best (1356, 1357)], all of which had previously been identified in cigarette MSS. Ten of the licorice pyrolysate components were phenols; four were dimethyl- or trimethylnaphthalenes.

Many of the compounds identified in licorice are the same as those identified in tobacco (3551, 3555). Thus, there will be similarities in their contributions to the composition of either pyrolysates from licorice *vs.* tobacco or the MSSs from a licorice-containing *vs.* a licorice-free tobacco blend. Differences will be reflected by the components unique to the material being investigated, e.g., glycyrrhizin in licorice, theobromine in cocoa, and nicotine in tobacco. As noted by Schumacher et al. (3555), 172 (83%) of the 209 components identified in licorice by 1981 had also been identified in tobacco and/or tobacco smoke. Later, a similar situation between cocoa composition and tobacco/tobacco smoke compositions will be discussed.

Sakuma et al. (25A62) reported the pyrolysis products from several naturally occurring polyphenols (chlorogenic acid, rutin). Rutin is a major polyphenol in both licorice and different tobacco types. It and chlorogenic acid yield substantial levels of catechol and substituted catechols on pyrolysis. All the identified volatile pyrolysis products from rutin have been identified in cigarette MSS.

In the late 1970s, Harllee and Leffingwell (1512, 1513) cataloged cocoa components identified to that date with particular emphasis on the volatile, flavorful components common to cocoa and tobacco or its smoke. Both tobacco and tobacco smoke as well as cocoa contain numerous fatty acid triglycerides (1512) and many of the same fatty acids (1512). At least 19 amino acids are common to cocoa and tobacco

(1512). Of 352 volatile components identified in cocoa by 1979, 209 (59%) had also been identified in tobacco and tobacco smoke (1513).

From his pyrolysis study on cocoa, Schlotzhauer (3447) reported that his results suggested the following:

> Cocoa powder added as tobacco flavorant would not significantly increase the phenol yield of smoke, but may affect the higher fatty acid content…

In the NCI study of the third set of experimental cigarettes (1332), the cigarette MSS composition and biological properties (mouse-skin-painting studies) of four cigarette samples were compared. These included three samples to each of which had been added individually a specified amount of glycerol (Code No. 80), sugar (Code No. 81), and cocoa (Code No. 82). The fourth sample was a control (Code No. 83) to which none of these casing materials/humectants had been added (1332, 2683). The results are summarized in Table 25.25 together with data from four Standard Experimental Blend III samples (SEB III, Code Nos. 72–75), the controls for the third set of experimental cigarettes. Variations in the analytical and biological data among these four control samples (Code Nos. 72–75) raised questions about any attempt to compare on a one-to-one basis the data from individual samples, e.g., the cocoa-treated sample (Code No. 82) *vs*. its control (Code No. 83), the sugar-treated sample (Code No. 81) *vs*. its control (Code No. 83), etc. Additional comments will be made about these data in the following section where humectants are discussed.

The phenol data (Code No. 82 *vs*. Code No. 83) in Table 25.25 indicate the prediction by Schlotzhauer (3447) appears to be valid: Inclusion of nominal levels of cocoa in the cigarette blend produced little change in the MSS phenol yield. Addition of 1% cocoa (Code No. 82 *vs*. Code No. 83) increased the phenol yield [mg/g of CSC] by 0.13 mg/g. This is about a 3% increase relative to Cigarette Code No. 83, well within the experimental error of the phenol determination.

25.4.2.2 Humectants (Glycerol, Propylene Glycol)

Humectants (glycerol, propylene glycol) are added to the tobacco blend to diminish the rate of postcigarette manufacture moisture loss. Cigarettes are usually manufactured with the blend at a 12% moisture content. As the cigarette loses moisture, i.e., becomes "dry" during transportation, shelf storage, its yield of smoke components changes adversely with increased yields not only of particulate-phase entities such as "tar" and nicotine but also vapor-phase components such as the aldehydes (acetaldehyde, acrolein) and ketones (acetone, methyl vinyl ketone) [Green et al. (1364)]. These changes usually are perceived by the consumer to be detrimental and unacceptable [Townsend (25A76)].

The pyrolysis of humectants, including glycerol and propylene glycol, was studied in the mid-1960s by Doihara et al. (1023, 1024) and Kröller (2192, 2195, 2196). Kröller examined the pyrolysates from nine humectants (including glycerol and propylene glycol, the most commonly used in the United States) for the yields of B[*a*]P and other PAHs generated during the pyrolysis. His B[*a*]P data are summarized in Table 25.26.

In the early studies of methods to control cigarette MSS composition and yield, particularly with regard to PAHs, Bentley and Burgan (286) asserted addition of glycerol at the 3% level to the tobacco blend substantially decreased (by as much as ≈60%) the B[*a*]P yield when the CSCs from glycerol-treated cigarettes *vs*. untreated tobacco were compared. Their finding was challenged by Wynder and Hoffmann (4332). Subsequently, with a reproducible analytical method

TABLE 25.25
NCI Study (Third Set of Experimental Cigarettes): Effect of a Humectant (Glycerol) or Casing Material (Sugar or Cocoa) on Cigarette Smoke Properties (1332, 2683)

					Relative to CSC				% TBA at Daily Dose of	
		Additive, %			µg/g		µg/g			
Code No.	Filler	Glyc	Sugar	Cocoa	Acr	Phenol	B[a]A	B[a]P	12.5 mg	25 mg
72	SEB III	2.80	5.30	0	3.36	3.86	1.43	1.16	28	50
73	SEB III	2.80	5.30	0	3.62	3.70	1.42	0.97	22	44
74	SEB III	2.80	5.30	0	3.30	3.90	1.36	0.95	30	46
75	SEB III	2.80	5.30	0	3.45	3.90	1.44	1.01	11(?)	44
Avge 72–75	2.80	5.30	0	3.44	3.84	1.41	1.02	23	46	
Avge 72–74	2.80	5.30	0	3.44	3.82	1.40	1.03	27	47	
83	SEB III	0	0	0	3.61	4.33	1.21	1.00	22	31
80	SEB III	2.95	0	0	3.46	3.82	1.23	1.09	22	47
81	SEB III	0	5.42	0	3.54	4.34	1.50	1.08	19	41
82	SEB III	0	0	1.00	3.22	4.46	1.40	1.06	28	49

CSC, cigarette smoke condensate; TBA, tumor-bearing animals; Glyc, glycerol; Acr, acrolein; B[*a*]A, benz[a]anthracene; B[*a*]P, B[*a*]P.

TABLE 25.26
B[*a*]P in the Pyrolysates from Various Humectants Used or Proposed for Use in Cigarette Fabrication

Humectant	B[*a*]P, ng/g Pyrolyzed
Diethylene glycol	15
Triethylene glycol	30
Glycerol	60
1,2-Propylene glycol	60
1,3-Propylene glycol	80
Polyethylene glycol 400	105
Sorbitol	130
Polyethylene glycol 600	289
Polyethylene glycol 1000	420
Tobacco, no additives	20–40

for B[*a*]P determination, Scherbak et al. (3440) and de Souza and Scherbak (953) reported that such levels of added glycerol did not have the dramatic effect claimed by Bentley and Burgan on PAHs (or B[*a*]P) generation during smoking. Scherbak et al. (3440) reported:

> Addition of glycerol to flue-cured tobacco up to the 6% level does not modify the formation of 3,4-benzpyrene or smoke particulate.

The effect of glycerol added to the cigarette blend on MSS composition and properties was studied by the NCI TWG in the third set of experimental cigarettes (1332, 2683). The results were summarized in Table 25.26. At the glycerol level (nearly 3%) used in the glycerol-treated sample (Code No. 80), it would be expected that the total particulate matter (TPM) would contain sufficient transferred glycerol to dilute other components by about 10%–12% [Greene et al. (1382), Laurene et al. (2300), Wynder and Hoffmann (4332), Hege (1603)]. This was not observed with B[*a*]A and B[*a*]P yields but was with the phenol yield [cf. data in Table 25.26 for samples of Code Nos. 80 and 83]. The effect of transfer of humectants from the tobacco blend to smoke plus their dilution of the products formed during the cigarette smoking process affects the biological properties (mutagenicity in the Ames bioassay with *S. typhimurium*) of the MSS particulate matter.

In a detailed study of the effect of various casing ingredients (sugars, cocoa, humectants) on smoke chemistry, Baker et al. (174c) determined the yields of various "Hoffmann analytes" when such ingredients were added in various mixtures. They concluded:

> Many of the casing ingredient mixtures either had no statistically significant effect on the level of analytes investigated in smoke relative to a control cigarette or the produced decreases of up to 44% in some case.

Sugars did increase the yield in MSS of formaldehyde.

25.5 CIGARETTE CONSTRUCTION MATERIALS (PAPER, ADHESIVES, ETC.)

Interest in cigarette MSS components possibly responsible for the epidemiological cigarette smoking–lung cancer association and the biological response observed in mice skin painted with massive CSC doses led to studies of the contribution of cigarette paper to MSS composition, primarily because as a cigarette construction factor, other than the tobacco blend, it contributed substantially (6%–7%) to the weight of a 1.0 g cigarette. In 1954, Cooper and Lindsey (819), based on fragmentary UV data, reported the presence of several PAHs, including B[*a*]P, in a "tar" obtained by burning cigarette paper in bulk. Similar findings on PAHs (and B[*a*]P) in the combustion products of cigarette paper, tobacco, and cigarettes were reported by Lefemine et al. (2335), Cardon et al. (594), and Alvord and Cardon (57). They also proposed an additive (ammonium sulfamate) for paper and/or tobacco to reduce pyrogenesis of PAHs. The ammonium sulfamate efficacy in decreasing B[*a*]P production in a burning cigarette was discussed by Wynder and Hoffmann [see pp. 521–523, 528 in (4322)] who noted that the additive gave discordant results in different investigations [no significant B[*a*]P reduction reported by Bentley and Burgan (286) or Pyriki et al. (3046) *vs.* substantial B[*a*]P reduction reported by Alvord and Cardon (57), Lindsey et al. (2370), and Candeli et al. (589)].

Whether cigarette paper contributed significantly to the PAHs in cigarette MSS was finally resolved by Wright (4281) who reported that PAHs (and particularly B[*a*]P) were indeed generated when cigarette paper was burned in bulk or pyrolyzed, but when it was burned in a cylindrical configuration such as that encountered around the cigarette tobacco rod, the yields of PAHs (particularly B[*a*]P) were insignificant.

Between 1963 and 1966, Kröller (2184–2195, 2200, 2203) reported the pyrolysis products from cigarette components permitted in cigarette fabrication in Germany. He estimated the amount of B[*a*]P generated by pyrolysis of each material at 700°C in air. In addition to tobacco itself (2191), the materials he studied included cellulose, starch, and a number of humectants, adhesives, and dyes consumed during the actual cigarette smoking process.

Kröller (2191, 2192) asserted his pyrolysis and the actual cigarette smoking process were qualitatively and quantitatively identical processes. Kröller's opinion of the equivalence of the fate of a material on pyrolysis in an inert atmosphere *vs.* its fate in the tobacco rod of a smoked cigarette parallels that of Wynder and Hoffmann (4332). In addition to phenanthrene, 4,5-methylenephenanthrene, and fluoranthene, Kröller reported the identification of four potent PAH mouse-skin tumorigens in his tobacco pyrolysate: DMB[*a*]A, 3-methylcholanthrene (now known as 1,2-dihydro-3-methylbenz[*j*]aceanthrylene), B[*a*]P, and DB[*a,h*]A. Despite their agreement with Kröller (2191, 2192) on the equivalence of the fate of a material in an inert atmosphere pyrolysis and the smoking process, Wynder and Hoffmann were critical of several Kröller's findings. For example, Wynder and Hoffmann (4332) questioned Kröller's identification of the

TABLE 25.27
B[*a*]P in the Pyrolysates from Various Materials Used or Proposed for Use in Cigarette Fabrication (2195)

Material	B[*a*]P, ng/g Pyrolyzed
Natural Dyes	
Logwood extract	<10
Buckthorn berry extract	20
Madder lake	120
Humic acid, sodium salt	270
Humectants	
Diethylene glycol	15
Triethylene glycol	30
Glycerol	60
1,2-Propylene glycol	60
1,3-Propylene glycol	80
Polyethylene glycol 400	105
Sorbitol	130
Polyethylene glycol 600	289
Polyethylene glycol 1000	420
Adhesives and Starches	
Alginic acid	30
Carob bean flour	60
Starch	70
Cellulose	80
Carboxymethylcellulose, sodium salt	120
Methylcellulose	180
Tragacanth	230
Dialdehyde starch	235
Cellulose monoacetate	285
Carboxymethylstarch	300
Guava gum	300
Gum arabic	320
Hydroxyethylcellulose	340
Agar–agar	470
Tobacco	
Tobacco (no additives)	20–40

methyl derivatives (DMB[*a*]A, 30-methylcholanthrene) in his pyrolysates and smoke samples. However, a methylbenz[*a*]anthracene had been identified in CSC by Rodgman and Cook (3273) in the late 1950s, and numerous methyl- and dimethylbenz[*a*]anthracenes were subsequently reported in CSC in the late 1970s by Snook et al. (3756, 3757).

Table 25.27, adapted from Kröller (2195), summarizes his data on the amounts of B[*a*]P generated during the pyrolysis of tobacco and numerous components used in cigarette fabrication.

More recently, several studies on the pyrolysis of various adhesives either used or proposed for use as seam pastes in cigarette fabrication were conducted by Best (25A06, 25A07). He reported that, in contrast to a starch pyrolysate, the pyrolysate from polyvinyl acetate showed high levels of acetic acid and B[*a*]P. BEST also examined the pyrolysates from a variety of proposed new cigarette papers (25A04, 25A05, 25A08).

In 1967, Wynder and Hoffmann [see pp. 350–351 in (4332)] noted that pyrolysis data on cigarette components should be considered carefully:

> Certain casing agents, saucing materials, and humectants are widely used in the manufacture of tobacco products. For all we know at this time, it is certainly a possibility that PAH may also be formed from these agents. One should keep in mind, however, that only small amounts of these materials are used for most smoking products.

Their latter statement would also apply to cigarette fabrication materials consumed during the smoking process such as the adhesives used on the cigarette paper seam and printing inks on the paper.

The data from Kröller (2195) on the B[*a*]P yields generated during cellulose and starch pyrolysis may be compared with those of Gilbert and Lindsey (1289), see Table 25.28. This provides an excellent example of the effect of changing pyrolysis conditions (pyrolysis at 650°C in air *vs.* pyrolysis at 700°C in N_2) when two different materials are considered. The different pyrolysis conditions give a ratio of 9.75 (0.78/0.080) for the B[*a*]P yields from cellulose, but a ratio of 2.43 (0.17/0.070) for the B[*a*]P yields from starch.

Inclusion of cellulose in the Kröller studies was because it constitutes the major part of cigarette paper, much of which is consumed during the smoking process. It was not included because cellulose, as wood pulp, is sometimes added by some manufacturers to their reconstituted tobacco sheet (RTS) to improve integrity and reduce fragmentation.

The effect of cellulose added to cigarette filler on cigarette MSS composition and properties in a mouse-skin-painting bioassay was examined in the mid-1970s in the NCI study of the first set of cigarettes (1329, 2683). The results are poorly defined because the cellulose was added (as wood pulp) at a 7.5% level to fillers made from the Standard Experimental Blend (SEB I) reconstituted into sheet material at three different densities.

TABLE 25.28
Pyrolysis of Cellulose and Starch: Comparison of B[*a*]P Data from Kröller with Those from Gilbert and Lindsey

	Pyrolysis Conditions		B[*a*]P, ng/mg of Material Pyrolyzed	
Investigator	Temp., °C	Atmosphere	Cellulose	Starch
Gilbert and Lindsey (1289)	650	N_2	0.78	0.17
Kröller (2195)	700	Air	0.080	0.070

25.6 FLAVORING INGREDIENTS

As outlined in Chapter 24 dealing with tobacco and/or smoke components used as flavorful additives, the numerous assertions about the possibly adverse effect of flavorful compounds added to tobacco were never accompanied by any supporting laboratory evidence. None of the information generated over the past decade that the added flavorants had little, if any, adverse effect on the chemical and biological properties of the smoke generated from the treated tobacco has been criticized by any investigator, governmental agency, or medical institute or any contradictory data presented. In an exemplary study by Baker and Bishop (172a), 291 flavorful additives were pyrolyzed, and in each case, the yields of the major components of the pyrolysate were determined. As outlined in Chapter 24, many of the compounds used as flavor additives are already components of tobacco and/or its smoke. The behavior of such an additive will not differ from its tobacco inherent counterpart. In addition to the pyrolysis study of Baker and Bishop (172a), there are also many studies in which the effect of added flavorants on the chemical and biological properties of cigarette MSS was determined. Many were summarized in 2004 by Rodgman [see Tables 1 and 7A in (3266)], but since then, much additional data have been published. Table 25.29 lists a variety of references pertinent to the use of tobacco and/or smoke components as additives, their pyrolysis, their effect on smoke composition when added individually to tobacco, and their effect on smoke composition when added as a component of a flavorant formulation. Among the references cited is that of Paschke et al. who, in their report on the effect of ingredients on the chemical and biological properties of MSS, tabulated detailed pyrolysis data on a number of individual tobacco and/or smoke components plus detailed pyrolysis data on a variety of materials studied as tobacco additives [see pp. 226–241, Table 5 in (2896)].

Table 25.30 lists a variety of references pertinent to compounds used as tobacco additives where the compounds are not known to be present in tobacco or its smoke. Included are references to their pyrolysis plus their effect on smoke composition when added as a component of a flavorant formulation.

Although Table 25.31 does not involve individual tobacco and/or tobacco smoke compounds, it is included because of the relationship of the entities to tobacco and/or tobacco products. The results of many of the studies cited were published in the early days of the examination of tobacco composition and the attempts to define the precursors in tobacco of various components in MSS. The studies on cocoa and licorice are included because of their level of use in tobacco products.

Table 25.29 deals with individual components that are either tobacco and/or tobacco smoke components, many of which are listed and discussed by Doull et al. (1053), Baker et al. (172a, 174a), Carmines (603), and Rodgman (3266) as additives in tobacco products. Table 25.30 deals with compounds not identified to date in tobacco and/or tobacco smoke but are listed as tobacco product additives. Since our primary concern throughout this project was the discussion of the contribution of individual tobacco components to smoke properties, neither Table 25.29 nor Table 25.30 includes the many complex mixtures (oils, extracts, resins, etc.) used as flavorful cigarette tobacco additives that have also been studied in detail with regard to their pyrolysates (172a, 172b) and their effect as tobacco additives on the chemical (174a, 174b, 630, 3370) and biological properties (174a, 25A24, 25A25, 25A27, 25A43, 25A49, 25A79) of cigarette smoke. Table 25.32 [updated from Table 6 in (3266)] summarizes the specific conclusions from many of such studies conducted between 1994 and 2005. A more detailed summary of the chemical and biological studies through mid-2004 of the complex mixture additives was presented by Rodgman [see Tables 2 and 7B in (3266)].

TABLE 25.29
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

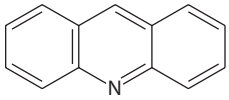
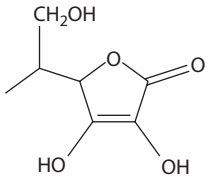
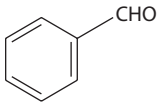
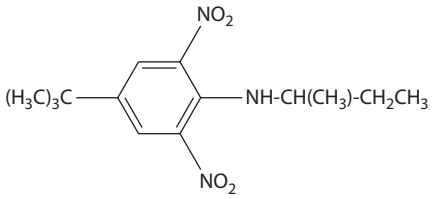
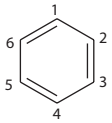
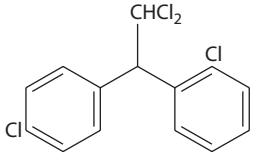
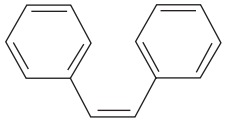
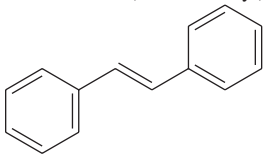
	CAS No.	Name (per CA Collective Index)	References to: Pyrolysis of Individual Component	Effect on MSS Composition, When Component Added: Individually	Effect on MSS Composition, When Component Added: In a Mixture
1.	64-19-7	Acetic acid CH_3-COOH	172a		174a, 174c, 603, 3370
2.	123-86-4	Acetic acid, butyl ester {butyl acetate} CH_3-COO-C_4H_9	172a		174a, 174b
3.	141-78-6	Acetic acid, ethyl ester {ethyl acetate} CH_3-COO-C_2H_5	172a, 2563		174a, 174b, 603, 3370
4.	142-92-7	Acetic acid, hexyl ester {hexyl acetate} CH_3-COO-$(CH_2)_5$-CH_3	172a		174a, 174b, 603, 3370
5.	123-92-2	Acetic acid, 3-methylbutyl ester {isoamyl acetate} CH_3-COO-$(CH_2)_2$-CH═$(CH_3)_2$	172a		174a, 174b, 603, 3370
6.	110-19-0	Acetic acid, 2-methylpropyl ester {isobutyl acetate} CH_3-COO-CH_2-CH═$(CH_3)_2$	172a, 2563		174a, 174b, 603, 3370
7.	103-45-7	Acetic acid, 2-phenylethyl ester {2-phenethyl acetate} CH_3-COO-$(CH_2)_2$-C_6H_5	172a		174a, 174b, 603, 3370
8.	109-60-4	Acetic acid, propyl ester {propyl acetate} CH_3-COO-$(CH_2)_2$-CH_3	172a		174a, 174b
9.	127-09-3	Acetic acid, sodium salt CH_3-COONa	2201, 3464, 3498		174a, 174b
10.	260-94-6	Acridine {benzo[*b*]quinoline} 	515		
11.	56-41-7	*L*-α-Alanine H_3C-CH(NH_2)-COOH	25A41, 25A44, 25A66		
12.	107-95-9	β-Alanine H_2N-$(CH_2)_2$-COOH	3499, 25A41, 25A44, 25A66		
13.	7664-41-7	Ammonia			174b
14.		9-^{14}C-Anthracene {anthracene-9-^{14}C}		25A74	
15.	147-81-9	*DL*-Arabinose HO-CH_2-$(CHOH)_3$-CH═O	3072a		
16.	50-81-7	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-} 	172a		174a, 174b
17.	100-52-7	Benzaldehyde 	172a, 25A70, 25A71		174a, 174b, 603, 3370
18.	120-14-9	Benzaldehyde, 3,4-dimethoxy- {veratraldehyde}	172a		174a, 174b, 603, 3370
19.	121-32-4	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}	172a		174a, 174b, 603, 3370
20.	4748-78-1	Benzaldehyde, 4-ethyl-	172a		174a, 174b
21.	90-02-8	Benzaldehyde, 2-hydroxy- {salicylaldehyde}	172a		174a, 174b, 603, 3370

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
22.	121-33-5	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}	172a, 2044, 25A70, 25A71	1105, 1358	174a, 174b, 603, 3370
23.	123-11-5	Benzaldehyde, 4-methoxy- {*p*-anisaldehyde}	172a, 25A70, 25A71		174a, 174b, 603, 3370
24.	529-20-4	Benzaldehyde, 2-methyl- {*o*-tolualdehyde}	172a		174a, 174b, 603, 3370
25.	620-23-5	Benzaldehyde, 3-methyl- {*m*-tolualdehyde}	172a		174a, 174b, 603, 3370
26.	104-87-0	Benzaldehyde, 4-methyl- {*p*-tolualdehyde}	172a		174a, 174b, 603, 3370
27.	122-03-2	Benzaldehyde, 4-(1-methylethyl)- {cuminaldehyde}	172a		174a, 174b
28.	33629-47-9	Benzenamine, 4-(1,1-dimethylethyl)-2, 6-dinitro-*N*-(1-methylpropyl)- {Butralin®} 	3585c		
29.	122-39-4	Benzenamine, *N*-phenyl- {diphenylamine}	515		
30.	71-43-2	Benzene 	705, 784, 1859, 3500		
31.	104-51-8	Benzene, butyl- C_6H_5-$(CH_2)_3$-CH_3	152		
32.	53-19-0	Benzene,1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*o*,*p*′-DDD, *o*,*p*′-TDE} 		713, 714	
33.	150-78-7	Benzene, 1,4-dimethoxy-	172a		174a, 174b, 603, 3370
34.	100-42-5	Benzene, ethenyl- {styrene} C_6H_5-CH=CH_2	1983		
35.	645-49-8	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*Z*)- 	1983		
36.	103-30-0	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*E*)- 	1983		

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

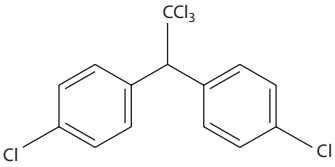
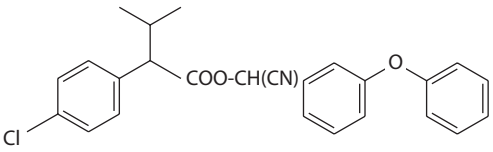
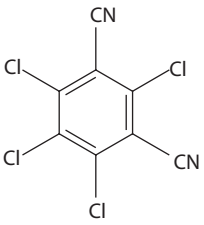
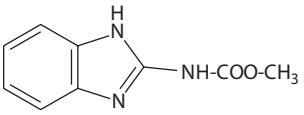
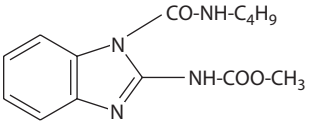
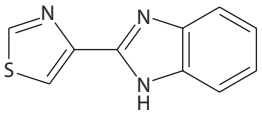
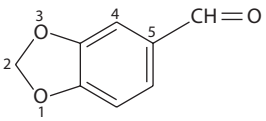
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
37.	100-41-4	Benzene, ethyl- C_6H_5-CH_2-CH_3	152		
38.	100-66-3	Benzene, methoxy- {anisole} C_6H_5-O-CH_3	172a, 25A70, 25A71		174b
39.	104-93-8	Benzene, 1-methoxy-4-methyl- {*p*-methylanisole}	172a		174a, 174b
40.	108-88-3	Benzene, methyl- {toluene} C_6H_5-CH_3	152, 1850, 3500		
41.		Benzene, ^{14}C-methyl- {toluene-^{14}C-methyl}	1850		
42.	99-87-6	Benzene, 1-methyl-4-(1-methylethyl)- {*p*-cymene}			603, 3370
43.	103-65-1	Benzene, propyl- C_6H_5-$(CH_2)_2$-CH_3	152		
44.	50-29-3	Benzene, 1,1′-(2,2,2-trichloroethylidene) bis[4-chloro- {*p,p*′-DDT} 	709	707, 708, 711–714	
45.	122-78-1	Benzeneacetaldehyde {phenylacetaldehyde} C_6H_5-CH_2-CHO	172a		174a, 174b, 603, 3370
46.	4411-89-6	Benzeneacetaldehyde, α-ethylidene- {2-phenyl-2-butenal}	172a		174a, 174b, 603, 3370
47.	103-82-2	Benzeneacetic acid {phenylacetic acid} C_6H_5-CH_2-COOH	172a		174a, 174b, 603, 3370
48.		Benzeneacetic acid, labeled with ^{14}C {phenylacetic acid-^{14}C}		1359	
49.	101-97-3	Benzeneacetic acid, ethyl ester {ethyl phenylacetate} C_6H_5-CH_2-COO-CH_2-CH_3	172a		174a, 174b, 603, 3370
50.	101-41-7	Benzeneacetic acid, methyl ester {methyl phenylacetate} C_6H_5-CH_2-COO-CH_3	172a		174a, 174b, 603, 3370
51.	51630-58-1	Benzeneacetic acid, 4-chloro- α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®} 	3585e		
52.	102-19-2	Benzeneacetic acid, 3-methylbutyl ester {isoamyl phenylacetate}	172a		174a, 174b, 603, 3370
53.	102-20-5	Benzeneacetic acid, 2-phenylethyl ester {phenethyl phenylacetate} C_6H_5-CH_2-COO-CH_2CH_2-C_6	172a		174a, 174b, 603, 3370

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
54.	1897-45-6	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro {Chlorothalonil®} 	3585c		
55.	84-74-2	1,2-Benzenedicarboxylic acid, dibutyl ester {dibutyl phthalate}	2206, 2896		
56.	64-04-0	Benzeneethanamine C_6H_5-CH_2-CH_2-NH_2	2905		
57.	60-12-8	Benzeneethanol phenethyl {alcohol} C_6H_5-CH_2CH_2-OH	172a		174a, 174b, 603, 3370
58.	100-51-6	Benzenemethanol {benzyl alcohol} C_6H_5-CH_2OH	172a		174a, 174b, 603, 3370
59.	104-21-2	Benzenemethanol, 4-methoxy-, acetate {anisyl acetate}	172a		174a, 174b, 603, 3370
60.	501-52-0	Benzenepropanoic acid {3-phenylpropionic acid, hydrocinnamic acid} C_6H_5-CH_2-CH_2-COOH	172a		174a, 174b
61.	122-97-4	Benzenepropanol {3-phenyl-1-propanol} C_6H_5-CH_2-CH_2-CH_2OH	172a		174b
62.	10605-21-7	1*H*-Benzimidazole-2-carbamic acid, methyl ester {Carbendazim®} 	3585b		
63.	17804-35-2	1*H*-Benzimidazole-2-carbamic acid, 1-(butylcarbamomyl)-, methyl ester {Benomyl®} 	3585b		
64.	148-79-8	1*H*-Benzimidazole, 2-(4-thiazolyl)- 	2207, 2896		
65.	120-57-0	1,3-Benzodioxole-5-carboxaldehyde {piperonal, heliotropin} 	172a		174a, 174b, 603, 3370

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

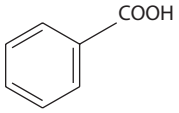
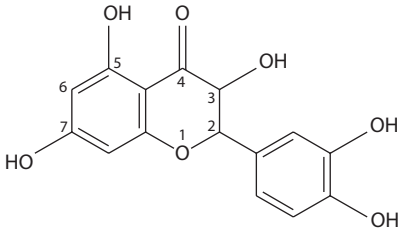
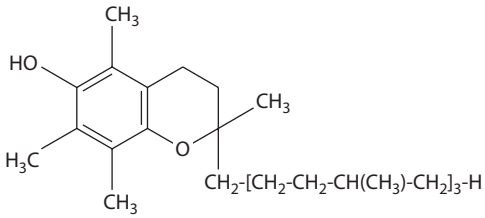
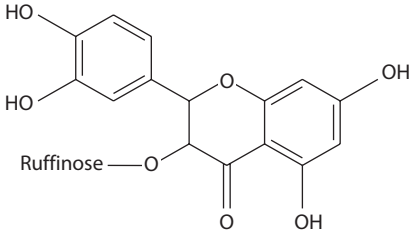
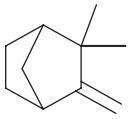
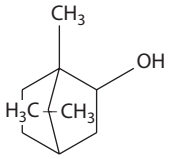
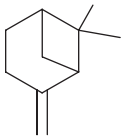
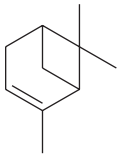
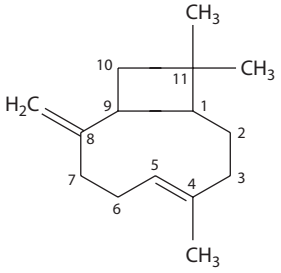
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
66.	65-85-0	Benzoic acid {benzenecarboxylic acid} 	172a		174a, 174b
67.	93-89-0	Benzoic acid, ethyl ester {ethyl benzoate}	172a		174a, 174b, 603, 3370
68.	93-58-3	Benzoic acid, methyl ester {methyl benzoate}	172a		174a, 174b
69.	120-51-4	Benzoic acid, phenylmethyl ester {benzyl benzoate}	172a		174a, 174b, 603, 3370
70.	118-61-6	Benzoic acid, 2-hydroxy-, ethyl ester {ethyl salicylate}	172a		174a, 174b
71.	119-36-8	Benzoic acid, 2-hydroxy-, methyl ester {methyl salicylate}	172a		174a, 174b, 603, 3370
72.	87-20-7	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester {isoamyl salicylate}	172a		174a, 174b
73.	117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3, 5,7-trihydroxy- {quercetin} 	4403		
74.	59-02-9	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- {α-tocopherol} 	172b		174a, 174b, 603, 3370
75.	153-18-4	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin} 	248, 2896, 3400, 3462, 4403, 25A62	5576	
76.		7,10-Benzo[*a*]pyrene-^{14}C {benz[*a*]pyrene-7,10-^{14}C}		25A74	

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

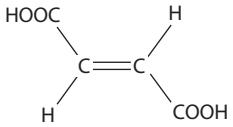
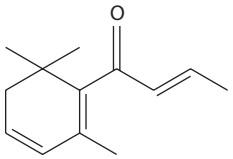
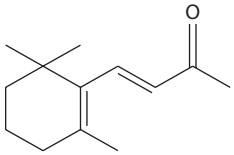
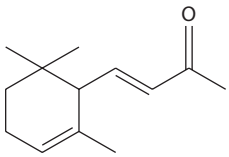
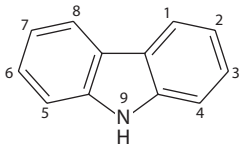
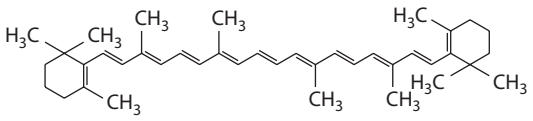
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
77.	79-92-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- {camphene} 			603, 3370
78.	507-70-0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *endo*- {borneol} 			603, 3370
79.	127-91-3 18172-67-3	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- {β-pinene} 	172a		174a, 174b, 603, 3370
80.	80-56-8 7785-26-4	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- {α-pinene} 	172a		174a, 174b, 603, 3370
81.	87-44-5	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4*E*,9S*)]- {β-caryophyllene} 	172a		174a, 174b, 603, 3370
82.	106-99-0	1,3-Butadiene $H_2C{=}CH\text{-}CH{=}CH_2$	154, 710		
83.	78-79-5	1,3-Butadiene, 2-methyl- {isoprene} $H_2C{=}C(CH_3)\text{-}CH{=}CH_2$	143, 2073, 2864b, 2896, 25A68		
84.	96-17-3	Butanal, 2-methyl- {2-methylbutyraldehyde} $H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH{=}O$	172a		174a, 174b
85.	590-86-3	Butanal, 3-methyl- {3-methylbutyraldehyde, isovaleraldehyde} $(H_3C)_2{=}CH\text{-}CH_2\text{-}CH{=}O$	172a		174a, 174b, 603, 3370
86.	87-69-4	Butanedioic acid, 2,3-dihydroxy- {*l*-tartaric acid}			174c

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
87.	6915-15-7	Butanedioic acid, hydroxy- {malic acid} HOOC-CHOH-CH_2-COOH	172a, 1279, 1289, 2201, 2896, 3456, 3486		174a, 174c
88.		Butanedioic acid, hydroxy-, labeled with ^{14}C {malic acid-^{14}C}	2763, 4249	2763, 4249	
89.	107-88-0	1,3-Butanediol {1,3-butylene glycol} H_3C-CHOH-CH_2-CH_2OH	1023, 2192, 2896		
90.	110-63-4	1,4-Butanediol {tetramethylene glycol} $HOCH_2$-$(CH_2)_2$-CH_2OH	2185		
91.	431-03-8	2,3-Butanedione {diacetyl, biacetyl} H_3C-CO-CO-CH_3	172a		174a, 174b, 603, 3370
92.	107-92-6	Butanoic acid {butyric acid} H_3C-$(CH_2)_2$-COOH	172a		174a, 174b, 603, 3370
93.	80-60-4	Butanoic acid, 2-amino- H_3C-CH_2-CH(NH_2)-COOH	3726		
94.	1118-85-0 3226-65-1	Butanoic acid, 2-amino-4-(methylsulfonyl)- {methionine sulfone, methionine S-oxide} H_3C-SO-$(CH_2)_2$-CH(NH_2)-COOH	3729		
95.	105-54-4	Butanoic acid, ethyl ester {ethyl butyrate} H_3C-$(CH_2)_2$-COO-C_2H_5	172a		174a, 174b, 603, 3370
96.	103-37-7	Butanoic acid, phenylmethyl ester {benzyl butyrate} H_3C-$(CH_2)_2$-COO-$CH_2C_6H_5$	172a		174a, 174b, 603, 3370
97.	116-53-0	Butanoic acid, 2-methyl- {2-methylbutyric acid} H_3C-CH_2-CH(CH_3)-COOH	172a		174a, 174b, 603, 3370
98.	7452-79-1	Butanoic acid, 2-methyl-, ethyl ester	172a		174a, 174b, 603, 3370
99.	503-74-2	Butanoic acid, 3-methyl- {isovaleric acid} $(H_3C)_2$=CH-CH_2-COOH	172a		174b, 603, 3370
100.	140-26-1	Butanoic acid, 3-methyl-, 2-phenylethyl ester {phenethyl isovalerate}	172a		174a, 174b, 603, 3370
101.	103-38-8	Butanoic acid, 3-methyl-, phenylmethyl ester {benzyl isovalerate}	172a		174a, 174b
102.	108-64-5	Butanoic acid, 3-methyl-, ethyl ester {ethyl isovalerate} $(H_3C)_2$=CH-CH_2-COO-C_2H_5	172a		174a, 174b, 603, 3370
103.	556-24-1	Butanoic acid, 3-methyl-, methyl ester {methyl isovalerate} $(H_3C)_2$=CH-CH_2-COO-CH_3	172a		603, 3370
104.	659-70-1	Butanoic acid, 3-methyl-, 3-methylbutyl ester {isoamyl isovalerate}	172a, 25A70, 25A71		174a, 174b, 603, 3370
105.	140-27-2	Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester			603, 3370
106.	61445-55-4 133201-39-5	Butanoic acid, 4-(methylnitrosoamino)- Butanoic acid, 4-[(nitrosomethyl)amino] {NMBA} CH_3-N(NO)-$(CH_2)_3$-COOH		464, 466	
107.	71-36-3	1-Butanol {*n*-butyl alcohol} H_3C-$(CH_2)_2$-CH_2OH	172a		174a, 174b, 603, 3370
108.	513-86-0	2-Butanone, 3-hydroxy- {acetoin} H_3C-CO-CHOH-CH_3	172a		174a, 174b, 603, 3370
109.	5471-51-2	2-Butanone, 4-(4-hydroxyphenyl)- {4-(*p*-hydroxyphenyl)-2-butanone}	172a		174a, 174b, 603, 3370

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
110.	110-17-8	2-Butenedioic acid (*E*)- {fumaric acid} 	3486		
111.	80-59-1	2-Butenoic acid, 2-methyl- {(*E*) = tiglic acid}	172a		174a, 174b
112.	23696-85-7	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)- {β-damascenone} 	172a		174a, 174b, 603, 3370
113.	23770-92-3 35044-68-9	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)- {damascone}	172a		174a, 174b, 603, 3370
114.	122-57-6	3-Buten-2-one, 4-phenyl- C_6H_5-CH=CH-CO-CH_3	172a		174a, 174b, 603, 3370
115.	14901-07-6	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- {β-ionone} 	172a, 3647		174a, 174b, 603, 3370
116.	127-41-3	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- {α-ionone} 	172a, 3647		174a, 174b, 603, 3370
117.	86-74-8	9*H*-Carbazole {dibenzo[*b,d*]pyrrole} 	515		
118.	7235-40-7	β,β-Carotene {β-carotene, all-*trans*} 	433, 1110		

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

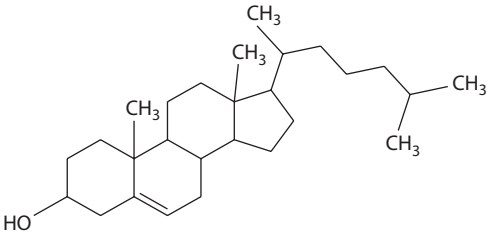
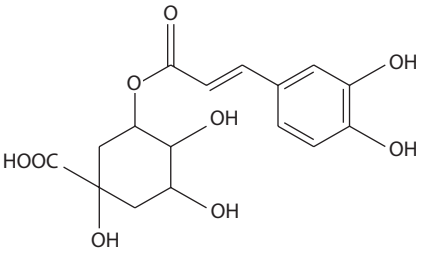
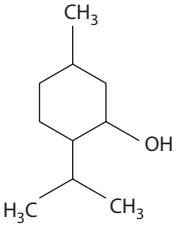
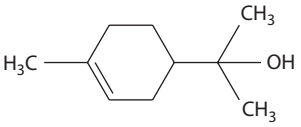
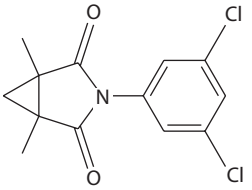
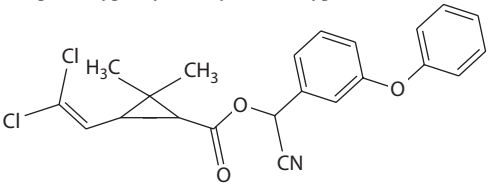
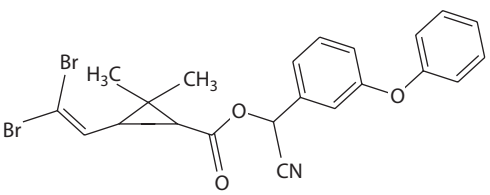
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
119.	9004-34-6	Cellulose	172b, 248, 1289, 1647, 2042, 2046, 2190, 2850, 2896, 3192, 3400, 3401, 3409, 3449, 3452, 3453, 3462, 3468, 25A19, 25A20, 25A29, 25A30, 25A33, 25A34, 25A42, 25A64, 25A77, 25A82		174a
120.		Cellulose, labeled with ^{14}C {cellulose-^{14}C}		2764, 25A31, 25A32	
121.	479-61-8 42617-16-3	Chlorophyll a	5539		
122.	57-88-5	Cholest-5-en-3-ol (3β)- {cholesterol} 	1171, 2080, 25A10, 25A54, 25A56, 25A57, 25A58, 25A69		
123.		Cholest-5-en-3-ol (3β)-, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {cholesteryl linolenate}	433		
124.		Cholest-5-en-3-ol (3β)-, 9-octadecenoate, [3β(*Z*),22*E*]- {cholesteryl oleate}	433		
125.		Cholest-5-en-3-ol (3β)-, octadecanoate, (3β,22*E*)- {cholesteryl stearate}	433		
126.	99-83-2	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- {α-phellandrene}	172a		174a, 174b, 603, 3370
127.	327-97-9 93451-46-8	Cyclohexanecarboxylicacid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid} 	2896, 3400, 3452, 3453, 3462, 4403, 25A62	5576	
128.	89-78-1	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {menthol} 	172a, 2896, 3497, 4036, 25A71	1106–1108	174a, 174b, 603, 3370

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
129.		Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-^{14}C(U) {^{14}C-menthol (U)}		1936, 2770	
130.	89-80-5	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}	172a		174a, 174b, 603, 3370
131.	98-55-5 10482-56-1	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {α-terpineol} 	172a		174a, 174b, 603, 3370
132.	80-26-2	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate {α-terpinyl acetate}	172a		174a, 174b, 603, 3370
133.	562-74-3	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- {4-carvomenthenol}	172a		174a, 174b, 603, 3370
134.	6485-40-1 99-49-0	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*l*-carvone}	172a		174a, 174b, 603, 3370
135.	89-81-6 6091-50-5	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- {*D*-piperitone}			603, 3370
136.	13494-06-9	1,2-Cyclopentanedione, 3,4-dimethyl-	172a		174a, 174b
137.	765-70-8	1,2-Cyclopentanedione, 3-methyl- {cyclotene}	172a		174a, 174b
138.	80-71-7	2-Cyclopenten-1-one, 2-hydroxy-3-methyl- {methylcyclopentenolone}	172a		174b, 603, 3370
139.	32809-16-8	1,2-Cyclopropanedicarboximide, *N* (3,5-dichlorophenyl)-1,2-dimethyl- {Procymidone®} 	3585c		
140.	52315-07-8	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano (3-phenoxyphenyl)methyl ester {Cypermethrin®} 	3585e		
141.	52918-63-5	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl) methyl ester {Deltamethrin®} 	3585e		

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

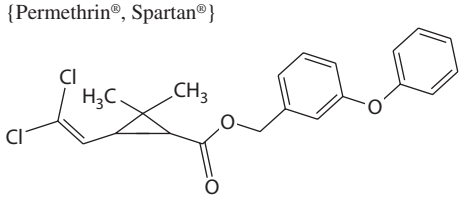
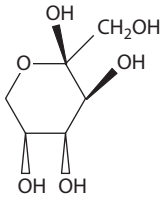
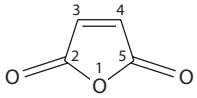
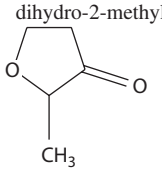
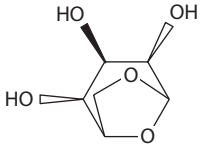
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
142.	52645-53-1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl)methyl ester {Permethrin®, Spartan®} 	3585e		
143.	52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto- (R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	2029, 3729, 25A23		
144.	24645-67-8	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-} $\{S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH\}_2$	2049, 2903, 3499, 3729, 25A23, 25A44		
145.	112-31-2	Decanal {capraldehyde}	172a		174a, 174b, 603, 3370
146.	124-18-5	Decane $H_3C\text{-}(CH_2)_8\text{-}CH_3$	151		
147.	334-48-5	Decanoic acid {capric acid} $H_3C\text{-}(CH_2)_8\text{-}COOH$	172a		174a, 174b, 603, 3370
148.	110-38-3	Decanoic acid, ethyl ester {ethyl caprate} $H_3C\text{-}(CH_2)_8\text{-}COO\text{-}C_2H_5$	172a		174a, 174b, 603, 3370
149.	112-30-1	1-Decanol {capric alcohol} $H_3C\text{-}(CH_2)_8\text{-}CH_2OH$	1644, 1645		603, 3370
150.	9004-53-9	Dextrin	172b, 2896, 3449		174a, 174b
151.	629-97-0	Docosane $H_3C\text{-}(CH_2)_{20}\text{-}CH_3$	248, 2896		
152.	143-07-7	Dodecanoic acid {lauric acid} $H_3C\text{-}(CH_2)_{10}\text{-}COOH$	172a		174a, 174b, 603, 3370
153.	106-33-2	Dodecanoic acid, ethyl ester {ethyl laurate} $H_3C\text{-}(CH_2)_{10}\text{-}COO\text{-}C_2H_5$	172a		174a, 174b, 603, 3370
154.	112-53-8	1-Dodecanol {lauryl alcohol} $H_3C\text{-}(CH_2)_{10}\text{-}CH_2OH$	1644, 1645		
155.	7212-44-4	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- {nerolidol}	172a		174a, 174b
156.	4602-84-0	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- {farnesol}	172a		174a, 174b
157.	544-85-4	Dotriacontane $H_3C\text{-}(CH_2)_{30}\text{-}CH_3$	142, 172a, 2256, 3466	1937	
158.	107-22-2	Ethanedial {glyoxal} O═CH-CH═O	2208, 2896		
159.	144-62-7	Ethanedioic acid {oxalic acid} HOOC-COOH	1289		
160.	43058-40-8	Ethanedioic acid, labeled with ^{14}C {oxalic acid-^{14}C}	2763, 4249	2763, 4249	
161.	64-17-5	Ethanol {ethyl alcohol}	172a		174a, 174b, 603, 3370
162.		1-^{14}C-Ethanol {ethyl alcohol-^{14}C}	1481		
163.	112-27-6	Ethanol, 2,2′-(1,2-ethanediylbis(oxy))bis- {triethylene glycol} $HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$	2192, 2896		
164.	1072-83-9	Ethanone, 1-(1*H*-pyrrol-2-yl)- {2-acetylpyrrole, methyl 2-pyrrolyl ketone}	172a		174a, 174b

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
165.	100-06-1	Ethanone, 1-(4-methoxyphenyl)- {acetanisole}	172a		174a, 174b, 603, 3370
166.	122-00-9	Ethanone, 1-(4-methylphenyl)- {4-methylacetophenone}	172a		174a, 174b, 603, 3370
167.	98-86-2	Ethanone, 1-phenyl- {acetophenone}	172a		174a, 174b, 603, 3370
168.	22047-25-2	Ethanone, 1-pyrazinyl- {acetylpyrazine}	172a		174a, 174b, 603, 3370
169.	74-85-1	Ethene {ethylene} $H_2C{=}CH_2$	710		
170.	74-86-2	Ethyne {acetylene} HC≡CH	149, 784, 2073		
171.	110-45-2	Formic acid, 3-methylbutyl ester			603, 3370
172.	104-57-4	Formic acid, phenylmethyl ester {benzyl formate}	172a		174a, 174b
173.	57-48-7	*D*-Fructose {levulose} 	1289, 1647, 2896, 3409, 3462, 4411		
174.		2,5-^{14}C- 2,5-Furandione {maleic anhydride-2,5-^{14}C} 		25A74	
175.	5989-33-3 60047-17-8	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*Z*)- {*cis*-linalool oxide}	172a		174a, 174b
176.	104-50-7	2(3*H*)-Furanone, 5-butyldihydro- {γ-octalactone}	172a		174a, 174b, 603, 3370
177.	695-06-7	2(3*H*)-Furanone, dihydro-5-ethyl- {γ-hexalactone}	172a		174a, 174b, 603, 3370
178.	706-14-9	2(3*H*)-Furanone, dihydro-5-hexyl- {γ-decalactone}	172a		174a, 174b, 603, 3370
179.	108-29-2	2(3*H*)-Furanone, dihydro-5-methyl- {γ-valerolactone}	172a		174a, 174b, 603, 3370
180.	104-61-0	2(3*H*)-Furanone, dihydro-5-pentyl- {γ-nonalactone}	172a		174a, 174b, 603, 3370
181.	105-21-5	2(3*H*)-Furanone, dihydro-5-propyl- {γ-heptalactone}	172a		174a, 174b, 603, 3370
182.	591-12-8	2(3*H*)-Furanone, 5-methyl- {4-hydroxy-3-pentenoic acid lactone, α-angelica lactone}	172a		174a, 174b
183.	3188-00-9	3(2*H*)-Furanone, dihydro-2-methyl- {2-methyltetrahydrofuran-3-one} 	172a		174a, 174b, 603, 3370
184.	59-23-4	*D*-Galactose	2896, 4411		
185.	498-07-7	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan} 	25A82		

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

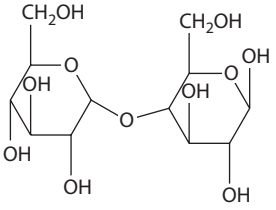
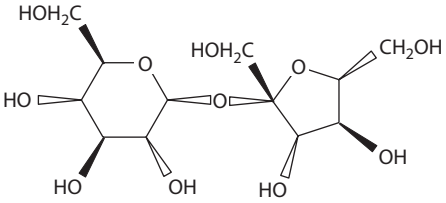
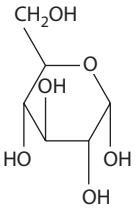
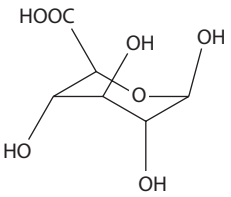
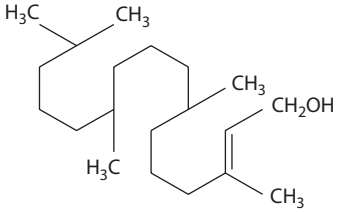
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
186.	69-79-4 4482-75-1 9005-84-9	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin, α-maltose} 	4411		
187.	57-50-1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose} 	172c, 248, 1289, 1647, 1958, 1960, 2204, 2896, 3409, 3449, 3462, 3473, 4411, 25A75		174c, 603, 3370
188.		^{14}C- α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose-^{14}C}		1264, 1265	
189.	50-99-7 26655-34-5	α-*D*-Glucose 	172c, 248, 1289, 1647, 1835d, 2042, 2896, 3409, 3468, 4411, 25A75		174b
190.	9050-36-6	^{14}C- α-*D*-Glucose {α-*D*-Glucose-^{14}C}		1264, 1265, 25A30, 25A74	
191.	576-37-4	Glucuronic acid 	2896, 3468		
192.	6899-05-4	Glutamic acid HOOC-$(CH_2)_2$-CH(NH_2)-COOH	2026, 3828a, 3862b, 3863a, 4365a, 25A44		
193.	56-40-6	Glycine H_2N-CH_2-COOH	1647, 2896, 3499, 25A44, 25A45, 25A66, 25A67		
194.	9034-32-6	Hemicellulose	2850		
195.	630-04-6	Hentriacontane [16-^{14}C] H_3C-$(CH_2)_{29}$-CH_3		1480	
196.	4313-03-5	2,4-Heptadienal O═CH-CH═CH-CH═CH-CH_2-CH═O	172a		174b, 603, 3370
197.	1604-28-0	3,5-Heptadien-2-one, 6-methyl-, (*E*)- $(H_3C)_2$═C═CH-CH═CH-CO-CH_3	172a		174a, 174b, 603, 3370
198.	111-14-8	Heptanoic acid {enanthic acid} H_3C-$(CH_2)_5$-COOH	172a		174b

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
199.	110-43-0	2-Heptanone {methyl pentyl ketone}	172a		174b, 603, 3370
200.	110-93-0	5-Hepten-2-one, 6-methyl-	172a		174a, 174b, 603, 3370
201.	57-10-3	Hexadecanoic acid {palmitic acid} $H_3C\text{-}(CH_2)_{14}\text{-}COOH$	172a, 25A28		174a, 174b
202.	628-97-7	Hexadecanoic acid, ethyl ester {ethyl palmitate} $H_3C\text{-}(CH_2)_{14}\text{-}COO\text{-}CH_2\text{-}CH_3$	172a		174a, 174b
203.	504-96-1	1-Hexadecene, 3-methylene-7,11,15-trimethyl- {neophytadiene} $H_2C{=}CH\text{-}C(=CH_2)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)CH_2\}_3\text{-}H$	2260		
204.	150-86-7	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(*E*)]]- {phytol} 	2260, 3466, 5067, 5539	5067, 5539	
205.	110-44-1	2,4-Hexadienoic acid, (*E,E*)- {sorbic acid} $H_3C\text{-}(CH{=}CH)_2\text{-}COOH$	742		174a, 174b
206.	66-25-1	Hexanal {caproic aldehyde} $H_3C\text{-}(CH_2)_4\text{-}CH{=}O$	172a		174b, 603, 3370
207.	110-54-3	Hexane $H_3C\text{-}(CH_2)_4\text{-}CH_3$	1481		
208.	50-70-4	Hexane, hexahydroxy- {sorbitol, glucitol} $HOCH_2\text{-}(CHOH)_4\text{-}CH_2OH$	172a, 2202, 2896		174a, 174b, 174c
209.	142-62-1	Hexanoic acid {caproic acid} $H_3C\text{-}(CH_2)_4\text{-}COOH$	172a		174b, 603, 3370
210.	123-66-0	Hexanoic acid, ethyl ester {ethyl caproate} $H_3C\text{-}(CH_2)_4\text{-}COO\text{-}C_2H_5$	172a		174a, 174b, 603, 3370
211.	4536-23-6	Hexanoic acid, 2-methyl- {2-methylhexanoic acid}			603, 3370
212.	111-27-3	1-Hexanol {caproyl alcohol} $H_3C\text{-}(CH_2)_4\text{-}CH_2OH$	172a, 1644, 1645		174b
213.	13190-97-1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3, 7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)- {solanesol} $H\text{-}[CH_2\text{-}C(CH_3){=}CH\text{-}CH_2]_9\text{-}OH$	433, 744, 1431, 1432	3269, 3291	
214.	6728-26-3	2-Hexenal, (*E*)-	172a		174b, 603, 3370
215.	4219-24-3	3-Hexenoic acid {hydrosorbic acid} $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}CH_2\text{-}COOH$	172a		174b
216.	928-95-0	2-Hexen-1-ol, (*E*)-	172a		174b
217.	2497-18-9	2-Hexen-1-ol, acetate, (*E*)-	172a		174b
218.	928-96-1	3-Hexen-1-ol, (*Z*)- {leaf alcohol}	172a		174b, 603, 3370
219.		3-Hexen-1-ol glucoside {leaf alcohol glucoside}	740		

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

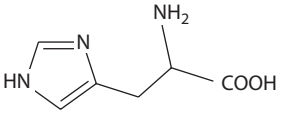
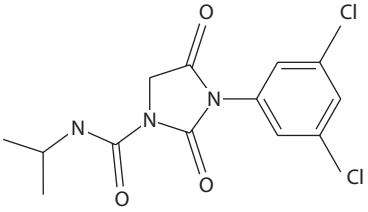
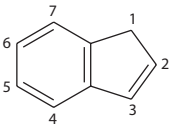
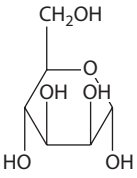
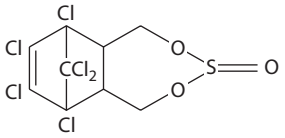
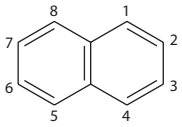
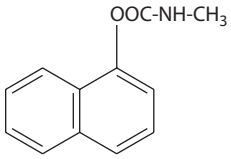
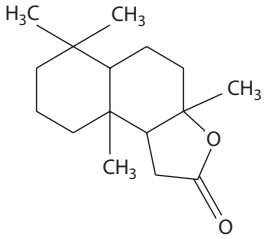
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
220.	71-00-1	*L*-Histidine 	3722a		
221.	368-16-1	*L*-Histidine, 3-methyl-	3722a		
222.	8064-26-4	Holocellulose	2046		
223.	454-29-5	*DL*-Homocysteine HS-$(CH_2)_2$-CH(NH_2)-COOH	3729		
224.	302-01-2	Hydrazine H_2N-NH_2	1507		
225.	36734-19-7	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®} 	3585c		
226.	95-13-6	1*H*-Indene 	146		
227.	73-32-5	*L*-Isoleucine H_3C-CH_2-CH(CH_3)-CH(NH_2)-COOH	25A41, 25A44, 25A66		
228.	63-42-3	Lactose	25A75		
229.	7005-03-0	Leucine $(H_3C)_2$═CH-CH_2-CH(NH_2)-COOH	2902, 3727a, 25A41, 25A44, 25A66, 25A67		
230.	9005-53-2	Lignin	1289, 1649, 2043, 2046, 2468a, 2851, 2896, 3429a, 3449, 3452, 3453, 3462, 3468		
231.	56-87-1	*L*-Lysine H_2N-$(CH_2)_4$-CH(NH_2)-COOH	2902, 2903, 3428, 3727a, 4102a, 25A65, 25A66		
232.	31103-86-3	Mannose 	3072a		

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
233.	115-29-7	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide {Thiodan®, Thiosulfan®, Endosulfan®} 	706		
234.	119-61-9	Methanone, diphenyl- {benzophenone} C_6H_5-CO-C_6H_5	172a		174a, 174b, 603, 3370
235.	63-68-3	*L*-Methionine H_3C-S-$(CH_2)_2$-CH(NH_2)-COOH	2049, 3729, 25A23		
236.	91-20-3	Naphthalene 	705		
237.		1-^{14}C-Naphthalene	144		
238.	119-64-2	Naphthalene, 1,2,3,4-tetrahydro- {tetralin}	145		
239.		1-^{14}C-Naphthalene, 1,2,3,4-tetrahydro- {1-^{14}C-tetralin}	147		
240.	63-25-2	1-Naphthalenol, methylcarbamate {Sevin®, Carbaryl®} 	3727		
241.	564-20-5	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {1,5,5,9-tetramethyl-13-oxatricyclo[8,3,0,0(4,9)]tridecane} {sclareolide} 		3269	174b, 603, 3370
242.	557-48-2	2,6-Nonadienal, (*E,Z*)-			603, 3370
243.	124-19-6	Nonanal {pelargonaldehyde} H_3C-$(CH_2)_7$-CH═O	172a		174a, 174b, 603, 3370
244.	112-05-0	Nonanoic acid {pelargonic acid} H_3C-$(CH_2)_7$-COOH	172a		174a, 174b, 603, 3370
245.	123-29-5	Nonanoic acid, ethyl ester H_3C-$(CH_2)_7$-COO-C_2H_5	172a		174a, 174b, 603, 3370

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

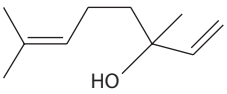
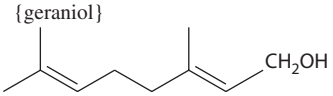
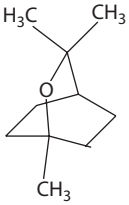
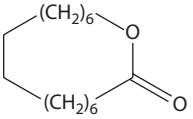
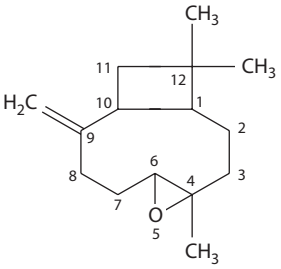
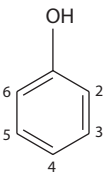
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
246.	821-55-6	2-Nonanone $H_3C\text{-}(CH_2)_6\text{-}CO\text{-}CH_3$	172a		174a, 174b
247.	57-11-4	Octadecanoic acid {stearic acid} $H_3C\text{-}(CH_2)_{16}\text{-}COOH$	1472, 3466		
248.	506-21-8	9,12-Octadecadienoic acid, (*E,E*)- {linoleic acid} $H_3C\text{-}(CH_2)_4\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}COOH$	3466, 25A28		
249.	26764-26-1	Octadecenoic acid {oleic acid}	25A28		
250.	5392-40-5	2,6-Octadienal, 3,7-dimethyl- {citral}	172a		174a, 174b, 603, 3370
251.	78-70-6	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool} 	172a		174a, 174b, 603, 3370
252.		1,6-Octadien-3-ol, 3,7-dimethyl-, labeled with ^{14}C {linalool-^{14}C}		317	
253.	115-95-7	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate {linalyl acetate}	172a		174a, 174b, 603, 3370
254.	106-24-1	2,6-Octadien-1-ol, 3,7-dimethyl-, (*E*)- {geraniol} 	172a, 1472		174a, 174b, 603, 3370
255.	106-25-2	2,6-Octadien-1-ol, 3,7-dimethyl-, (*Z*)- {nerol}	172a		174a, 174b, 603, 3370
256.	124-13-0	Octanal $H_3C\text{-}(CH_2)_6\text{-}CH{=}O$	172a		174a, 174b, 603, 3370
257.	124-07-2	Octanoic acid {caprylic acid} $H_3C\text{-}(CH_2)_6\text{-}COOH$	172a		174a, 174b, 603, 3370
258.	106-32-1	Octanoic acid, ethyl ester {ethyl caprylate}	172a		174a, 174b, 603, 3370
259.	111-87-5	1-Octanol {caprylic alcohol} $H_3C\text{-}(CH_2)_6\text{-}CH_2OH$	172a, 1644, 1645		174a, 174b
260.	13877-91-3	1,3,6-Octatriene, 3,7-dimethyl- {ocimene} $H_2C{=}CH\text{-}C(CH_3){=}CH\text{-}CH_2\text{-}CH{=}C(CH_3)_2$			603, 3370
261.	106-23-0	6-Octenal, 3,7-dimethyl- {citronellal} $(H_3C)_2{=}C{=}CH\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH{=}O$	172a		174a, 174b
262.	3391-86-4	1-Octen-3-ol	172a		174a, 174b
263.	106-22-9	6-Octen-1-ol, 3,7-dimethyl- {*dl*-citronellol}	172a		174a, 174b, 603, 3370
264.	470-82-6	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- {eucalyptol, 1,8-cineole} 	172a		174a, 174b, 603, 3370
265.	106-02-5	Oxacyclohexadecan-2-one {ω-pentadecalactone, exaltolide} 	172a		174a, 174b, 603, 3370

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
266.	1139-30-6	5-Oxatricyclo[8.2.0.04,6]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- {β-caryophyllene oxide} 	172a		174a, 174b
267.	9000-69-5	Pectin	172b, 174d, 248, 1289, 2850, 2896, 3429, 3468, 3651, 3979a		174a, 174c
268.		Pectin, labeled with ^{14}C {pectin-^{14}C}		2764	
269.	629-99-2	Pentacosane $H_3C\text{-}(CH_2)_{23}\text{-}CH_3$	2260		
270.	110-62-3	Pentanal {valeraldehyde} $CH_3\text{-}(CH_2)_3\text{-}CH{=}O$	172a		174a, 174b, 603, 3370
271.	600-14-6	2,3-Pentanedione $H_3C\text{-}CH_2\text{-}CO\text{-}CO\text{-}CH_3$	172a		174a, 174b
272.	109-52-4	Pentanoic acid {valeric acid} $H_3C\text{-}(CH_2)_3\text{-}COOH$	172a		174a, 174b, 603, 3370
273.	539-82-2	Pentanoic acid, ethyl ester {ethyl valerate} $H_3C\text{-}(CH_2)_3\text{-}COO\text{-}C_2H_5$	172a		174a, 174b
274.	97-61-0	Pentanoic acid, 2-methyl- {2-methylvaleric acid}	172a		174a, 174b, 603, 3370
275.	105-43-1	Pentanoic acid, 3-methyl- {β-methylvaleric acid, 3-methylpentanoic acid}	172a		174a, 174b
276.	123-76-2	Pentanoic acid, 4-oxo- {levulinic acid} $H_3C\text{-}CO\text{-}(CH_2)_2\text{-}COOH$	741, 25A02		
277.	107-87-9	2-Pentanone $H_3C\text{-}(CH_2)_2\text{-}CO\text{-}CH_3$	172a		174a, 174b
278.	96-22-0	3-Pentanone $H_3C\text{-}CH_2\text{-}CO\text{-}CH_2\text{-}CH_3$	25A61		
279.	108-95-2	Phenol 	3500		
280.	90-05-1	Phenol, 2-methoxy- {guaiacol}	172a		174a, 174b
281.	93-51-6	Phenol, 2-methoxy-4-methyl- {4-methylguaiacol}	172a		174a, 174b, 603, 3370
282.	97-54-1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}	1649, 2896, 3468		

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

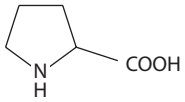
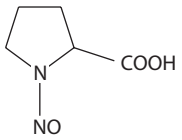
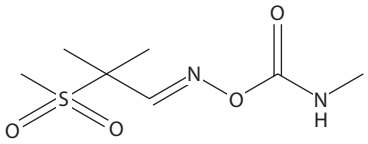
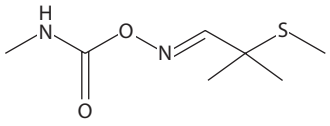
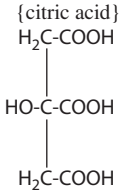
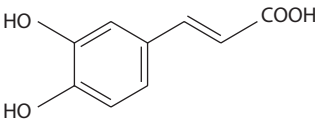
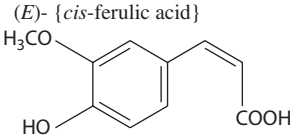
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
283.	499-75-2	Phenol, 2-methyl-5-(1-methylethyl)- {carvacrol}	172a		174a, 174b
284.	644-35-9	Phenol, 2-propyl-	1649, 2896, 3468		
285.	7786-61-0	Phenol, 4-ethenyl-2-methoxy- {4-vinylguaiacol}	172a		174a, 174b
286.	123-07-9	Phenol, 4-ethyl- {*p*-ethylphenol}	172a		174a, 174b
287.	89-83-8	Phenol, 5-methyl-2-(1-methylethyl)- {thymol}	172a		174a, 174b
288.	91-10-1	Phenol, 2,6-dimethoxy- {syringol}	172a		174a, 174b
289.	63-91-2	*L*-Phenylalanine C_6H_5-CH_2-CH(NH_2)-COOH	2903, 2905, 3727a, 3829, 25A44, 25A65, 25A66		
290.	147-85-3	*L*-Proline 	1647, 1967, 2896, 2903, 3499, 3726, 3727a, 25A44		
291.	18610-59-8	*L*-Proline, 1-hydroxy-	1967, 25A44		
292.	7519-36-0	*L*-Proline, 1-nitroso- {NPRO} 		464, 466	
293.	78-84-2	Propanal, 2-methyl- {isobutyraldehyde} $(H_3C)_2$=CH-CH=O	172a		174a, 174b, 603, 3370
294.	1646-88-4	Propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino)carbonyl]oxime {Aldoxycarb®} 	3585d		
295.	116-06-3	Propanal, 2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb®} 	3585d		
296.	3268-49-3	Propanal, 3-(methylthio)- {methional}	172a		174a, 174b
297.	57-55-6	1,2-Propanediol {propylene glycol} H_3C-CHOH-CH_2OH	172a, 1023, 2192, 2896		174a, 174b, 174c, 603, 3370
298.	77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid} 	172a, 1289, 2201, 2896, 3456, 3486		174a, 174c, 603, 3370
299.	58308-53-5	1,2,3-Propanetricarboxylic-1,3-$^{14}C_2$ acid, 2-hydroxy- {citric acid-^{14}C}	2763, 4249	2763, 4249	

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
300.	77-93-0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester {triethyl citrate}	172a		174a, 174b
301.	56-81-5	1,2,3-Propanetriol {glycerol} $HOCH_2$-CHOH-CH_2OH	172a, 1023, 2196, 2896, 3813		174a, 174b, 603, 3370
302.	63346-81-6	1,2,3-Propanetriol, labeled with ^{13}C {glycerol-^{13}C}		5028, 5583	
303.	4254-13-1	1,2,3-Propanetriol, labeled with ^{14}C {glycerol-^{14}C}	300–302, 310	300–302, 310, 25A46	
304.	79-09-4	Propanoic acid {propionic acid} H_3C-CH_2-COOH	172a, 1279, 25A61		174a, 174b
305.	105-37-3	Propanoic acid, ethyl ester {ethyl propionate} H_3C-CH_2-COO-C_2H_5	172a		174a, 174b, 603, 3370
306.	50-21-5 598-82-3	Propanoic acid, 2-hydroxy- {lactic acid} H_3C-CHOH-COOH	172a, 3456		174a, 174b, 174c
307.	97-64-3	Propanoic acid, 2-hydroxy-, ethyl ester {ethyl lactate} H_3C-CHOH-COO-C_2H_5	172a		174a, 174b, 603, 3370
308.	16595-31-6	Propanoic acid, 2-hydroxy-, sodium salt {sodium lactate} H_3C-CHOH-COONa	1279, 2201, 2896, 3486		
309.	79-31-2	Propanoic acid, 2-methyl- {isobutyric acid} $(H_3C)_2$=CH-COOH	172a		174a, 174b, 603, 3370
310.	127-17-3	Propanoic acid, 2-oxo- {pyruvic acid} H_3C-CO-COOH	172a		174a, 174b, 603, 3370
311.	10478-42-9	Propanoic acid, 3-(methylnitrosoamino)- {NMPA} CH_3-N(NO)-$(CH_2)_2$-COOH		464, 466	
312.	78-83-1	1-Propanol, 2-methyl- {isobutyl alcohol} $(H_3C)_2$=CH-CH_2OH	172a		174a, 174b, 603, 3370
313.	104-55-2	2-Propenal, 3-phenyl- {cinnamaldehyde}			603, 3370
314.	331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid} 	1840a, 1981		
315.	1014-83-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*cis*-ferulic acid} 	1840a		
316.	140-10-3	2-Propenoic acid, 3-phenyl-, (*E*)- {*trans*-cinnamic acid}	1983		
317.	621-82-9	2-Propenoic acid, 3-phenyl- {cinnamic acid} C_6H_5-CH=CH-COOH	172a		174a, 174b, 603, 3370
318.		2-Propenoic acid, 3-phenyl-, sodium salt	1983		
319.	122-69-0	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester {cinnamyl cinnamate}	172a		174a, 174b, 603, 3370
320.	103-36-6	2-Propenoic acid, 3-phenyl-, ethyl ester {ethyl cinnamate}	172a		174a, 174b, 603, 3370

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

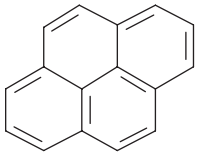
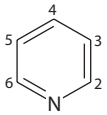
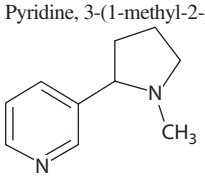
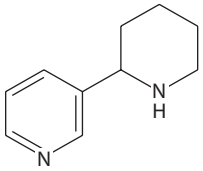
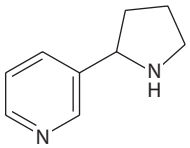
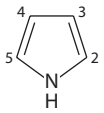
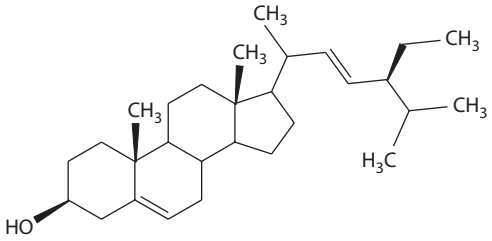
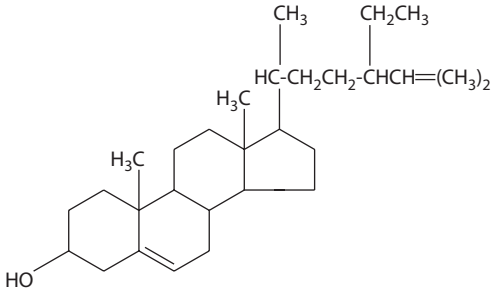
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
321.	103-26-4	2-Propenoic acid, 3-phenyl-, methyl ester {methyl cinnamate}	172a, 25A70, 25A71		174a, 174b, 603, 3370
322.	7779-65-9	2-Propenoic acid, 3-phenyl-, 3-methylbutyl ester	172a		174a, 174b, 603, 3370
323.	103-41-3	2-Propenoic acid, 3-phenyl-, phenylmethyl ester {benzyl cinnamate}	172a		174a, 174b, 603, 3370
324.	104-54-1	2-Propen-1-ol, 3-phenyl- {cinnamyl alcohol}	172a		174a, 174b, 603, 3370
325.	698-76-0	2*H*-Pyran-2-one, tetrahydro-6-propyl- {δ-octalactone}	172a		174a, 174b, 603, 3370
326.	4940-11-8	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy- {ethylmaltol}	172a		174a, 174b, 603, 3370
327.	118-71-8	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}	172a		174a, 174b, 603, 3370
328.	15707-24-1	Pyrazine, 2,3-diethyl-	172a		174a, 174b, 603, 3370
329.	5910-89-4	Pyrazine, 2,3-dimethyl-	172a		174a, 174b
330.	123-32-0	Pyrazine, 2,5-dimethyl-	172a		174a, 174b, 603, 3370
331.	108-50-9	Pyrazine, 2,6-dimethyl-	172a		174a, 174b
332.	13360-65-1	Pyrazine, 2-ethyl-3,6-dimethyl- = pyrazine, 6-ethyl-2,5-dimethyl-	172a		174a, 174b, 603, 3370
333.	13925-07-0	Pyrazine, 2-ethyl-3,5-dimethyl- = pyrazine, 3-ethyl-2,6-dimethyl-	172a		174a, 174b, 603, 3370
334.	15707-23-0	Pyrazine, 2-ethyl-3-methyl-	172a		174a, 174b, 603, 3370
335.	109-08-0	Pyrazine, methyl- = pyrazine, 2-methyl-	172a, 1852		174a, 174b
336.	1124-11-4	Pyrazine, tetramethyl-	172a		174a, 174b, 603, 3370
337.	14667-55-1	Pyrazine, trimethyl-	172a		174a, 174b, 603, 3370
338.	129-00-0	Pyrene {benzo[*def*]phenanthrene} 	154		
339.	123-33-1	3,6-Pyridazinedione, 1,2-dihydro- {maleic hydrazide, MH, MH-30}	704, 1507, 2906, 2907, 3585c, 3723, 3728, 25A13		
340.		^{13}C-3,6-Pyridazinedione, 1,2-dihydro-	3725		
341.	110-86-1	Pyridine 	1852		
342.	109-06-8	Pyridine, 2-methyl- {2-picoline}	1852		
343.	108-99-6	Pyridine, 3-methyl- {3-picoline}	1852		
344.	108-89-4	Pyridine, 4-methyl- {4-picoline}	1852		
345.	54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} 	172a, 515, 1923a, 2006, 3499, 3967, 4027, 4275a		
346.	54-11-5	^{14}C-Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine-^{14}C}	3512	3512	

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
347.	494-52-0	Pyridine, 3-(2-piperidinyl)-, (S)- {*l*-anabasine} 	1075a, 5582		
348.	494-97-3	Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine} 	175		
349.	109-97-7	1*H*-Pyrrole {azole} 	2903, 2908		
350.	6898-95-9	Serine $HO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	2047, 2048, 25A44		
351.	9005-25-8	Starch	248, 1289, 2200, 2896, 25A40		174a
352.	70226-57-2	Starch, labeled with ^{14}C {starch-^{14}C}		2764	
353.	83-48-7	Stigmasta-5,22-dien-3-ol, (3β,22*E*)- {stigmasterol} 	142, 433, 1214		
354.	83-46-5	Stigmast-5-en-3-ol, (3β)- {β-sitosterol} 	435, 705, 1214, 3466	3269, 3291	

(*continued*)

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

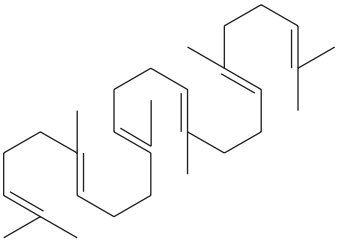
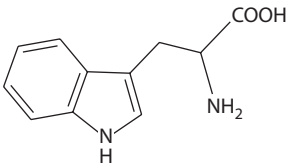
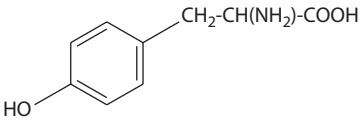
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
355.	111-02-4	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-*E*)- {squalene} 	433, 3466, 5581		
356.	646-31-1	Tetracosane $H_3C\text{-}(CH_2)_{22}\text{-}CH_3$	248, 2896		
357.	124-06-1	Tetradecanoic acid, ethyl ester {ethyl myristate} $H_3C\text{-}(CH_2)_{12}\text{-}COO\text{-}C_2H_5$	172a		174a, 174b
358.	110-02-1	Thiophene 	1849		
359.	554-14-3	Thiophene, 2-methyl-	1849		
360.		Thiophene, 2-^{14}C-methyl-	1849		
361.	72-19-5	*L*-Threonine $H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	2048, 3499		
362.	73-22-3	*L*-TRY 	1835a, 2449, 2902, 2903, 3499, 3727a, 3829, 3862d, 4370a, 4387a, 25A01, 25A65, 25A67, 25A78		
363.	60-18-4	*L*-Tyrosine 	25A44, 25A65		
364.	3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (*E*)- {geranylacetone} $H(CH_2\text{-}C(CH_3){=}CH\text{-}CH_2)_2\text{-}CH_2\text{-}CO\text{-}CH_3$	172a		174a, 174b, 603, 3370
365.	112-12-9	2-Undecanone {methyl nonyl ketone} $H_3C\text{-}(CH_2)_8\text{-}CO\text{-}CH_3$	172a		174a, 174b
366.	57-13-6	Urea $H_2N\text{-}CO\text{-}NH_2$	172a, 25A83		174a, 174b, 603, 3370
367.	7004-03-7	Valine $(H_3C)_2{=}CH\text{-}CH(NH_2)\text{-}COOH$	1968, 3726, 25A41, 25A44, 25A66		

TABLE 25.29 (continued)
Pyrolysis of Tobacco and Tobacco Smoke Components plus Their Effect on Smoke Composition When Added to Tobacco

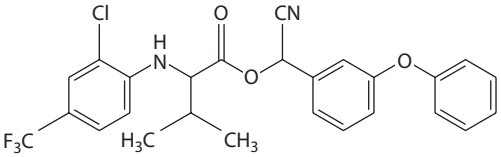
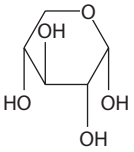
			References to		
				Effect on MSS Composition, When Component Added	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
368.	102851-06-9	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®} 	3585e		
369.	7732-18-5	Water			174c
370.	25990-60-7	Xylose 	3072a		

TABLE 25.30
Pyrolysis of Nontobacco and Nontobacco Smoke Components and/or Their Effect on Smoke Composition When Added to Tobacco

			References to	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Effect on MSS Composition, When Component Added in a Mixture
1.	105-87-3	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl acetate}	172a	174a, 174b, 603, 3370
2.	150-84-5	Acetic acid, 3,7-dimethyl-6-octenyl ester {citronellyl acetate}	172a	174a, 174b
3.	151-05-3	Acetic acid, 1,1-dimethyl-2-phenylethyl ester {α,α-dimethylphenethyl acetate}		603, 3370
4.	3681-71-8	Acetic acid, 3-hexen-1-yl ester, (*Z*)- {*cis*-3-hexen-1-yl acetate}	172a	174b
5.	140-39-6	Acetic acid, 4-methylphenyl ester {*p*-tolyl acetate}	172a	174b, 603, 3370
6.	143-13-5	Acetic acid, nonyl ester {nonyl acetate}		603, 3370
7.	2442-10-6	Acetic acid, 1-octen-3-yl ester {1-octen-3-yl acetate}		603, 3370
8.	24851-98-7	Acetic acid, 2-pentyl-3-oxo-1-cyclopentyl-, methyl ester {methyl dihydrojasmonate}	172a	174a, 174b
9.	103-54-8	Acetic acid, 3-phenyl-2-propenyl ester {cinnamyl acetate}	172a	174a, 174b
10.	76-49-3	Acetic acid, *endo*-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl ester {bornyl acetate}		603, 3370
11.	141-97-9	Acetoacetic acid, ethyl ester {ethyl acetoacetate}	172a	174a, 174b
12.	53956-04-0	Ammonium glycyrrhizinate[a]		174a, 174b
13.	1336-21-6	Ammonium hydroxide	172a	
14.	10031-82-0	Benzaldehyde, 4-ethoxy- {*p*-ethoxybenzaldehyde}	172a	174a, 174b
15.	1319-88-6	Benzaldehyde glyceryl acetal	172a	174a, 174b
16.	698-27-1	Benzaldehyde, 2-hydroxy-4-methyl-{2-hydroxy-4-methylbenzaldehyde}	172a	174a, 174b
17.	151-10-0	Benzene, 1,3-dimethoxy- {*m*-dimethoxybenzene}	172a	174a, 174b, 603, 3370
18.	1076-56-8	Benzene, 3-methoxy-1-methyl-4-(1-methylethyl)- {4-isopropyl-3-methoxy-1-methylbenzene}	172a	174a, 174b
19.	104-87-0	Benzeneacetaldehyde, 4-methyl- {*p*-tolylacetaldehyde}		174b
20.	122-43-0	Benzeneacetic acid, butyl ester {butyl phenylacetate}		603, 3370
21.	102-22-7	Benzeneacetic acid, 3,7-dimethyl-2,6-octadieny-1-yl ester {geranyl phenylacetate}		603, 3370
22.	5421-17-0	Benzeneacetic acid, hexyl ester {hexyl phenylacetate}		603, 3370
23.	101-94-0	Benzeneacetic acid, 4-methylphenyl ester {*p*-tolyl phenylacetate}		603, 3370
24.	102-13-6	Benzeneacetic acid, 2-methylpropyl ester {isobutyl phenylacetate}	172a	174a, 603, 3370
25.	105-13-5	Benzenemethanol, 4-methoxy- {anisyl alcohol}	172a	174a, 174b, 603, 3370
26.	122-91-8	Benzenemethanol, 4-methoxy-, formate {anisyl formate}	172a	174a, 174b, 603, 3370
27.	102-17-0	Benzenemethanol, 4-methoxy-, phenylacetate {anisyl phenylacetate}	172a	174a, 174b, 603, 3370
28.	7549-33-9	Benzenemethanol, 4-methoxy-, propanoate {anisyl propionate}	172a	174a, 174b
29.	93-92-5	Benzenemethanol, α-methyl-, acetate {α-methylbenzyl acetate}	172a	174a, 174b
30.	104-53-0	Benzenepropanal {3-phenylpropionaldehyde}	172a	174a, 174b
31.	13341-72-5	Benzofuranone, dimethyltetrahydro- {dimethyltetrahydrobenzofuranone-}		603, 3370
32.	134-20-3	Benzoic acid, 2-amino-, methyl ester {methyl anthranilate}		603, 3370
33.	87-19-4	Benzoic acid, 2-hydroxy-, 2-methylpropyl ester {isobutyl salicylate}		603, 3370
34.	118-58-1	Benzoic acid, 2-hydroxy-, phenylmethyl ester {benzyl salicylate}		603, 3370
35.	120-47-8	Benzoic acid, 4-hydroxy-, ethyl ester {ethyl *p*-hydroxybenzoate}	2208, 2896	
36.	94-13-3	Benzoic acid, 4-hydroxy-, propyl ester {propyl *p*-hydroxybenzoate}		603, 3370
37.	121-98-2	Benzoic acid, 4-methoxy-, methyl ester {methyl anisate}	172a	174a, 174b
38.	94-46-2	Benzoic acid, 3-methylbutyl ester {isoamyl benzoate}		603, 3370
39.	126-64-7	Benzoic acid, 3,7-dimethyl-1,6-octadien-3-yl ester {linalyl benzoate}	172a	174a, 174b
40.	532-32-1	Benzoic acid, sodium salt {sodium benzoate}	2208, 2896	174a, 174b
41.	125-12-2	Bicyclo[2,2,1]heptan-2-ol, 1,7,7,-trimethyl-, acetate {isobornyl acetate}	172a	174a, 174b
42.	87-69-4	Butanedioic acid, 2,3-dihydroxy- {*l*-tartaric acid}	172a, 2201, 2896,	174a, 174c
43.	7492-70-8	Butanoic acid, 2-butoxy-1-methyl-2-oxoethyl ester {butyl butyryl lactate}		603, 3370
44.	109-21-7	Butanoic acid, butyl ester {butyl butyrate}	172a	174a, 174b, 603, 3370

TABLE 25.30 (continued)
Pyrolysis of Nontobacco and Nontobacco Smoke Components and/or Their Effect on Smoke Composition When Added to Tobacco

	CAS No.	Name (per CA Collective Index)	References to: Pyrolysis of Individual Component	References to: Effect on MSS Composition, When Component Added in a Mixture
45.	106-29-6	Butanoic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl butyrate}	172a	174a, 174b, 603, 3370
46.	10094-34-5	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester {α,α-dimethylphenethyl butyrate}		603, 3370
47.	539-90-2	Butanoic acid, 2-methylpropyl ester {isobutyl butyrate}	172a	174a, 174b
48.	540-18-1	Butanoic acid, pentyl ester {amyl butyrate}	172a	174b, 603, 3370
49.	106-27-4	Butanoic acid, 3-methylbutyl ester {isoamyl butyrate}	172a	174a, 174b, 603, 3370
50.	10032-15-2	Butanoic acid, 2-methyl-, hexyl ester {hexyl 2-methylbutyrate}		603, 3370
51.	109-19-3	Butanoic acid, 3-methyl-, butyl ester {butyl isovalerate}	172a	174a, 174b, 603, 3370
52.	55066-56-3	Butanoic acid, 3-methyl-, 4-methylphenyl ester {*p*-tolyl 3-methylbutyrate}		1053
53.	16409-46-4	Butanoic acid, 3-methyl-, 5-methyl-2-(1-methylethyl)- cyclohexyl ester {menthyl isovalerate}	172a	174b
54.	103-52-6	Butanoic acid, phenylethyl ester {phenethyl butyrate}	172a	174a, 174b, 603, 3370
55.	104-20-1	2-Butanone, 4-(4-methyoxyphenyl)- {4-(*p*-methoxyphenyl)-2-butanone}	172a	174a, 174b
56.	10544-63-5	2-Butenoic acid, ethyl ester, (*E*)- {ethyl *trans*-2-butenoate}	172a	174a, 174b
57.	1504-55-8	3-Buten-2-ol, 4-phenyl- {4-phenyl-3-buten-2-ol}		1053
58.	76-69-6	3-Buten-2-one, 4-(2,5,6,6-tetramethyl-2-cyclohexen-1-yl)- {α-irone}	172a	174a, 174b
59.	3008-43-3	2,3-Cyclohexanedione, 1-methyl- {1-methyl-2,3-cyclohexadione}	172a	174a, 174b
60.	16409-45-3 89-48-5	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate {menthyl acetate}	172a	174a, 174b
61	38462-22-5	Cyclohexanone, 2-(1-mercapto-1-methylethyl)-5-methyl- {*p*-Mentha-8-thiol-3-one}	172a	174a, 174b
62.	491-07-6	Cyclohexanone, 2-methyl-5-(1-methylethyl)- {*dl*-isomenthone}	172a	174a, 174b
63.	495-62-5	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl- {bisabolene}		603, 3370
64.	586-62-9	Cyclohexene, 1-methyl-4-(methylethylidene)- {terpinolene}	172a	174a, 174b, 603, 3370
65.	2244-16-8	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)- {*d*-carvone}	172a	174a, 174b
66.	23747-48-0	5*H*-Cyclopenta[*b*]pyrazine, 6,7-dihydro-5-methyl- {5*H*-5-methyl-6,7-dihydrocyclopenta[*b*]pyrazine}	172a	174a, 174b
67.	21835-01-8	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- {3-ethyl-2-hydroxy-2-cyclopenten-1-one}	172a	174a, 174b
68.	110-40-7	Decanedioic acid, diethyl ester {diethyl sebacate}		603, 3370
69.	111-46-6	Ethanol, 2,2′-oxybis- {diethylene glycol}	2192, 2896	
70.	89-74-7	Ethanone, 1-(2,4-dimethylphenyl)- {2,4-dimethylacetophenone}		603, 3370
71.	24295-03-2	Ethanone, 1-(2-thiazolyl)- {2-acetylthiazole}	172a	174a, 174b, 603, 3370
72.	105-86-2	Formic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl formate}	172a	174a, 174b, 603, 3370
73.	33467-73-1	Formic acid, 3-hexenyl ester, (*E*)- {3-hexenyl formate, (*E*)-}	172a	174b
74.	638-49-3	Formic acid, pentyl ester {amyl formate}		603, 3370
75.	28664-35-9	2(3*H*)-Furanone, 2,5-dihydro-4,5-dimethyl-3-hydroxy- {4,5-dimethyl-3-hydroxy-2,5-dihydrofuran-2-one}	172a	174a, 174b
76.	104-67-6	2(3*H*)-Furanone, dihydro-5-heptyl- {γ-undecalactone}	172a	174a, 174b, 603, 3370
77.	2305-05-7	2(3*H*)-Furanone, dihydro-5-octyl- {γ-dodecalactone}	172a	174a, 174b, 603, 3370
78.	3658-77-3	3(2*H*)-Furanone, 2,5-dimethyl-4-hydroxy- {2,5-dimethyl-4-hydroxy-3(2*H*)-furanone}	172a	174a, 1974b, 603, 3370
79.	27538-09-6	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl- {3-ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone}	172a	174a, 174b
80.	698-10-2	2(5*H*)-Furanone, 5-ethyl-3-hydroxy-4-methyl- {5-ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone}	172a	174a, 174b, 603, 3370
81.	1405-86-3	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid(3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid, glycyrrhizin}	2896, 25A87	

(*continued*)

TABLE 25.30 (continued)
Pyrolysis of Nontobacco and Nontobacco Smoke Components and/or Their Effect on Smoke Composition When Added to Tobacco

	CAS No.	Name (per CA Collective Index)	References to: Pyrolysis of Individual Component	References to: Effect on MSS Composition, When Component Added in a Mixture
82.	106-30-9	Heptanoic acid, ethyl ester {ethyl heptanoate}	172a	174a, 174b, 603, 3370
83.	6728-31-0	4-Heptenal {4-heptenal}	172a	174b
84.	1119-44-4	3-Hepten-2-one {3-hepten-2-one}		603, 3370
85.	7779-50-2	ω-6-Hexadecenlactone {ω-6-Hexadecenlactone}	172a	174a, 174b, 603, 3370
86.	590-00-1 24634-61-5	2,4-Hexadienoic acid, potassium salt {potassium sorbate}	2208, 2896	174a, 174b, 603, 3370
87.	2198-61-0	Hexanoic acid, 3-methylbutyl ester {isoamyl hexanoate}	172a	174a, 603, 3370
88.	540-07-8	Hexanoic acid, pentyl ester {amyl hexanoate}	172a	174a, 174b
89.	3452-97-9	1-Hexanol, 3,5,5-trimethyl- {3,5,5-trimethyl-1-hexanol}	172a 3	174a, 174b
90.	21834-92-4	2-Hexenal, 5-methyl-2-phenyl- {5-methyl-2-phenyl-2-hexenal}		603, 3370
91.	13419-69-7	2-Hexenoic acid, (*E*)- {2-hexenoic acid, (*E*)-}	172a	174b, 603, 3370
92.	551-08-6	1(3*H*)-Isobenzofuranone, 3-butylidene {3-butylidenephthalide}		603, 3370
93.	17369-59-4	1(3*H*)-Isobenzofuranone, 3-propylidene {3-propylidenephthalide}	172a	174a, 174b, 603, 3370
94.	3738-00-9	Naphtho[2,1-*b*]furan, dodecahydro-3a,6,6,9a-tetramethyl- {ambroxide}	172a	174a, 174b
95.	7786-44-9	2,6-Nonadien-1-ol {2,6-nonadien-1-ol}	172a	174a, 174b
96.	31502-14-4	2-Nonen-1-ol {2-nonen-1-ol}	120	603, 3370
97.	141-12-8	2,6-Octadien-1-ol, 3,7-dimetyyl-, acetate, (*Z*)- {neryl acetate}	172a	174a, 174b
98.	107-75-5	Octanal, 3,7-dimethyl-7-hydroxy- {hydroxycitronellal}	172a	174a, 174b
99.	2035-99-6	Octanoic acid, 3-methylbutyl ester {isoamyl octanoate}	172a	174a, 174b
100.	502-47-6	6-Octenoic acid, 3,7-dimethyl- {3,7-dimethyl-6-octenoic acid}	172a	174a, 174b, 603, 3370
101.	6812-78-8 141-25-3	7-Octen-1-ol, 3,7-dimethyl- {rhodinol}	172a	174a, 174b, 603, 3370
102.	111-12-6	2-Octynoic acid, methyl ester methyl {2-octynoate}	172a	174a, 174b
103.	591-68-4	Pentanoic acid, butyl ester {butyl valerate}	172a	174a, 174b
104.	127-42-4	4-Penten-3-one, 5-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {methyl-α-ionone}	172a	174a, 174b
105.	94-86-0	Phenol, 2-ethoxy-5-(1-propenyl)- {5-propenylguaethol}	172a	174a, 174b, 603, 3370
106.	2785-89-9	Phenol, 4-ethyl-2-methoxy- {4-ethylguaiacol}		174a, 174b
107.	103-95-7	Propanal, 2-methyl-3-[4-(1-methylethyl)]phenyl- {2-methyl-(*p*-isopropylphenyl)-propionaldehyde, cyclamen aldehyde}	172a	174a, 174b
108.	105-53-3	Propanedioc acid, diethyl ester {diethyl malonate}	172a	174a, 174b
109.	866-84-2	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, potassium salt {potassium citrate}		174a, 174b
110.	68-04-2	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, sodium salt {sodium citrate}		174a, 174b
111.	26446-35-5	1,2,3-Propanetriol, monoacetate {monoacetin}	2206, 2896	
112.	102-76-1	1,2,3-Propanetriol, triacetate {triacetin}	172a, 2896	174a, 174b, 603, 3370
113.	105-68-0	Propanoic acid, 3-methylbutyl ester {isoamyl propionate}	172a	174a, 174b
114.	97-89-2	Propanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester {citronellyl isobutyrate}		603, 3370
115.	97-62-1	Propanoic acid, 2-methyl-, ethyl ester {ethyl isobutyrate}	172a	174a, 174b
116.	65416-14-0	Propanoic acid, 2-methyl-, 2-methyl-4-oxo-4*H*-pyran-3-yl ester {maltyl isobutyrate}		603, 3370
117.	103-93-5	Propanoic acid, 2-methyl-, 4-methylphenyl ester {*p*-tolyl isobutyrate}	172a	174a, 174b, 603, 3370
118.	78-35-3	Propanoic acid, 2-methyl-, 3,7-dimethyl-1,6-octadien-3-yl ester {linalyl isobutyrate}	172a	174a, 174b
119.	109-15-9	Propanoic acid, 2-methyl-, octyl ester {octlyl isobutyrate}		603, 3370
120.	103-48-0	Propanoic acid, 2-methyl-, phenylethyl ester {phenethyl isobutyrate}	172a	174a, 174b, 603, 3370
121.	103-28-6	Propanoic acid, 2-methyl-, phenylmethyl ester {benzyl isobutyrate}	172a	174a, 174b
122.	103-59-3	Propanoic acid, 2-methyl-, 3-phenyl-2-propenyl ester {cinnamyl isobutyrate}		174a, 174b

TABLE 25.30 (continued)
Pyrolysis of Nontobacco and Nontobacco Smoke Components and/or Their Effect on Smoke Composition When Added to Tobacco

			References to	
	CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Effect on MSS Composition, When Component Added in a Mixture
123.	13532-18-8	Propanoic acid, 3-(methylthio)-, methyl ester {methyl 3-methylthiopropionate}	172a	174a, 174b
124.	122-63-4	Propanoic acid, phenylmethyl ester {benzyl propionate}		603, 3370
125.	122-84-9	2-Propanone, 1-(4-methoxyphenyl)- {1-(*p*-methoxyphenyl)-2-propanone}	172a	174a, 174b
126.	122-40-7	2-Propenal, 3-phenyl-, α-pentyl- {α-amylcinnamaldehyde}	172a	174a, 174b
127.	499-12-7	1-Propene, 1,2,3-tricarboxylic acid {aconitic acid}	3486	603, 3370
128.	122-67-8	2-Propenoic acid, 3-phenyl-, 2-methylpropyl ester {isobutyl cinnamate}	172a	174a, 174b, 603, 3370
129.	103-53-7	2-Propenoic acid, 3-phenyl-, phenylethyl ester {phenethyl cinnamate}	172a	174a
130.	16409-43-1	Pyran, 4-methyl-2-(2-methylpropen-1-yl)-tetrahydro- {rose oxide}	172a	174a, 174b
131.	3301-94-8	2*H*-Pyran-2-one, 6-butyltetrahydro- {δ-nonalactone}	172a	174a, 174b
132.	713-95-1	2*H*-Pyran-2-one, 6-heptyltetrahydro- {δ-dodecalactone}	172a	174a, 174b, 603, 3370
133.	710-04-3	2*H*-Pyran-2-one, 6-hexyltetrahydro- {δ-undecalactone}	172a	174a, 174b
134.	823-22-3	2*H*-Pyran-2-one, 6-methyltetrahydro- {δ-hexalactone}	172a	174a, 174b
135.	2721-22-4	2*H*-Pyran-2-one, 6-nonyltetrahydro- {tetradecalactone}	172a	174a, 174b
136.	705-86-2	2*H*-Pyran-2-one, 6-pentyltetrahydro- {δ-decalactone}	172a	174b, 603, 3370
137.	2847-30-5	Pyrazine, 2-methoxy-3-methyl- {2-methyl-3-methoxypyrazine}	172a	174b, 603, 3370
138.	2882-22-6	Pyrazine, 2-methoxy-5-methyl- {2-methyl-5-methoxypyrazine}	172a	174b
139.	2882-21-5	Pyrazine, 2-methoxy-6-methyl- {2-methyl-6-methoxypyrazine}	172a	174b
140.	13708-12-8	Quinoxaline, 5-methyl- {5-methylquinoxaline}	172a	174a, 174b
141.	34413-35-9	Quinoxaline, 5,6,7,8-tetrahydro- {5,6,7,8-tetrahydroquinoxaline}	172a	174a, 174b
142.	110-27-0	Tetradecanoic acid, 1-methylkesthyl ester {isopropyl myristate}	172a	174a, 174b
143.	137-00-8	5-Thiazoleethanol, 4-methyl- {4-methyl-5-thiazole ethanol}	172a	174a, 174b

[a] The Doull et al. list (1053) does not include this item per se but does include glycyrrhizin, ammoniated (see Table 24.1, item No. 184).

TABLE 25.31
Pyrolysis of Miscellaneous Tobacco Product Components plus Their Effect on Smoke Composition When Added to Tobacco

		References to		
			Effect on MSS Composition, When Component Added	
CAS No.	Name (per CA Collective Index)	Pyrolysis of Individual Component	Individually	In a Mixture
	Cocoa	172b, 2896, 3447		174a, 174c, 603, 3370
	Hydrocarbons, aliphatic, tobacco-derived	2257, 3616	3269, 3291	
	Licorice	172b, 743, 1356, 2204, 2896		174a, 174c
	Phytosterols, tobacco-derived	4346		
	Polyphenol pigment, tobacco-derived	725a, 726		
	Tobacco	162, 163, 170, 171a, 172c, 276, 277, 369, 521, 522, 532, 536, 1357, 1651, 2071, 2072, 2196, 3190, 3468, 3616, 4150–4153, 4279, 4319, 4332, 25A35, 25A63		
	Tobacco extract	722, 3456, 3458, 3465–3467, 3470, 3472, 3616, 3877, 4355, 25A35		

TABLE 25.32
Summary of Tobacco Ingredient Studies from 1994 to 2005

Analysis	Date	Number of Ingredients Studied	Reported Findings/Conclusions	Reference
Detailed literature survey of ingredients added to U.S. tobacco products	1994	599	"…it was concluded that there was no evidence that any ingredient added to cigarette tobacco produces harmful effects under the conditions of use in cigarettes"	Doull et al. (1053)
Effect of added tobacco ingredients on cigarette MSS chemistry	2002	333	"The smoke chemistry data revealed changes towards both higher and lower amounts of various smoke constituents… This suggests that the addition of 333 commonly used ingredients to cigarettes in three groups did not add to the toxicity of the smoke, even at the exaggerated levels tested…" "An overall assessment of our data suggests that these ingredients, when added to the tobacco, do not add to the toxicity of smoke, even at the elevated levels used in this series of studies."	Carmines (603); Rustemeier et al. (3370)
	2002	482	"In most cases, the flavour mixtures had no statistically significant effect on the smoke yields relative to the control cigarette. In a few cases, the small increases or decreases were observed for some analytes relative to the control cigarette. The smoke yields of the experimental cigarettes were well within the ranges observed in the three reference cigarettes."	Baker and Smith (25A03)
	2004	482	"The significances of differences between the test and control cigarettes were determined using both the variability of the data on the specific occasion of the measurement, and also taking into account the long-term variability of the analytical measurements over the one-year period in which analyses were determined in the present study. This long-term variability was determined by measuring the levels of the 44 'Hoffmann analytes' in a reference cigarette on many occasions over the one-year period of this study." "…It was found that, in most cases, the mixtures of flavouring ingredients (generally added in parts per million levels) had no statistically significant effect on the analyte smoke yields relative to the control cigarette."	Baker et al. (174b)
Effect of added tobacco ingredients on cigarette MSS biology:	1997	≈152	"Although the mutagenic activities appeared to be similar, there were statistically significant differences in mutagenic activities among the sample."	Bioresearch [for RJRT] (25A09); Rodgman (3263, 3264)
(a) In vitro genotoxicity and cytotoxicity	2002		[*Note*: The differences were primarily due to the increase in mutagenicity of the CSC when the humectants (glycerol, propylene glycol) were not added to the cigarette tobacco and thus were not present as diluents in the CSC]	
	2002	333	"Within the sensitivity and specificity of the test systems, the in vitro mutagenicity and cytotoxicity of the cigarette smoke were not increased by the addition of the ingredients."	Carmines (603); Roemer et al. (25A49)
	2002	482	"The data has been analyzed and demonstrates no additional activity from the flavoured cigarettes above that of the control products."	Massey et al. (25A43)
(b) MSS inhalation	1997 2002	2 (Glycerol, propylene glycol)	"It was concluded that addition of the tested humectants singly or in combination had no meaningful effect on the site, extent or frequency of respiratory tract changes associated with smoke exposure in rats."	Gaworski et al. (25A27)

TABLE 25.32 (continued)
Summary of Tobacco Ingredient Studies from 1994 to 2005

Analysis	Date	Number of Ingredients Studied	Reported Findings/Conclusions	Reference
	1997	1 (Menthol)	"The results of this 13-week inhalation study indicated that the addition of 5000 ppm menthol to tobacco had no substantial effect on the character or extent of the biological responses normally associated with inhalation of mainstream cigarette smoke in rats."	Gaworski et al. (25A24)
	1998	170	"The results indicate that the addition of flavoring ingredients to cigarette tobacco had no discernible effect on the character or extent of the biologic responses normally associated with inhalation of mainstream cigarette smoke in rats."	Gaworski et al. (25A25)
	2002	333	"The data indicate that the addition of these 333 commonly used ingredients, added to cigarette in three groups, did not increase the inhalation toxicity of the smoke, even at the exaggerate levels used."	Carmines (603); Vanscheeuwijck et al. (25A79)
(c) Mainstream CSC and skin painting	1999	150	"While tumor incidence, latency and multiplicity data occasionally differed between test and comparative reference CSC groups, all effects appeared to be within normal variation for the model system. Furthermore, none of the changes appeared to be substantial enough to conclude that the tumor promotion capacity of CSC obtained from cigarettes containing cigarettes with ingredients was discernibly different from the CSC obtained from reference cigarettes containing tobacco processed without ingredients."	Gaworski et al. (25A26)
Pyrolysis of tobacco ingredients under conditions simulating those in the cigarette burning zone	2004	291	"The results are compatible with parallel studies in which the ingredients are added to tobacco and the effect on cigarette smoke constituents are measured. In general, the number of "Hoffmann analytes" detected among the pyrolysis products of the ingredients, and their levels, are low…Of the 291 tobacco ingredients pyrolysed, almost a third transfer out of the pyrolysis zone intact, and almost two thirds transfer at least 95% intact."	Baker and Bishop [see pp. 245–246 in (172a)]
	2005	159	"…a further 159 non-volatile and complex ingredients, as well as ingredient mixtures have been pyrolyzed…For the pyrolysis of many of the non-volatile ingredients, no 'Hoffmann analytes' were detected among the products."	Baker and Bishop (172b)

26 Carcinogens, Tumorigens, and Mutagens *vs.* Anticarcinogens, Inhibitors, and Antimutagens

26.1 CARCINOGENS, TUMORIGENS, AND MUTAGENS

In 1990, the U.S. Environmental Protection Agency (EPA) issued several draft documents in which it defined environmental tobacco smoke (ETS) as a carcinogen and designated it as a "group A carcinogen" (1148, 1148a). Subsequently, EPA issued a final report on this topic (1148b). Data from various epidemiological studies on the incidence of lung cancer in nonsmokers exposed to ETS were interpreted by the EPA as indicating that ETS was causally related to lung cancer in the ETS-exposed nonsmokers. In addition to these epidemiological data, EPA relied on data from studies on tobacco smoke composition, particularly the many studies dealing with the composition of mainstream smoke (MSS) as well as the smaller number of studies dealing with sidestream smoke (SSS) composition. Of the limited number of SSS components for which quantitative data have been obtained on per cigarette yields, many are delivered at higher per cigarette levels in SSS than in MSS. Many of the SSS components quantified are those that have been considered as contributors to respiratory tract or other disease problems, based upon results reported from laboratory animal experiments with individual compounds. EPA extrapolated these SSS (and MSS) qualitative and quantitative composition data directly to ETS with little regard for the profound quantitative differences between MSS and SSS composition and the highly diluted ETS system and the biological implications of these differences (3255, 3255a, 3257). Of prime concern to EPA were those MSS and SSS components which, in one biological system or other, had been described as tumorigenic at doses far in excess of those encountered in MSS or SSS (1148).

The cigarette MSS components of greatest concern to EPA were 35 MSS components listed by Hoffmann and Wynder (1808) in 1986, a list derived from the 1986 International Agency for Research on Cancer (IARC) monographs on tobacco smoking (1869, 1870) and expanded in 1990 to 43 MSS (and tobacco) components by Hoffmann and Hecht (1727). The Hoffmann and Hecht list was the first of many lists issued from 1990 through 2001 by Hoffmann et al. (1727, 1740, 1741, 1743, 1744, 1773), by the Occupational Safety and Health Administration (OSHA) in 1994 (2825), and by Fowles and Bates in 2001 (1217). These listings involved tobacco and tobacco smoke components previously reported to be tumorigenic, carcinogenic, or biologically active in various bioassays with individual components. The components of tobacco smoke were particularly emphasized (3265). Eventually, many of the listed MSS components, because of their multiple listings by Hoffmann et al., became defined as "Hoffmann analytes."

Table 26.1 is a tabulation of toxicants in tobacco and tobacco smoke from the IARC 1986 publication (1870) plus the seven lengthy publications coauthored from 1986 through 2001 by Hoffmann and his American Health Foundation colleagues (1727, 1740, 1741, 1743, 1744, 1773, 1808).

In their 1990 list, Hoffmann and Hecht (1727) classified 43 tobacco and/or tobacco smoke components as "tumorigenic agents in tobacco smoke." It is interesting to note that Hoffmann and Hecht used the term "tumorigenic" rather than "carcinogenic" to define the components. A similar list was issued by Hoffmann et al. (1773) in 1993. In 1994, OSHA (2825) tabulated 43 tobacco smoke components for which it claimed there was "sufficient evidence" of carcinogenicity in humans or animals. For some unknown reason, the OSHA list included only 42 items. Obviously, polonium-210 was inadvertently omitted. OSHA listed many of the same components as Hoffmann and Hecht but included several components not listed by Hoffmann and Hecht (1727) and vice versa.

In 1997, Hoffmann and Hoffmann (1740) classified 60 tobacco and/or tobacco smoke components as "carcinogens in tobacco and cigarette smoke." Several components listed by Hoffmann and Hecht but omitted by OSHA were also omitted by Hoffmann and Hoffmann. A major addition, accounting for much of the increase from 43 to 60, was the inclusion of the highly mutagenic *N*-heterocyclic amines.

EPA (1148) incorrectly assessed the health consequences with regard to lung cancer of the components in the Hoffmann–Hecht list by stating:

> Of the 99 compounds in tobacco smoke that have been studied in detail, at least 43 are complete carcinogens,* each able on its own to cause the development of cancer in humans or animals.

The EPA erred in its assessment of the 43 components in the Hoffmann–Hecht list since most have been shown not to be (1) tumorigenic to any human tissue or (2) tumorigenic to lung tissue in laboratory animals. These facts are addressed by comments from Hoffmann and Hecht in the text accompanying their tabulation. In addition, the few compounds that

* OSHA cited the U.S. Surgeon General's 1989 report (4012) which, in turn, reproduced the table subsequently presented in Hoffmann and Hecht (1727).

TABLE 26.1
Tumorigens, Carcinogens, and Toxicants Listed by Hoffmann et al.

Component	1986 IARC (1870)[a]	1986 Hoffmann and Wynder (1808)	1990 Hoffmann and Hecht (1727)	1993 Hoffmann et al. (1773)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)	2001 Hoffmann and Hoffmann (1743)	2001 Hoffmann et al. (1744)
Number of tumorigens and/or toxicants	52	35	43	43	60	70	68	69
PAHs								
B[*a*]A	20–70 ng 40–70 ng[b] 4–76 ng[c]	40–70 ng[d] 40–60 ng[e]	20–70 ng	20–70 ng	20–70 ng	20–70 ng	20–70 ng	20–70 ng
B[*e*]A	4–22 ng 30 ng[b]	30 ng[d]	4–22 ng	4–22 ng	4–22 ng	4–22 ng	4–22 ng	4–22 ng
B[*j*]A	6–21 ng 60 ng[b]	60 ng[d]	6–21 ng	6–21 ng	6–21 ng	6–21 ng	6–21 ng	6–21 ng
B[*k*]A	6–12 ng	NL[f]	6–12 ng	6–12 ng	6–12 ng	6–12 ng	6–12 ng	6–12 ng
B[*a*]P	20–40 ng 10–50 ng[b] 5–78 ng[c]	10–50 ng[d] 10–40 ng[g]	20–40 ng	20–40 ng	20–40 ng	20–40 ng	20–40 ng	20–40 ng
Chrysene	40–60 ng[b]	40–60 ng[d]	40–60 ng	40–60 ng	NL	NL	NL	NL
Chrysene, 5-methyl-	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng	0.6 ng
DB[*a,h*]A	4 ng	40 ng	4 ng	4 ng	4 ng	4 ng	4 ng	4 ng
NC	P[h], NYL[f]	NL[f]	NL	NL	NL	P, NYL[i]	P, NYL[i]	P, NYL[i]
DB[*b*]C	P[h], NYL[f]	NL[f]	NL	NL	NL	NL	NL	NL
DB[*a,i*]P	1.7–3.2 ng 2–3 ng[b] 17–32 ng[c]	NL	1.7–3.2 ng	1.7–3.2 ng	1.7–3.2 ng	NL[i]	NL[i]	NL[i]
DB[*d*]P[d]	P, NYL	P, NYL	P, NYL	P, NYL	P, NYL	1.7–3.2 ng[i]	1.7–3.2 ng[i]	1.7–3.2 ng[i]
Indeno[1,2,3-*cd*]pyrene	4–20 ng	4 ng	4–20 ng	4–20 ng	4–20 ng	4–20 ng	4–20 ng	4–20 ng
Aza-Arenes								
Pyridine	16–40 µg	NL	NL	NL	20–200 µg[j]	10–40 µg	20–200 µg[k] 16–40 µg[l]	20–200 µg[m]
Quinoline	NL[f]	NL	1–2 µg	0.2–1.3 g	1–2 µg	2–180 ng	1–2 ng[n]	1–2 µg[n]
Dibenz[*a,h*]acridine[o]	0.1 ng	0.1 ng[d]	0.1 ng	0.1 ng	0.1 ng	0.1 ng	0.1 ng	0.1 ng
Dibenz[*a,j*]acridine	2.7 ng 3–10 ng[b]	3–10 ng[d]	3–10 ng	3–10 ng	3–10 ng	3–10 ng	3–10 ng	3–10 ng
7*H*-Dibenzo[*c,g*]carbazole	0.7 ng	0.7 ng[d]	0.7 ng	0.7 ng	0.7 ng	0.9 ng	0.7 ng	0.7 ng
NNAs								
NDMA	2–20 ng 1–200 ng[b]	1–180 ng[o] 2–180 ng[e]	0.1–180 ng	0.1–180 ng	0.1–180 ng	2–180 ng	2–180 ng	2–1000 ng
N-Nitrosoethylmethylamine	0–2.7 ng 0.1–10 ng[b]	1–40 ng[o] 0,1–40 ng[e]	3–13 ng	3–13 ng	3–13 ng	3–13 ng	3–13 ng	3–13 ng
NDEA	0–2.8 ng 0–10 ng[b]	0.1–28 ng	0–25 ng	0–25 ng	0–2.8 ng	0–2.8 ng	0–2.8 ng	0–2.8 ng
N-Nitrosodi-*n*-propylamine	0–1 ng	0–1 ng	NL	NL	NL	0–1.0 ng	0–1.0 ng	0–1.0 ng

N-Nitrosodi-*n*-butylamine	0–3 ng	0–3 ng	NL	NL	NL	0–30 ng	0–30 ng	0–30 ng
NPYR	0–110 ng 2–42 ng[b]	2–110 ng[o] 2–42 ng[e]	1.5–110 ng	NL	3–60 ng	3–110 ng	3–110 ng	3–110 ng
NPIP	0–9 ng	0–9 ng	NL	NL	NL	0–9 ng	0–9 ng	0–9 ng
NDELA	0–36 ng 0–90 ng[b]	0–40 ng	0–36 ng	NL	0–68 ng	0–68 ng	0–68 ng	0–68 ng
NSAR	NL	NL	NL	NL	NYL	ND[f]	NL	NL
NNN	0.2–3.0 µg 0.13–0.25 µg[b]	0.12–3.7 µg	0.12–3.7 µg	0.12–3.7 µg	0.12–3.7 µg	120–3.700 ng[p]	0.12–3.7 µg[p]	0.12–3.7 µg[p]
NNK	0.08–0.77 µg 0.08–0.7 µg[b]	0.12–0.95 µg	0.08–0.77 µg	0.08–0.77 µg	0.08–0.77 µg	0.08–0.77 µg	0.08–0.77 µg	0.08–0.77 µg
NAB	0–150 ng 0–200 ng[b]	40–400 ng[o] 120 ng[e]	0.14–4.6 µg	0.14–4.6 µg	0.14–4.6 µg	0–150 ng	NL	NL
N′-Nitrosoanatabine	NL 0–3.7 µg[b]	NL	NL	NL	NL	NL	NL	NL
NMOR	NL	NL	ND[q] in MSS	ND in MSS	ND in MSS	ND in MSS	NL	NL
Aromatic Amines								
Aniline	NL	360 ng	360 ng	NL	NL	360–655 ng	360–655 ng[l]	NL
2-Toluidine	32–160 ng 30–200 ng[b]	30–160 ng	30–200 ng	30–200 ng	30–200 ng	30–337 ng	30–337 ng	30–337 ng
Aniline, 2,6-dimethyl-	NL	NL	NL	NL	NL	NL	4–50 µg[n]	4–50 ng[n]
1-Naphthylamine	NL 3–4 ng[b]	NL	NL	NL	NL	NL	NL	NL
2-Naphthylamine	1.7–22 ng 1–22 ng[b]	4.3–27 ng	1–22 ng	1–22 ng	1–22 ng	1–334 ng	1–334 ng	1–334 ng
Biphenyl, 3-amino	NL	NL	NL	NL	NL	NL	NL	NL
Biphenyl, 4-amino-	2.4–4.6 ng 2–5 ng[b]	2.4–4.6 ng	2–5 ng	2–5 ng	2–5 ng	2–5.6 ng	2–5.6 ng	2–5.6 ng
N-Heterocyclic Amines[q]								
A*a*C	NL	NL	NL	NL	25–260 ng	25–260 ng	25–260 ng	25–260 ng
MeA*a*C	NL	NL	NL	NL	2–37 ng	2–37 ng	NL	2–37 ng
Glu-P-1	NL	NL	NL	NL	0.37–0.89 ng	6.37[n]–0.89 ng	0.37[n]–0.89 ng	0.37–0.89 ng
Glu-P-2	NL	NL	NL	NL	0.25–0.88 ng	0.25–0.88 ng	0.25–0.88 ng	0.25–0.88 ng
PhIP	NL	NL	NL	NL	11–23 ng	11–23 ng	11–23 ng	11–23 ng
IQ	NL	NL	NL	NL	0.26 ng	0.3 ng	0.3 ng	0.3 ng
MeIQ	NL	NL	NL	NL	NL	NL	NL	NL
Trp-P-1	NL	NL	NL	NL	0.29–0.48 ng	0.3–0.5 ng	0.3–0.5 ng	0.3–0.5 ng
Trp-P-2	NL	NL	NL	NL	0.82–1.1 ng	0.8–1.1 ng	0.8–1.1 ng	0.8–1.1 ng
Aldehydes and Ketones								
Formaldehyde	70–100 µg 20–88 µg[b]	5–100 µg	70–100 µg	70–100 µg	70–100 µg[r] 20–100 µg[j]	70–100 µg	70–100 µg 20–100 µg[k]	70–100 µg[r] 20–100 µg[m]
Acetaldehyde	500–1200 µg 18–1400 µg[b]	500–1200 µg	18–1400 µg	18–1400 µg	18–1400 µg[r] 400–1400 µg[j]	500–1400 µg[s]	500–1400 µg[s] 400–1400 µg[k]	500–1400 µg[s] 400–1400 µg[m]

(*continued*)

TABLE 26.1 (continued)
Tumorigens, Carcinogens, and Toxicants Listed by Hoffmann et al.

Component	1986 IARC (1870)[a]	1986 Hoffmann and Wynder (1808)	1990 Hoffmann and Hecht (1727)	1993 Hoffmann et al. (1773)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)	2001 Hoffmann and Hoffmann (1743)	2001 Hoffmann et al. (1744)
Propionaldehyde	NL	NL	NL	NL	NL	NL	NL	NL
Butyraldehyde	NL	NL	NL	NL	NL	NL	NL	NL
Crotonaldehyde	10–20 µg	NL	10–20 µg	10–20 µg	NL	10–20 µg	NL	NL
Acrolein	60–100 µg 25–140 µg[b]	50–100 µg	NL	NL	60–140 µg[j]	60–140 µg	60–140 µg[k]	60–240 µg[m]
Acetone	100–250 µg	100–250 µg	NL	NL	100–650 µg[j]	NL	100–650 µg[k]	NL
2-Butanone	NL	NL	NL	NL	NL	NL	NL	NL
Volatile Hydrocarbons								
1,3-Butadiene	NL	NL	NL	NL	20–75 µg[r] 25–40 µg[j]	20–75 µg	20–75 µg 25–40 µg[k]	20–75 µg 25–40 µg[m]
Isoprene	NL	NL	NL	NL	450–1000 µg[r] 200–400 µg[j]	450–1.00 µg[s]	450–1000 µg[s] 200–400 µg[k]	450–1000 µg[s] 200–400 µg[m]
Benzene	20–50 µg	20–50 µg	12–48 µg	12–48 µg	12–70 µg[r] 6–70 µg[j]	20–70 µg	20–70 µg 12–50 µg[k]	20–70 µg 6–70 µg[m]
Toluene	NL	NL	NL	NL	5–90 µg[j]	NL	20–60 µg[k]	5–90 µg[m]
Styrene	10 µg	NL	NL	NL	10 µg	10 µg	10 µg	10 µg
Miscellaneous Organic Compounds								
Acetamide	38–56 µg[b]	NL	NL	NL	NL	38–56 µg	38–56 µg	38–56 µg
Acrylonitrile	3.2–15 µg[b]	3.2–15 µg	3.2–15 µg	3.2–15 µg	3.2–15 µg	3–15 µg	3–15 µg	3–15 µg
Acrylamide	NL	NL	NL	NL	P, NYL	P, NYL	P, NYL	P, NYL
Hydrazine, 1,1-dimethyl-	P, NYL	NL	P, NYL	P, NYL	NYL	P, NYL	P, NYL	P, NYL
Maleic hydrazide	NL	NL	NL	NL	NL	1.16 µg	1.16 µg[l]	
Methanol	NL	NL	NL	NL	80–180 µg[j]	100–250 µg	80–180 µg[k] 100–250 µg[l]	80–180 µg[m]
Methyl isocyanate	NL	NL	NL	NL	NL	1.5–5 µg	NL	NL
Nitromethane	NL	NL	NL	NL	NL	NL	0.3–0.6 µg	0.5–0.6 µg
2-Nitropropane	0.2–2.2 µg 0.73–1.21 µg[b]	0.2–2.2 µg	0.73–1.21 µg	0.73–1.21 µg	0.73–1.21 µg	0.2–2.2 µg	0.7–1.2 µg	0.7–1.2 µg
Nitrobenzene	NL	NL	NL	NL	NL	25 µg	25 µg	25 µg
Vinyl chloride	1.3–16 ng 1–16 ng[b]	1.3–16 ng	1–16 ng	1–16 ng	1–16 ng	11–15 ng	11–15 ng	11–15 ng
Ethyl carbamate	20–38 ng	20–38 ng	20–38 ng	20–38 ng	20–38 ng	20–38 ng	20–38 µg	20–38 µg

Ethylene oxide	NL	NL	NL	NL	7 µg	7 µg	7 µg	7 µg
Propylene oxide	NL	NL	NL	NL	NL	NL	12–100 ng	0–100 ng
Di(2-ethylhexyl) phthalate	NL	NL	NL	NL	20 µg	20 µg	NL	NL
Furan	NL	NL	NL	NL	18–30 µg[r] 20–40 µg[j]	18–30 ng[s]	18–37 ng[s]	18–37 µg[s]
Benzo[*b*]furan	NL	NL	NL	NL	P, NYL	P, NYL	P, NYL	P, NYL
Phenols								
Phenol	60–140 µg	60–140 µg	80–60	NL	NL	80–160 µg	80–160 µg[l]	60–180 µg[t]
o-Cresol	14–30 µg	NL	NL	NL	NL	NL	NL	NL
m-Cresol	NL	NL	NL	NL	NL	NL	NL	NL
p-Cresol	NL	NL	NL	NL	NL	NL	NL	NL
Catechol	40–350 µg	25–360 µg[d] 100–350 µg[g] 140–500 µg[e]	200–400 µg	NL	NL	200–400 µg	100–360 µg 200–400 µg[l]	90–2000 µg 100–200 µg[t]
Resorcinol	8–80 µg[b]	NL	NL	NL	NL	NL	NL	NL
Hydroquinone	88–155 µg[b]	110–300 µg	NL	NL	NL	NL	NL	NL
Methyleugenol	NL	NL	NL	NL	NL	20 ng	20 ng	20 ng
Caffeic acid	NL	NL	NL	NL	NL	NL	<3 µg	<3 µg
Chloroaromatic Compounds								
DDT	NL 0.7–1.2 µg[b]	NL	NL	NL	800–1200 ng	800–1.200 ng[s]	800–1200 µg	800–1200 µg
DDE	NL	NL	NL	NL	200–370 ng	200–370 ng	200–370 µg	200–370 µg
Polychlorodibenzo-*p*-dioxins	NL	NL	NL	NL	NL	NL	NL	NL
Polychlorodibenzofurans	NL	NL	NL	NL	NL	NL	NL	NL
Inorganic Components								
Hydrazine	24–43 ng	24–43 ng	24–43 ng	24–43 ng	24–43 ng	24–34 µg[n]	24–43 ng[n]	24–43 ng
Hydrogen sulfide	NL	NL	NL	NL	20–90 µg[j]	10–90 µg	20–90 µg[k]	20–90 µg[m]
Arsenic	1–25 µg	NL	40–120 ng	40–120 ng	40–120 ng	40–120 ng	40–120 µg	40–120 µg
Beryllium	NL	NL	NL	NL	NL	0.3 µg	0.5 ng	0.5 ng
Cadmium	9–70 ng	NL	41–62 ng	41–62 ng	41–62 ng	NL	7–350 ng	7–350 ng
Chromium VI	4–70 ng	NL	4–70 ng	4–70 ng	4–70 ng	4–70 ng	4–70 ng	4–70 ng
Cobalt	0.2 ng	NL	NL	NL	NL	0.13–0.2 ng	0.13–0.2 ng	0.13–0.2 ng
Nickel	0–600 ng[b]	20–3000 ng	0–600 ng	0–600 ng	0–600 ng	0–600 ng	0–600 ng	0–600 ng
Mercury	NL	NL	NL	NL	NL	4 ng	NL	
Lead	P[c]	NL	35–85 ng	35–85 ng	35–85 ng	34–85 ng	34–85 ng	34–85 ng
Polonium-210	0.03 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi	0.03–1.0 pCi
Selenium	P[c]	NL	NL	NL	NL	NL	NL	NL

(*continued*)

TABLE 26.1 (continued)
Tumorigens, Carcinogens, and Toxicants Listed by Hoffmann et al.

Component	1986 IARC (1870)[a]	1986 Hoffmann and Wynder (1808)	1990 Hoffmann and Hecht (1727)	1993 Hoffmann et al. (1773)	1997 Hoffmann and Hoffmann (1740)	1998 Hoffmann and Hoffmann (1741)	2001 Hoffmann and Hoffmann (1743)	2001 Hoffmann et al. (1744)
Additional Components								
Nicotine	1.0–2.3 mg	1–2.5 mg	1.0–3.0 mg	NL	0.1–3.0 mg[u]	1.0–3.0 mg	1.0–3.0 mg[v]	0.1–3.0 mg[t]
Carbon monoxide	10–23 mg	10–23 mg	NL	NL	14–23 mg[j]	10–23 mg	14–23 mg[k]	14–23 mg[m]
Ammonia	50–130 µg	50–170 µg[g] 50–130 µg[e]	NL	NL	10–130 µg[j]	10–130 µg	10–130 µg[k]	10–130 µg[m]
Nitrogen oxides	100–600 µg	50–600 µg	NL	NL	100–600 µg[j]	100–600 µg	100–600 µg[k]	100–600 µg[m]
Hydrogen cyanide	400–500 µg	400–500 µg	NL	NL	400–500 µg[j]	400–500 µg	400–500 µg[k]	400–500 µg[m]

[a] See Table 19 in (1870).
[b] See Appendix 2 in (1870).
[c] See Table 20 in (1870).
[d] See Table 5 in (1808).
[e] See Table 13 in (1808).
[f] NL, not listed; NYL, no per cigarette MSS yield listed; ND, not detected.
[g] See Table 11 in (1808).
[h] P, present, as listed in Appendix 2 in (1870).
[i] The yield range listed for dibenz[*a,l*]pyrene is incorrect. It is the range usually listed for dibenzo[*a,i*]pyrene. The P, NYL designation should also apply to dibenzo[*a,l*]pyrene.
[j] See Table 1 in (1740).
[k] See Table 5-1 in (1743).
[l] See Table 5-3 in (1743).
[m] See Table 2 in (1744).
[n] Compare yields listed in Tables in (1741, 1743, 1744).
[o] See Table 6 in (1808).
[p] Compare yield listed in Table 1 in (1741) with those listed in (1727, 1740, 1743, 1744).
[q] A*a*C, 2-amino-9*H*-pyrido[2,3-*b*]indole; MeA*a*C, 2-amino-3-methyl-9*H*-pyrido[2,3-*b*]indole; Glu-P-1, 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole; Glu-P-2, 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole; PhIP, 2-amino-1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridine; IQ, 2-amino-3-methyl-3*H*-imidazo[4,5-*f*]quinoline; MeIQ, 2-amino-3,4-dimethyl-3*H*-imidazo[4,5-*f*]quinoline; Trp-P-1, 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole; Trp-P-2, 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole.
[r] See Table 3 in (1740).
[s] Compare yield listed in Table 1 in (1741), Table 5-4 in (1743), and Table 4 in (1744).
[t] See Table 3 in (1744).
[u] See Table 2 in (1740).
[v] See Table 5-2 in (1743).

have been reported to produce tumors in laboratory animals have done so at dose levels far in excess of those encountered in MSS, SSS, or ETS.

Careful examination of the Hoffmann–Hecht list reveals significant flaws which, if they had been considered at all by the EPA, would have profoundly affected its conclusions concerning ETS. It has been known for over five decades that classifying a substance as "tumorigenic" or "carcinogenic" can be misleading. These terms should not be misinterpreted or overinterpreted. Users of tables with headings "tumorigenic" or "carcinogenic" must be aware of the meaning and limitations of the terms "tumorigenicity" and "carcinogenicity" when applied to specific compounds or elements.

The misunderstanding and misinterpretation of these terms are not new. The term "carcinogenesis" and by extension derivative terms were defined precisely as early as 1923, and its original definition is still listed in various medical dictionaries: *Carcinogenesis is the process whereby a carcinoma is generated*. In the 27th edition (1051c) of Dorland's medical dictionary, this definition of carcinogenesis is the same as that listed in the 13th edition (1051b). Some investigators incorrectly use the term "carcinogenesis" for the production of any tumor type not just a carcinoma. The correct term, if used in this manner, is "tumorigenesis." The term "carcinogen" is often applied, again often incorrectly, to any factor that induces any type of tumor. Common in the past, but seldom used now, was the term "sarcogenesis" used to describe sarcoma production, the end point in studies in which a compound injected subcutaneously induced a sarcoma.

Within 25 years of the first successful experiments to produce tumors in animals by skin painting with solutions of coal tar by Yamagiwa and Ichikawa (4361) and within a decade of the first successful skin-tumor inductions with pure compounds such as dibenz[*a,h*]anthracene (DB[*a,h*]A) [Kennaway and Hieger (2078)] and benzo[*a*]pyrene (B[*a*]P) [Cook et al. (796a, 797), Barry et al. (194)], the misuse and misunderstanding of the term "carcinogenicity" had reached such proportions that Shear, an outstanding and highly regarded U.S. investigator of chemical carcinogenesis, was invited to put the term in perspective. In 1941, Shear and Leiter (3627) published an article in which their admonitions regarding overinterpretation of these terms are as significant today as they were then:

> The term 'carcinogenic potency' … is not to be considered as an invariable property inherent in a compound but is merely a summary of the results of particular experiments and is valid only for animals of the species, strain, sex, age, diet, etc., of the particular animal employed as well as the dose, menstruum, mode and site of application, etc., of the compound in question … Conclusions regarding the potency of any given compounds should therefore be interpreted in the light of the data upon which they are based.

In 1951, Hartwell compiled the 2nd edition (1544) of his survey on compounds tested for carcinogenicity since the demonstrated carcinogenicity of DB[*a,h*]A and B[*a*]P in mouse-skin-painting experiments. To further the understanding of the terms "carcinogen" and "carcinogenicity" and to minimize their future misuse, Hartwell quoted liberally from the Shear–Leiter publication. He added several important points, one of which was the following: There is a tendency on the part of some to consider carcinogenicity or lack of carcinogenicity as characteristic properties of chemical compounds. In other words, some researchers treat carcinogenicity as a fixed property of a compound. This is not a valid approach to thinking about "carcinogens." Carcinogenicity is a variable property, depending on a number of factors. It differs from other properties of a compound that are fixed, e.g., melting point, boiling point, refractive index, specific gravity, crystalline form. As noted by Shear and Leiter (3627), by Hartwell (1544), and by many others, a substance or factor can show a range from carcinogenicity to noncarcinogenicity to anticarcinogenicity, and the response will differ in the laboratory depending on the animal used (species, strain, sex, age), route of administration (inhalation, ingestion, injection [subcutaneous, intravenous, intraperitoneal], skin painting, douching), mode of administration (single *vs*. multiple doses, neat, in solution, as an aerosol or as a vapor), diet supplied to the animals, and cage care.

Hartwell also cautioned:

> Another pitfall is the attempt to carry over, without reservation, to man, conclusions based on animal experiments. We do not know whether man is more or less susceptible than mice to particular carcinogens. Some animal species, such as the rat, rabbit, and dog are much more resistant than is the mouse, and vice versa, while in the monkey none of the powerful carcinogens has been shown to produce tumors.

From an examination of Table 26.1, it is obvious that several classes of components account for the greatest number of tumorigens classified as significant in tobacco smoke. Further examination of the number of references cited for each of them in the pertinent chapters of this book indicates the magnitude of the research conducted on each class both within and outside the tobacco industry since the early 1950s. Sequentially, polycyclic aromatic hydrocarbons (PAHs), azaarenes, *N*-nitrosamines (NNAs), and *N*-heterocyclic amines in tobacco smoke have attracted much attention on their identification, quantitation, precursors, and reduction or elimination. Tumorigenic components in these four classes account for nearly 60% of the total listed. The following pages contain brief descriptions of the history and chronology of the four classes of tobacco smoke components.

The components listed in Table 26.1 and by Osha (2825) and Fowles and Bates (1217) raise numerous questions as to why many of them were included. First, attempts to attribute the "carcinogenicity" of cigarette MSS to a particular component are questionable. Scores of citations over the past five decades have been issued by eminent scientists and health organizations in which it is stated that no single MSS component or class of components acting either individually or in concert can explain observations in human smokers or in laboratory animals treated with heroic doses of MSS. For example, comments on B[*a*]P in particular or other tumorigenic PAHs in general include

those by Cook (793) [cf. (796a, 797)] who wrote the following about B[*a*]P in cigarette smoke:

> The tarry condensates of the smoke obtained by smoking cigarettes in machines … have 3,4-benzpyrene, but the amount is exceedingly small and there is considerable doubt about whether the concentration is high enough to produce carcinogenic action.

In 1981, the U.S. Surgeon General [see p. 36 in (4009)] stated:

> The contribution of BaP or PAH in general to mouse skin carcinogenesis by cigarette smoke condensate cannot be fully measured at this time … In the smoking and health program of the National Cancer Institute … no significant dependence of carcinogenic potency on BaP content was observed.

The American Association for Cancer Research (26A02) in its 1984 position paper on smoking wrote:

> Studies have presented the profile of the known carcinogens in tobacco. At present, there is no direct method to assign priority to any of these substances as putative causal agents in human lung cancer.

That year, Peto and Doll (26A127) stated the following: But 30 years of laboratory research has yet to identify reliably the important carcinogenic factors in cigarette smoke.

The U.S. Surgeon General [see p. 200 in (4010)], on the subject of NNAs in tobacco smoke, stated:

> There is lack of direct evidence that these compounds are also human carcinogens. This was also the view of Magee who first demonstrated the tumorigenicity of *N*-nitrosamines in laboratory animals. In 1983, Magee (26A89) noted: A role for nitrosamines in the causation of human cancer has not been established.

On the basis of the data available, the aromatic amines, including β-naphthylamine, were discounted in the U.S. Surgeon General's 1981 and 1982 reports:

> The presence of β-naphthylamine in cigarette smoke has been demonstrated [Hoffmann et al. (1747)], along with other carcinogenic aromatic amines [Patrianakos et al. (2900)]. The yield was so low that [the researchers] did not believe these agents contributed significantly to the risk of bladder cancer in smokers [see p. 41 in (4009)].

> On the basis of quantitative data for aromatic amines in cigarette smoke, an etiological significance of these traces of carcinogenic amines in bladder cancer is questionable, even if one were to consider the total of the aromatic amines and their metabolites [see pp. 207–208 in (4010)].

Similar comments about other components on the various lists have been published: arsenic (4010), nickel (4010), polonium-210 (4009, 4010), and benzene (4005).

Many of these MSS and/or tobacco components should be excluded from the lists on the basis of explicit comments in the literature by numerous knowledgeable authorities on their tumorigenicity to laboratory animals at levels determined in MSS, their lack of tumorigenicity in most instances on inhalation, and the equivocal evidence showing their tumorigenicity in humans at levels in MSS. All but 4 of the 43 components have never produced respiratory tract tumors in laboratory animals exposed to the component via inhalation. Many have never been tested in an inhalation system, and one component of great interest (B[*a*]P) has only produced lung carcinoma via inhalation in animals at an extraordinarily massive dose.

The following situation should not be overlooked: the MSS yield determined two, three, or four decades ago for a component is not relevant to the MSS yield found by analysis for the component from more recent or current cigarettes. For example, MSS values for dibenz[*a,h*]acridine and 7*H*-dibenzo[*c,g*]carbazole were obtained with 1959–1960 cigarettes, MSS values for dibenz[*a,j*]acridine from 1959 to 1960 and from 1963 cigarettes, the MSS value for DB[*a,h*]A is from 1963 cigarettes, the MSS value for 5-methylchrysene (5-MeC) is from 1973 cigarettes, and the MSS value for *N*-nitrosodiethanolamine (NDELA) is from commercial cigarettes manufactured in or before 1981. It is well recognized, as indicated in Figure 26.1, that the variety of cigarette design technologies (efficient filtration, filter-tip additives, processed tobacco materials [reconstituted tobacco sheet, RTS, expanded tobaccos], air dilution [porous paper, filter-tip perforations], and paper additives) has progressively reduced the sales-weighted average MSS total particulate matter (TPM) by almost 70% from 40 mg/cig in the early 1950s to less than 12 mg/cig in the late 1980s. These eight cigarette design technologies have been defined, even by various opponents of cigarette smoking, as significant in the design of a "less hazardous" cigarette [Wynder and Hoffmann (4319, 4332), USPHS (4005, 4009), Gori (1333), Hoffmann and Hoffmann (1740, 1743, 1744)].

At the same time that the reduction of delivery of MSS TPM was accomplished, the composition of the MSS was altered. For example, for MSS TPM, the B[*a*]P content—expressed as ng B[*a*]P/mg TPM—has decreased about 33% (from 1.2 to 0.8 ng/mg TPM) during the same time period. The U.S. Surgeon General in his 1979 report (4005) summarized the B[*a*]P data for a commercial cigarette sold in the United States from 1954 to 1979.

As noted by Rodgman and Green (3300), Gold et al., colleagues of Ames, as recently as 1998, questioned the extrapolation of laboratory animal tumorigenesis data generated by the use of a maximum tolerated dose (MTD) to a human situation. They stated (1318a):

> Extrapolation of cancer potency results from MTD studies to real-life exposures is not scientifically supportable.

From these considerations and the information presented later, it is obvious that many of the components could and should be removed from the various Hoffmann et al. lists that subsequently led to the "Hoffmann analyte" phenomenon.

In its 1994 report on indoor air quality, OSHA (2825) dealt at some length with ETS. It presented a list of 43 tobacco smoke components for which it claimed "there is 'sufficient evidence' of carcinogenicity in humans or animals." Comparison of the OSHA list with that of Hoffmann–Hecht (Table 26.1) reveals

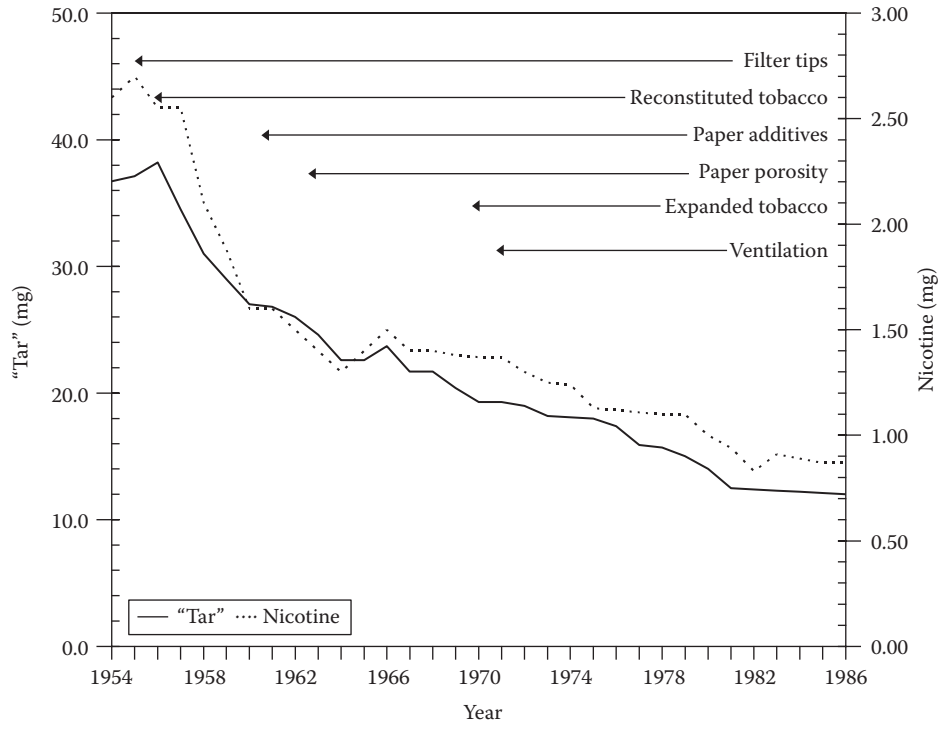


FIGURE 26.1 "Tar" and nicotine deliveries, sales-weighted average basis.

numerous similarities plus some differences. OSHA (2825) described 10 of its listed 43 tobacco smoke "carcinogens" in the following less-than-positive terms:

Formaldehyde	*Probable* human carcinogen
N-Nitrosodimethylamine (NDMA)	*Probable* human carcinogen
N-Nitrosodiethylamine (NDEA)	*Probable* human carcinogen
N-Nitrosopyrrolidine (NPYR)	*Probable* human carcinogen
2-Toluidine	Listed only as an irritant, *not as a carcinogen*
Benz[*a*]anthracene (B[*a*]A)	*Listed only* as an animal carcinogen
N′-Nitrosonornicotine (NNN)	*Listed only* as an animal carcinogen
4-(*N*-Methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK)	*No relevant information available* on health effects
NDELA	*Probable* human carcinogen
Cadmium	*Probable* human carcinogen

Despite these and other equivocal statements, OSHA stated with great certainty:

> The corroborative evidence of the carcinogenic activity of tobacco smoke provided by animal bioassays and in vitro studies and the chemical similarity between mainstream smoke and ETS clearly establish the plausibility that ETS is … a human lung carcinogen …

Of the components in the various lists, the four classes of tobacco smoke components investigated in greatest detail during the past five decades were the PAHs, aza-arenes, NNAs, and the *N*-heterocyclic amines. Because of the wealth of background information available on PAHs demonstrated to be tumorigenic in laboratory animals, extensive research (isolation, identification, quantitation, precursors, removal, prevention of formation, etc.) was conducted in the 1950s and 1960s on this compound class in tobacco smoke. The reason for selection of this class of compounds was obvious.

It has been estimated that more research funds were expended since the 1930s on the study of tumorigenic PAHs in general (and B[*a*]P in particular) than on any other class of compounds. The results of thousands of investigations on PAHs (their synthesis, biological properties [tumorigenicity, mutagenicity], metabolism, sources [air pollutants, industrial oils and tars, tobacco smoke, foodstuffs, beverages, etc.], isolation, quantitation, reduction, etc.) have been published. Similar studies, but to a much lesser degree, have been conducted on the aza-arenes. Since the early 1950s, over 500 PAHs and slightly fewer than 300 aza-arenes have been reported as tobacco smoke components. The per cigarette yields of most of the PAHs and aza-arenes are in the subnanogram range.

In the early 1950s, the discovery of the tumorigenicity by Barnes and Magee (192) of an NNA in laboratory animals initiated a flurry of research on the NNAs, initially in foodstuffs and subsequently (mid-1960s) in tobacco smoke. In contrast to the great number of PAHs and aza-arenes identified in tobacco smoke, fewer than 70 NNAs have been identified in tobacco and/or tobacco smoke to date (see Table 15.8). In the mid-1970s, Japanese investigators in their investigations of various cooked foodstuffs reported the isolation and identification of several *N*-heterocyclic amines derived pyrogenetically from amino acids and proteins [Sugimura et al. (3829, 3829a), Sugimura (3828b, 3828c)]. Subsequently, several of the *N*-heterocyclic amines were reported to possess inordinately high mutagenicities in the Ames test with

Salmonella typhimurium, be tumorigenic in the mouse-skin-painting bioassay, and to be present in cigarette smoke condensate (CSC) at low nanogram or subnanogram levels [Sato et al. (3415a), Yamashita et al. (4367, 4368)]. Fewer than a dozen of the highly mutagenic *N*-heterocyclic amines have been reported as CSC components.

26.1.1 Polycyclic Aromatic Hydrocarbons

In the case of the PAHs in general and the 13 specific PAHs listed in Table 26.1, many of the assertions about them in tobacco smoke since the early 1950s have either been shown to be incorrect or, in several instances, highly equivocal.

Several sources of PAHs in cigarette MSS, originally considered to be the major sources of the PAHs, were shown to be either incorrect (effluents from lighting source [matches, butane- or hexane-fueled lighters]) or insignificant (PAH-containing air pollutants deposited on the surface of the tobacco leaf during growing, harvesting, and curing) or primarily derived from cigarette paper combustion.

Long-chained saturated hydrocarbons (SHCs) were originally defined as the major precursors in tobacco of PAHs in tobacco smoke. Subsequently, it was shown that the contributions of tobacco terpenes and phytosterols to the levels of MSS or SSS PAHs exceeded those of the SHCs.

In the mid- to late 1950s, it was proposed (3241, 3242) that the per cigarette yields of MSS PAHs would be diminished by removal of SHCs, phytosterols, and terpenes from the tobacco by extraction with nonpolar solvents such as hexane, a process dubbed the "dry cleaning" of tobacco.* It was proposed that the reduced MSS PAH level in the CSC from cigarettes fabricated with extracted tobacco would be accompanied by reduced tumorigenicity to mouse skin of the extracted tobacco CSC [Wynder and Wright (4354)]. In 1982, Brunnemann and Hoffmann, members of a research group that formerly proposed removal of waxlike compounds considered to be the precursors of the PAHs in smoke, advocated addition of such compounds to tobacco (480).

Also in the late 1950s, it was proposed to use high-nitrate tobacco in the tobacco blend or add nitrate to the blend to modify the combustion process during smoking to decrease the MSS PAH yields [Hoffmann and Wynder (1797, 1798)]. In direct contrast was a 1982 proposal: Because of the involvement of nitrate and nitrogen oxides generated from it in the pyrogenesis of NNAs, use low-nitrate tobaccos in the blend or remove the nitrate from tobacco as a means to control NNAs in MSS (and SSS) (480).

* The concept of extraction of tobacco with an organic solvent to remove PAH precursors was not new. Roffo (3327) reported that extraction of tobacco with organic solvents such as ethyl alcohol, chloroform, acetone, petroleum ether, paraffin hydrocarbons, or benzene resulted in a reduction of the tumorigenicity of the tar generated by destructive distillation of the extracted tobacco compared to the tar generated by destructive distillation of the unextracted (control) tobacco. Roffo did not study the smokes from cigarettes fabricated with the extracted and unextracted tobaccos. Roffo suggested that the extraction removed the phytosterols from the tobacco which he considered the major precursor of the PAHs in the destructive distillate and in tobacco smoke.

The proposal that high-molecular-weight PAHs, including B[*a*]P, could be removed from MSS by selective filtration was shown to be incorrect. Selective filtration from MSS is possible only with compounds that have an appreciable vapor pressure, i.e., they are found in both the particulate and vapor phases of MSS. For example, the low-molecular-weight phenols and the volatile NNAs are sufficiently volatile to be selectively filtered from MSS, but the vapor pressures of most PAHs of interest (B[*a*]P, DB[*a,h*]A, B[*a*]A) are too low for selective filtration to be effective.

B[*a*]P in MSS was proposed as an "indicator" of (1) the tumorigenicity of mainstream CSC to mouse skin, (2) the levels of PAHs with four or more rings, and (3) the levels of tumorigenic PAHs. In none of these cases is the level of B[*a*]P a valid "indicator." (Similarly, phenol, proposed as an "indicator" of the level of low-molecular-weight promoting phenols in cigarette MSS, was shown not to be a valid "indicator.")

Assertions that the probability was extremely low that alkylated PAHs (methyl- and dimethyl-PAHs) would occur in tobacco smoke were demonstrated to be incorrect. Subsequently, even polyalkylated PAHs such as pentamethyl- and hexamethyl-PAHs were identified in tobacco smoke, their major precursor being the high-molecular-weight tobacco terpenes such as solanesol [Snook et al. (3757)].

Assertions that cyclopentabenzanthracenes could not occur in tobacco smoke were incorrect. Numerous cyclopentabenzanthracenes were identified in MSS, their major precursor being the phytosterols [Snook et al. (3736, 3756, 3758, 3759)].

PAHs in tobacco smoke are formed by either (1) a degradation-combination mechanism or (2) an aromatization mechanism involving a single molecule. Studies showed that both mechanisms are operative.

To bolster several arguments concerning PAHs in MSS, it was incorrectly asserted by some investigators that the fate of an individual tobacco component during experimental pyrolysis in an inert atmosphere and at a temperature approximating that of the cigarette coal was the same as its fate in the tobacco matrix during the cigarette smoking process. This assertion was shown to be incorrect by several investigators, including Schmeltz et al. (3512), members of the same group that originally proposed the equivalency of the fate of tobacco components during pyrolysis and the smoking process.

The tumorigenicity of CSC to mouse skin is due to its content of PAHs with four or more fused rings. Even though it was claimed that the PAHs are the only initiators in CSC, the levels and tumorigenicities of the PAHs in CSC accounted for no more than 2%–2.5% of the observed tumorigenic response in mouse or other rodent-skin-painting bioassays.

With so many incorrect or equivocal assertions about the MSS PAHs issued by antitobacco smoking investigators over the last four decades (see Table 26.2), it was somewhat surprising that either OSHA or EPA was so willing to accept the premise that the 13 PAHs in the Hoffmann–Hecht and/or the OSHA lists contributed significantly to the alleged tumorigenic effects of MSS and ETS in the respiratory tract of active and passive smokers, respectively.

TABLE 26.2
PAH Paradoxes

Assertion	Contradiction
Major source of PAHs in cigarette MSS is the lighting source (match, flammable fuel-charged lighter, gas burner in laboratory)	The PAH level in cigarette MSS was independent of lighting source: Cigarettes lit by an electric lighter gave the same PAH levels as those lit by matches, fuel-charged cigarette lighters, or a gas flame
Because bulk pyrolysis of cigarette paper yielded PAHs, cigarette paper (representing about 5% of the cigarette weight) was defined as the major source of PAHs in cigarette MSS [Cooper et al. (817), Cardon et al. (594)]	Comparison of PAH yields, including B[*a*]P, produced by bulk pyrolysis of cigarette paper *vs*. pyrolysis of the paper in a cylindrical form approximating its configuration in the cigarette revealed that the cylindrical configuration combustion produced very little PAHs (or B[*a*]P) *vs*. bulk pyrolysis [Wright (4281)]
PAHs in cigarette MSS are the result of transfer of PAHs from the surface of air-pollutant-contaminated tobacco to MSS	MSS PAH level was not due to transfer of contaminant PAHs transfer from the tobacco rod to smoke: B[*a*]P injected into the tobacco rod produced very little increase in the MSS B[*a*]P level. Most of the injected B[*a*]P was destroyed during smoking process
Since none of the factors noted earlier (means of cigarette lighting, cigarette paper, air pollutant contamination) were the source of PAHs in cigarette MSS, the source must be one or more of the tobacco components. However, even in 1957, the presence of B[*a*]P in tobacco smoke was questioned [cf. Fieser (1181)]	Because the fragmentary evidence presented, the presence of PAHs, particularly B[*a*]P, in tobacco smoke was questioned by such noted PAH experts as Fieser (1181) whose colleagues identified B[*a*]P in roasted coffee beans but were unable to identify it in tobacco smoke. Eventually, because of the isolation by Hoffmann of B[*a*]P in crystalline form from cigarette MSS (4307), its presence in MSS became universally accepted
According to Wynder and Hoffmann, PAHs in cigarette smoke were the only major tumor initiators in mouse-skin carcinogenesis (4332): "The many detailed data obtained in studies of tobacco carcinogenesis on mouse skin exclude with some certainty that major tumor initiators other than the PAH type play a role in this assay system."	Mouse-skin-painting studies with B[*a*]P solutions at concentrations much in excess of that in CSC produced no skin carcinomas in rabbits or mice
B[*a*]P, because of its potency in skin-tumor carcinogenesis and level in MSS, was considered the major PAH of concern in tobacco smoke. In the 1981 Surgeon General's report (4009), it is stated: "Benzo[*a*]pyrene] appears to be the most important single member of this class of compounds [the PAHs], taking into consideration both its concentration and its relative carcinogenic potency."	[Wynder et al. (4351), Warshawsky et al. (26A180)]. Similarly, use of more reasonable doses of CSC in skin-painting studies instead of the massive doses usually used resulted in neither papilloma nor carcinoma formation [Wynder et al. (4351), Gori (1329, 1330, 1332, 1333), NCI (2683)].
Initially, Fieser did not believe the evidence was sufficient to demonstrate that B[*a*]P was present in tobacco smoke. He stated that if B[*a*]P were present, its precursor would be tobacco cellulose (1181)	Subsequent studies indicated the major precursors in tobacco of PAHs in its smoke were not cellulose and lignin but were the lipophilic tobacco components. Rodgman and Cook (3269, 3286, 3291) and Severson et al. (3616) reported that terpenoids, phytosterols, and SHCs were PAH precursors
Removal of lipophilic PAH precursors from tobacco by solvent extraction reduced the MSS PAH levels and the tumorigenicity (mouse-skin-painting) of the CSC [Wynder (4294), Wright (4282), Wynder and Wright (4354)]. This led to recommendations to remove the lipophilic tobacco components. Later, Wynder et al. (4332) minimized the effectiveness of the removal of the lipophilic tobacco components. Wynder and Hoffmann (4310) defined tobacco extraction as "impractical both technically and economically." Wynder and Hecht (4306d) and the Surgeon General (4005) described tobacco extraction as "of academic interest." Eventually, Wynder's colleagues recommended addition of lipophilic compounds, e.g., *n*-hentriacontane, to tobacc*o* (480) to offset effect of nitrate-derived NO_x in NNA formation	Biological activity of CSC from extracted tobacco was decreased but to a much lesser extent than decrease in MSS PAH (and B[*a*]P) yields. This resulted from two unanticipated effects of extraction on the tobacco and its smoke: Extracted lipophilic compounds included various inhibitors (SHCs) and anticarcinogens (α-tocopherol, β-sitosterol, cholesterol, *D*-limonene, duvanediols) which have been reported to offset the tumorigenicity of PAHs.\ • Residual tobacco after extraction contains higher levels of lignin, cellulose, and pectins. All of these generate promoting/cocarcinogenic phenols during the smoking process: levels of low-molecular-weight phenols in MSS were increased
PAHs in cigarette smoke are generated by one or other of the following mechanism: • Organic compounds in tobacco are degraded to simpler molecules during the pyrolysis processes occurring in the burning cigarette, and these simpler molecules recombine to PAHs (degradation-combination mechanism) [cf. Badger et al. (142, 143) and earlier papers]. • During the pyrolysis processes occurring in the burning cigarette, high-molecular-weight compounds in tobacco undergo unimolecular cyclization, dehydration, aromatization, ring expansion, etc., to form PAHs (aromatization reaction) [Rodgman and Cook (3269, 3286)]	The mechanism of PAH formation is not an either-or situation. Laboratory data indicated that both mechanisms were operative in PAH formation in the burning cigarette. Evidence for the unimolecular aromatization reaction was provided by pyrolysis data and cigarette "spiking" data with phytosterols. In this instance, the relatively high levels of chrysene and cyclopentaphenanthrene *vs*. B[*a*]P were more readily explained by the unimolecular aromatization of the tetracyclic sterol

(*continued*)

TABLE 26.2 (continued)
PAH Paradoxes

Assertion	Contradiction
Inhaled cigarette smoke is the responsible agent for respiratory tract cancer, particularly squamous cell carcinoma of the lung, in smokers. It was implied in the late 1950s and in the 1960s that the responsible agent in MSS may be the PAHs, particularly B[*a*]P	Inhalation experiments with laboratory animals exposed for their lifetime to cigarette MSS consistently failed to produce pulmonary squamous cell carcinoma [Essenberg (1161–1163), Leuchtenberger et al. (26A81, 26A82, 26A83), Henry and Kouri (1621, 1622)], the lung tumor type reported to be associated with smoking in humans. Similar exposures of laboratory animals to vehicular exhaust gases produced pulmonary squamous cell carcinoma [Mauderly et al. (2505)]. Inhalation studies with B[*a*]P at levels comparable to those in cigarette MSS were consistently negative. Tumor production at extremely high levels of inhalation exposure to B[*a*]P was described as "equivocal" [RTECS (3085)]. From a study with roofers exposed via inhalation to levels of B[*a*]P equivalent to the daily inhalation of MSS from over 700 cigarettes, Selikoff et al. (3584a) concluded: "If a high level of exposure to benzo[*a*]pyrene has any relation to lung cancer, the effect must be small… If a high level of occupational exposure to benzo[*a*]pyrene by way of inhalation results in little if any increase in the risk of lung cancer—then it seems unlikely that the extremely small amount of benzo[*a*]pyrene in cigarette smoke can account for the high degree of association between cigarette smoking and lung cancer."
Since B[*a*]P and other known tumorigenic PAHs account for so little (<2%) of the observed biological effect in mouse-skin-painting studies, two possibilities were proposed: A PAH whose tumorigenicity was equivalent to that of B[*a*]P was present at a substantially higher level (25–50 times) than B[*a*]P, or there was an unknown "supercarcinogenic" PAH in CSC, present at a level similar to that of B[*a*]P but whose activity was 25–50 times that of B[*a*]P [Wright (4282)]	After a year and a half unsuccessful search, attempts to find either the highly tumorigenic PAH present at a high level or the "supercarcinogenic" PAH were discontinued [Wright (4282)]. Neither proposal has resurfaced since the late 1950s
Since B[*a*]P in CSC acting alone accounts for less than 2% and the total PAH fraction accounts for less than 3% of the observed biological response in mouse-skin-painting studies and no "supercarcinogenic" PAHs is present, additional mechanisms are needed to explain the biological effect: The mechanisms of promotion and cocarcinogenesis of tobacco smoke components (phenols, etc.) may explain the observed effect in skin-painting studies with CSC	The promoting/cocarcinogenic effect of phenols on PAH tumorigenicity was offset by the following: • Removal of the low-molecular-weight phenols by selective filtration of smoke "does not change significantly the biological activity of the resulting condensate." [Hecht et al. (1582, 1583)]. • Phenol inhibited the tumorigenicity of PAHs such as B[*a*]P [Van Duuren et al. (4029, 4035)]. • Inclusion of known initiators, promoters, and cocarcinogens in tobacco smoke in the calculation explained less than 5% of the observed biological effect in skin-painting studies
Wynder and Hoffmann (4317) reported that doubling the level of tumorigenic 17 PAHs in CSC produces "a statistically significant increase in tumor yield."	The following contradictory evidence was reported: Increasing the B[*a*]P level in CSC by a factor of 10 produced no increase in the tumorigenicity of CSC [Roe (3310, 3311)]. Increasing the level of B[*a*]P by a factor of 30 produced no increase in the tumorigenicity of the CSC in mouse-skin-painting studies [Lazar et al. (2320)]
As proposed many times by Wynder, Hoffmann et al. (1766, 4304, 4317, 4319, 4330, 4355), the B[*a*]P level in CSC is an "indicator" (or "marker") of the following: • The levels of the tetracyclic and higher PAHs, particularly those that are tumorigenic • The tumorigenicity of the CSC in mouse-skin-painting studies	Ample evidence indicated these premises are invalid: • No significant correlation between levels of B[*a*]P and other PAHs in pyrolysates from pyrolysis studies [Lam (2255, 2257)] • Contradictory data provided from the studies of Wynder et al. (4355, 4356), Campbell and Lindsey (583), and Severson et al. (3616) • No significant correlation between levels of B[*a*]P and chrysene as reported by Rodgman and Cook (3269) or B[*a*]P and B[*a*]A [Gori (1329, 1330, 1332, 1333)] in cigarette smoking studies • No significant correlation between tumorigenicity of over 130 test and reference CSCs to mouse skin and their B[*a*]P and/or B[*a*]A content [Gori (1329, 1330, 1332, 1333), NCI (2683)] • In non-CSC-related studies, Warshawsky et al. (26A180) found in their study of the carcinogenic potential of mixtures that the carcinogenic "activity of a mixture cannot be accounted for by the level of benzo[*a*]pyrene present."

TABLE 26.2 (continued)
PAH Paradoxes

Assertion	Contradiction
Tumorigenicity of PAHs, e.g., B[*a*]P, is inhibited by representative hydrocarbons ($C_{31}H_{64}$ and $C_{35}H_{72}$) in the SHC fraction of CSC at SHC–B[*a*]P ratios much less than that found in CSC [4314, see p. 370 in (4332)]	Inhibitors and anticarcinogens more potent in their effect against PAHs than the SHC fraction in mouse-skin carcinogenesis were identified in CSC (phytosterols, α-tocopherol, duvanediols, *D*-limonene): their concentrations relative to that of the PAHs are far in excess of that required to elicit anticarcinogenesis
Reports of the presence of DMB[*a*]A in MSS CSC [Pietzsch (2962), Kröller (2191)] were criticized because "the formation of a dialkylated benz[*a*] anthracene during pyrolysis appears questionable." [Cook (796), Wynder and Hoffmann (4332)]	Snook et al. (3756, 3757) reported identification of numerous alkyl-, dialkyl-, and multialkyl-B[*a*]As in CSC. Subsequent research indicated a host of mono- to penta-alkyl-PAHs in the CSC. Their major precursors were tobacco terpenoid compounds, e.g., solanesol, neophytadiene
Report of presence of 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene) in CSC [Kröller (2191)] was criticized by Wynder and Hoffmann (4332): "Since this carcinogenic hydrocarbon has not yet been found in any other combustion product, it remains a doubtful assumption that it is present in tobacco smoke."	Several benzo[*a*]cyclopentanthracenes, structurally similar to 1,2-dihydro-3-methylbenz[*j*]aceanthrylene (3-methylcholanthrene, a methylbenzo[*a*]cyclopent[*fg*]anthracene), have been identified in CSC: These included an unmethylated benzocyclopentanthracenes, originally reported erroneously as 1,2-dihydrobenz[*j*]aceanthrylene (cholanthrene) by Rodgman and Cook, (3273), 2,3-dihydro-1*H*-benzo[*a*]cyclopent[*h*]anthracene, and 9,10-dihydro-9*H*-benzo[*a*]cyclopent[*j*]anthracene [Bonnet and Neukomm (394, 397–399), Ahlmann (39), Bonnet (392), Pyriki (3033), Rodgman and Cook (3273)]
Dibenzo[*a,l*]pyrene (dibenzo[*def,p*]chrysene) is present in CSC and the pyrolysate from saturated tobacco hydrocarbons [Wynder et al. (4355)]. It was identified on the basis of agreement between spectral data for the isolate and those published for a synthetic PAH [Lyons and Johnston (2430), Lyons (2427, 2428), Wynder and Wright (4354), Rodgman and Cook (3273), Pyriki (3033), Bonnet and Neukomm (398, 399)]	Lavit-Lamy and Buu-Hoï (2314) demonstrated that the synthetic PAH originally defined as dibenzo[*a,l*]pyrene (dibenzo[*def,p*]chrysene) and spectrally identical with the tobacco smoke isolate was actually dibenz[*a,e*]aceanthrylene (dibenzo[*a,e*]-fluoranthene), a fact accepted by Hoffmann and Wynder (1798). Dibenzo[*def,p*]chrysene (dibenzo[*a,l*]pyrene) was subsequently identified in tobacco smoke by Snook et al. (3756), but no quantitative data were reported. In citations of dibenzo[*a,l*]pyrene as a "tumorigenic agents in tobacco smoke," Hoffmann et al. (1727, 1740, 1741, 1743, 1744, 1773), IARC (1869, 1870), and EPA (1148) indicated only that it was "present." Whether its "presence" was based on the erroneous dibenzo[*a,l*]pyrene reports from the 1950s or the authentic dibenzo[*a,l*]pyrene report of Snook et al. (3756) is unclear
Addition of nitrate to the tobacco blend significantly reduced MSS yields of "tar," PAHs, and phenols. The odd-electron compound NO generated during the smoking process interrupted the free radical mechanism of formation of PAHs [Hoffmann and Wynder (1797)]. The % TBA of the resulting CSC was also reduced by about 80%. On the basis of these results, nitrate addition or use of high-nitrate tobaccos was proposed	Reductions in these deliveries were confirmed (3246, 3286), but they were less than those originally proposed. In fact, in the first NCI–TWG study (1329), doubling the nitrate level produced the following changes: "Tar," −7%; phenanthrene, −9%; B[*a*]P, +23%; B[*a*]A, −17%; phenol, −10%; nitric oxide; +111%. Doubling the nitrate level decreased the % TBA by about 20%. Later data showed that adding nitrate increased volatile NNAs and TSNAs in smoke. Nitrate removal or use of low-nitrate tobaccos was proposed [Brunnemann and Hoffmann (480)]. Hoffmann et al. included NNAs and TSNAs in their list of tumorigens or carcinogens in tobacco smoke
According to Hoffmann and Wynder, increasing the number of cuts/inch (decreasing the cut width) for the tobacco filler reduces the delivery of CSC and B[*a*]P (1793)	The 1963 Hoffmann–Wynder findings were not confirmed either at RJRT or in the NCI–TWG study on the first set of experimental cigarettes [Gori (1329)]. In the latter study, the B[*a*]P and B[*a*]A yields for the normal filler cut (32 cpi) were less than those for the coarse (20 cpi) and fine (60 cpi) cuts
PAHs are removed selectively by filters treated with reagents (chloranil, picric acid, 2,4,7-trinitrofluorenone) that form stable complexes with individual PAHs[Szent-Gyorgi (3847)]	Complexing reagents such as chloranil or 2,4,7-trinitrofluorenone did not selectively reduce MSS yields of individual PAHs [Rodgman and Cook (3275)]. The complexing agent is unable to react with the nonvolatile individual PAHs in the milieu of thousands of compounds in the particles of the smoke aerosol

(*continued*)

TABLE 26.2 (continued)
PAH Paradoxes

Assertion	Contradiction
Because of the nature of the cigarette smoke aerosol, Wynder and Hoffmann (4311) considered selective filtration of a specific smoke component or class of smoke components such to be an "impossibility." However, the next year, they reversed their view, noting that selective filtration is not "impossible" [Wynder and Hoffmann, (4314)]	Wynder and Hoffmann (4314) reversed their view on the impossibility of selective filtration when they found that relatively volatile smoke components, e.g., low-molecular-weight phenols, are selectively removed from the MSS by filters incorporating certain plasticizers such as triacetin [cf. Laurene et al. (2312)]. Some years later, the same phenomenon was observed with volatile NNAs [Fredrickson (1236), Brunnemann et al. (514)]
Single compound pyrolysis at 800°C in an inert atmosphere (N_2 or He) is equivalent to the conditions existing in a smoked cigarette [Wynder and Hoffmann (4319, 4332)]. This proposal was an attempt to justify drawing conclusions on PAHs in MSS on the basis of pyrolysis data	On the basis of numerous laboratory data, this premise was criticized by several investigators [Bell et al. (248), Benner et al. (276, 277), Schlotzhauer and Schmeltz (3466, 3467), Chortyk and Schlotzhauer (722), Baker (163, 166, 167, 171a, 171b), Baker and Robinson (174d)]. Proponents of the equivalence of inert-atmosphere pyrolysis of a tobacco component and its behavior in a burning cigarette during the smoking process misinterpreted one set of data and disregarded another: "The atmosphere immediately behind the burning coal is oxygen-deficient compared to the oxygen level of the air entering the cigarette at the lit end and the smoke exiting the cigarette at the mouth end but it is *not* oxygen-free. The oxygen level in the tobacco rod a short distance (1–2 mm) behind the tobacco rod–fire cone interface is influenced by diluting air entering the tobacco rod through the cigarette paper and this diluting air increases as the cigarette paper porosity increases." The ultimate contradiction was provided from the laboratory of the original claimants. Schmeltz et al. (3512) reported that the fate of radiolabeled nicotine on pyrolysis was entirely different from its fate in the smoking process: "These results suggest to us that pyrolysis experiments may be of limited value for establishing the fate of nicotine and possibly other tobacco components in a burning cigarette."
Severson et al. (1979) describe "the pyrolytic conditions that yielded [PAH] profiles of tobacco pyrolyzates that could be correlated with [cigarette smoke condensate] profiles…"	The anticipated correlation was not attained: When the tobacco, a tobacco extract, and the residual extracted tobacco were pyrolyzed, neither the amounts obtained for the individual PAHs other than B[*a*]P, the phenols, nor the acids (volatile or nonvolatile) in the tobacco pyrolysate matched the totals of the amounts in the extract pyrolysate plus the amounts in the residual tobacco pyrolysate. For the individual PAHs (except for B[*a*]P) and the acids, the totals of the amounts from the extract pyrolysate plus residue pyrolysate were higher than the amounts from the tobacco pyrolysate. For the individual phenols, the opposite was the case: The totals were less!
Between the early 1950s and 1984, literally hundreds of articles were published on PAHs in tobacco smoke with particular emphasis on the tumorigenicity of many of them (3262, 3306a, 3306b, 3307, 3713, 3714)	Despite the many published articles prior to 1984 on PAHs in tobacco smoke, none of the authors contributing to the Searle-edited over 1400-page American Chemical Society's monograph on chemical carcinogens (3568) mentioned any of the tumorigenic PAHs reported in cigarette smoke

26.1.2 Other Classes of Carcinogens, Tumorigens, and Mutagens

26.1.2.1 Aza-Arenes

Within a few years of the discovery of the tumorigenicity to mouse skin of the PAHs DB[*a,h*]A (2078) and B[*a*]P (194, 796a, 797), investigations on the tumorigenicity of aza-arenes began. The aza-arenes selected for study were those structurally related to the PAHs already demonstrated to be tumorigenic. The first aza-arenes studied were those corresponding structurally to the dibenzanthracenes in which one *mesocarbon* was replaced by a nitrogen atom. From a comparison of their tumorigenicities (mouse-skin-painting experiments), Barry et al. (194) reported that the tumorigenicity of several dibenzacridines was much less than the corresponding PAH, e.g., dibenz[*a,h*]acridine (I) was reported to be much less tumorigenic than DB[*a,h*]A (IV) under the same experimental conditions (Figure 26.2).

For the PAHs, much of the early research on their synthesis and tumorigenicity was conducted by the Kennaway group

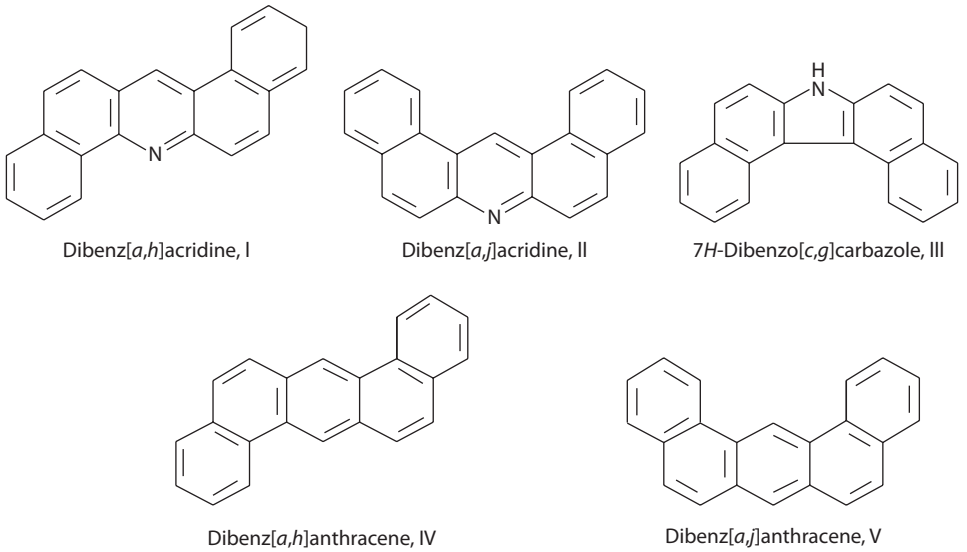


FIGURE 26.2 Structural similarity of several PAHs and aza-arenes.

(Barry, Cook, Hewett, Hieger, Lindsey, Schoental) in the United Kingdom, by groups headed by Fieser and Newman in the United States, and by the Clar group in Germany. For the aza-arenes such as the benzacridines, much of the early research was conducted by the Lacassagne group (Buu-Hoï, Daudel, Lavit-Lamy, Zajdela) in France.

It has been known for nearly six decades [cf. review by Lacassagne et al. (2247a)] from the comparative tumorigenicity studies involving structurally similar PAHs and aza-arenes that the aza-arenes are much less tumorigenic than the PAHs to mouse skin [cf. DB[*a,h*]A (IV) *vs*. dibenz[*a,h*]acridine (I) and DB[*a,j*]A (V) *vs*. dibenz[*a,j*]acridine (II) or 7*H*-dibenzo[*c,g*]carbazole (III)]. These observations on tumorigenicity plus the reported amounts of the three aza-arenes in cigarette MSS relative to the amount of B[*a*]P certainly raise doubts as to the importance of the aza-arenes as significant tobacco smoke tumorigens. In Table 26.1, B[*a*]P is listed as occurring in cigarette MSS in yields ranging from 20 to 40 ng/cig, whereas the yields of aza-arenes I, II, and III are listed at 0.1, 3–10, and 0.7 ng/cig, respectively. Even though a more realistic range for B[*a*]P in the MSS of cigarettes marketed over the past two decades would be 5–20 ng/cig rather than 20–40 ng/cig, the ratios of B[*a*]P yield to those of dibenz[*a,h*]acridine and 7*H*-dibenzo[*c,g*]carbazole are substantial. This of course assumes that the yields for the three aza-arenes that were included in Table 26.1 are correct! It is obvious that the listed aza-arene yields are not meaningful for recently manufactured cigarettes whose design includes technologies not used in the late 1950s and early 1960s when Van Duuren et al. (4027) reported their findings on aza-arenes in cigarette MSS.

The listing of single delivery values rather than a range for dibenz[*a,h*]acridine (0.1 ng/cig) and 7*H*-dibenzo[*c,g*]carbazole (0.7 ng/cig) indicates the MSS yields cited are those reported from a single study, which appears to be that of Van Duuren et al. (4027). Wynder and Hoffmann (4319, 4332) cited their own unpublished 1963 findings [Candeli et al. (587)] that they could not detect dibenz[*a,h*]acridine in cigarette MSS. Such findings were never published in a peer-reviewed journal. Thus, the upper limit (10 ng/cig) of the range for MSS yield of dibenz[*a,j*]acridine is that reported by Hoffmann, coauthor of all but one of the lists in Table 26.1.

Single MSS yields for dibenz[*a,h*]acridine and 7*H*-dibenzo[*c,g*]carbazole in MSS based on a cigarette manufactured in 1959–1960 or 1963 are hardly representative of more recently manufactured cigarettes. It is well recognized that a variety of cigarette design technologies (efficient filtration, filter-tip additives, processed tobacco materials [RTS, expanded tobaccos], air dilution [porous paper, filter-tip perforations], and paper additives) have progressively reduced the sales-weighted average mainstream TPM by almost 70% from 40 mg/cig in the early 1950s to less than 12 mg/cig currently. At the same time that the reduction of delivery of mainstream TPM was accomplished, the composition of the MSS was also altered. For example, for mainstream TPM, the B[*a*]P content—expressed as ng B[*a*]P/mg TPM—has decreased about 33% (from 1.2 to 0.8 ng/mg TPM) during the same time period. The 1979 U.S. Surgeon General's report (4005) summarized the B[*a*]P data for a commercial cigarette sold in the United States from 1954 to 1979. In addition to changes in the composition of mainstream TPM, changes in mainstream vapor-phase composition also occurred.

Nicotine and the tobacco proteins and amino acids are proposed as the major precursors of aza-arenes [Chortyk and Schlotzhauer (722)]. Thus, the decrease in cigarette nicotine content and delivery since 1960 should certainly influence the pyrogenesis of the dibenzacridines and dibenzocarbazole during the tobacco smoking process. The levels of nicotine in U.S. cigarette tobacco blends (and MSS) decreased on average more than 40% between 1960 and the late 1980s.

In addition, inconsistencies among numerous isolation studies raise serious questions about the actual presence of

these three aza-arenes in the MSS (or SSS) from cigarettes manufactured after the mid-1960s. Results from German, Japanese, and American groups of investigators on their search for dibenz[*a,h*]acridine (I), dibenz[*a,j*]acridine (II), and 7*H*-dibenzo[*c,g*]carbazole (III) in mainstream CSC and/or nicotine pyrolysates are summarized in Table 26.3. Only Van Duuren et al. (4027) in their published report and Candeli et al. (587) in their unpublished report have detected any of these three aza-arenes in cigarette MSS!

Examination of the results summarized in Table 26.3 indicates that Van Duuren et al. (4027) reported the identification of the three aza-arenes in mainstream CSC and two of them (I and II) in a nicotine pyrolysate. However, Candeli et al. (587) failed to identify I but did identify II in mainstream CSC. The Candeli et al. findings reported in 1963 on II in mainstream CSC were not confirmed in 1979 by investigators from the same laboratory [Schmeltz et al. (3512)]. Two later studies (3499, 3512) confirmed the 1960 finding by Van Duuren et al. that 7*H*-dibenzo[*c,g*]carbazole was not present in a nicotine pyrolysate.

Examination of the detailed chromatograms presented in a study on aza-arenes in MSS and SSS by Grimmer et al. (1409) indicates the presence of several benzacridines (benz[*a*]acridine, benz[*c*]acridine). However, no gas chromatographic peaks corresponding to standard dibenz[*a,h*]acridine and dibenz[*a,j*]acridine peaks are visible in the chromatograms of the aza-arene fraction from either the MSS or SSS.

The failures by numerous talented research groups (Table 26.3) to detect the two dibenzacridines, I and II, in tobacco smoke cannot be attributed to difficulties or problems in the analytical procedures. Motohashi et al. (26A113) reviewed the analytical procedures that enabled investigators to identify several benzacridines and their homologs plus dibenz[*a,h*]acridine and dibenz[*a,j*]acridine in a variety of environmental samples (urban air; gasoline engine exhaust; diesel engine exhaust; street dust; sediment from lake, river, and saltwater sources). Motohashi et al. (26A113) also reviewed in some detail the reports by Schmeltz et al. (3499), Snook et al. (3750), Grimmer et al. (1409), and Kamata et al. (2021) on the identification of various benzacridines in tobacco smoke, but they did not mention the reported identification of dibenz[*a,h*]acridine and dibenz-[*a,j*]acridine in MSS by Van Duuren et al. (4027).

In summary, the situation with regard to the four aza-arenes considered to be significant "tumorigens" in tobacco smoke by Hoffmann et al., OSHA (1994), and/or EPA (which relied on the 1990 Hoffmann–Hecht list) is as follows:

- OSHA did not list quinoline as a significant tumorigen, whereas EPA did.
- Only one laboratory, that of Van Duuren, reported the presence of dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole, listed in Table 26.1 as tumorigens in tobacco smoke.

TABLE 26.3
Dibenz[*a,h*]acridine {I}, Dibenz[*a,j*]acridine {II}, and 7*H*-Dibenzo[*c,g*]carbazole {III} in Nicotine Pyrolysates (Pyr) and CSC

	Dibenz[*a,h*]acridine		Dibenz[*a,j*]acridine		7*H*-Dibenzo[*c,g*]carbazole	
Investigators	**Pyr**	**CSC**	**Pyr**	**CSC**	**Pyr**	**CSC**
Van Duuren et al. (4027)	Yes	Yes	Yes	Yes	No	Yes
Candeli et al. (587); Wynder and Hoffmann (4319, 4332)	NE	No	NE	Yes	NE	NE
Kaburaki et al. (2006)	No	NE	No	NE	NE	NE
Schmeltz et al. (3499)	No	NE	No	NE	No	NE
Schmeltz et al. (3512)	No	No	No	No	No	No
Snook (3733)	NE	No	NE	No	NE	No
Snook et al. (3750)	NE	No	NE	No	NE	No
Grimmer et al. (1409)	NE	No	NE	No	NE	No
Kamata et al. (2021)	NE	No	NE	No	NE	NE
Sasaki and Moldoveanu (3414)	NE	No	NE	No	NE	NE
Rustemeier et al. (3370)	NE	No	NE	Yes	NE	NE

Yes, compound identified; No, compound not found or identified; NE, substrate not examined for compound in question.

Examination of these results indicates that Van Duuren et al. (4027) reported the identification of the three *N*-heterocyclic compounds {I, II, and III} in mainstream CSC and two of them {I and II} in a nicotine pyrolysate; whereas, Candeli et al. (587) failed to identify I but did identify {II} in mainstream CSC. The 1963 Candeli et al. findings on {II} in mainstream CSC were not confirmed in 1979 by investigators (3512) from the same laboratory: Hoffmann participated in both the 1963 and 1979 studies. Two studies (3499, 3512) confirmed the 1960 report by Van Duuren et al. that 7*H*-dibenzo[*c,g*]carbazole {III} was not present in a nicotine pyrolysate.

- One other laboratory reported the presence of dibenz[*a,j*]acridine in MSS but not the other two aza-arenes [Candeli et al. (587), see Wynder and Hoffmann (4319, 4332)]. Candeli et al. reported the MSS yield for dibenz[*a,j*]acridine to be roughly four times that reported by Van Duuren et al. (4027). This disparity in per cigarette MSS yield should have triggered additional research on its presence and level in MSS. However, the 1963 finding by Candeli et al. has never appeared in a peer-reviewed journal.
- Failure to detect the three aza-arenes dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, and 7*H*-dibenzo[*c,g*]carbazole in cigarette MSS and/or in nicotine pyrolysates was reported in at least nine studies conducted periodically between 1970 and 2002 (Table 26.3).
- In comparable tumorigenicity studies, the aza-arenes are much less tumorigenic to mouse skin than their corresponding PAH analogs and much less tumorigenic than B[*a*]P [Barry et al. (194)]. The MSS yields of the three aza-arenes listed by OSHA and EPA, if they are present at all in MSS, are much less than that of B[*a*]P.
- Even when the repeated failure to confirm their presence in tobacco smoke is ignored, the combination of their significantly lower levels *vs*. that of B[*a*]P of the three aza-arenes in cigarette MSS plus their significantly lower tumorigenicity in the mouse-skin-painting bioassay raises serious questions about their inclusion in a table listing the "significant tumorigens in tobacco smoke."

26.1.2.2 *N*-Nitrosamines

Hoffmann and Hecht (1727) did not acknowledge that the MSS yields listed for both the volatile NNAs and the tobacco-specific *N*-nitrosamines (TSNAs) could be incorrect (and high) because of the artifactual formation of both types of NNAs during MSS (and SSS) collection for analysis as reported by Caldwell and Conner (573). EPA and OSHA accepted without question the mainstream volatile NNA and TSNA yields tabulated by Hoffmann and Hecht (1727) and cited by the U.S. Surgeon General in his 1989 report (4012).

The artifactual formation of NNAs during the collection and analysis of MSS and SSS has been noted many times over the years, and it has not been limited to the determination of NNAs in cigarette smoke. A similar problem was noted with the determination of NNAs in foodstuffs. Neurath et al. (2750) were one of the earliest groups of investigators to discuss this problem in cigarette smoke. More recently, Brunnemann et al. (457), from their study of the levels of NNAs in MSS and SSS, reported lower levels than previously reported for volatile NNAs in MSS, attributing the lower levels to the avoidance of artifactual formation of NNAs during smoke collection and analysis. They wrote

> In fact, several of the cigarettes which were machine smoked earlier and analyzed without precautions, when smoked by us under the same conditions but with precautions, yielded 25 to 100% lower values for DMN [*N*-nitrosodimethylamine] and NPY [*N*-nitrosopyrrolidine] for the mainstream smoke …
>
> The nitrate content of the tobacco appears to be a determining factor for the concentration of volatile nitrosamines in the smoke. Selective removal of these nitrosamines does occur with cellulose acetate filter tips but not with charcoal filter tips.

Guerin et al. [see p. 236 in (1445)], in their review of NNAs in ETS commented on four ETS-related studies, those of Brunnemann et al. (457), Stehlik et al. (3812), Matsushita and Mori (2495), and Klus et al. (2134a). Guerin et al. summarized the results on the determination of NNAs in natural and artificial ETS environments as follows:

> The concentration of nitrosodimethylamine in commonly encountered ETS-contaminated indoor air is likely to range from <10–40 ng/m^3. Nitrosodiethylamine and nitrosopyrrolidine are likely to be present at similar but lower concentrations. Extrapolating from studies of artificial environments suggest NNN and NNK concentrations in common environments will range from <1–3 ng/m^3.

They also noted that occasionally, NDMA concentrations may show excursions to be 100 ng/m^3 or more.

It was noted previously (Table 26.1) that many claims about PAHs in tobacco smoke, particularly those demonstrated to be tumorigenic to the skin of rodents, were subsequently demonstrated to be either incorrect or equivocal. However, the points of contention about NNAs in tobacco smoke are fewer than the number listed for tobacco smoke PAHs (see Table 26.4).

26.1.2.3 *N*-Heterocyclic Amines

While many of the *N*-heterocyclic amine mutagens are present in tobacco smoke, the extensive research on this class of compounds was initiated and extended because of their presence in many foodstuffs consumed by many people. Table 26.5 summarizes some details of these *N*-heterocyclic amines in tobacco smoke.

As in the case of the tumorigens whose activity has been shown to be substantially reduced by administration of anticarcinogens [see reviews (3255, 3257, 3300)], Lee et al. (2327c) reported that the mutagenicities (Ames test) of several *N*-heterocyclic amine mutagens, each of which shows inordinately high mutagenicity, are substantially reduced by CSC. The compounds studied by Lee et al. were 2-amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-1), 2-aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole (Glu-P-2), 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1), and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2), 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ), and 2-amino-3,4-dimethylimidazo[4,5-*f*]quinoline (MeIQ).

Table 26.6 summarizes the chronology of the studies dealing with the *N*-heterocyclic amines in tobacco smoke and in commonly consumed foodstuffs.

TABLE 26.4
NNAs in Tobacco Smoke

Assertion	Contradiction
Druckrey and Preussmann (1057) proposed that conditions were appropriate (presence of nitrogen oxides, water, and secondary amines, pH < 7.0) in a burning cigarette for pyrogenesis of NNAs such as NDMA. Boyland et al. (422, 423) proposed that the presence in tobacco smoke of nornicotine and anabasine, nitrogen oxides, and water made it highly likely that NNN and *N′*-nitrosoanabasine (NAB) would be formed	
Serfontein and Hurter (3595, 3597) reported the identification of NNAs in cigarette MSS	First claims by Serfontein and Hurter (3595, 3597) of identification of NNAs in cigarette MSS were challenged with counterclaims that NNAs were artifactually produced during smoke generation, collection, and analysis [cf. Neurath et al. (2751)]. Neurath et al. (2751) reported the presence of an NNA but subsequently discovered the identified compound was produced artifactually during the smoke processing
Since volatile NNAs and TSNAs occur in tobacco, a part of the NNAs in cigarette MSS is a result of direct transfer of NNAs from tobacco to smoke; the remainder results from formation and transport during the smoking process [Adams et al. (29)]. For NNK, the transfer from tobacco to smoke ranges from 6.9% to 11.0% of the amount in the tobacco; this represents about 30% of the NNK in MSS. The remainder in MSS is formed during the smoking process [Hoffmann et al. (1734), Hecht et al. (564)]	The premise of the pyrogenesis of NNN and NNK during the cigarette smoking process was challenged by Fischer et al. (1193, 1199) who reported that these compounds occur in cigarette MSS only by transfer from the tobacco rod
The problem of artifactual formation of NNAs has persisted from the mid-1960s to the present [Neurath et al., (2751), Fredrickson (1236), Krull et al. (26A77), Eisenbrand et al. (26A27), Caldwell and Conner (573)]. Continual improvement in smoke collection and analytical procedures has progressively reduced the analytical error	
TSNAs in CSC have little or no influence on the host response in skin-painting studies. Little of the volatile NNAs remain in the CSC after collection and preparation for the skin-painting bioassay. The only NNAs to consistently elicit a positive response at the application site in skin-painting studies are the alkyl-*N*-nitrosourethanes, none of which has been identified in tobacco or tobacco smoke to date.	
Hundreds of rodent-skin-painting studies with CSC and its fractions have been conducted since the first successful production of carcinoma in mice painted with CSC [see (4319, 4332, and references cited), Gori (1329, 1330, 1332, 1333), NCI (2683)]. Even in the massive NCI decade-long study, no attempt was made to correlate NNA content with bioassay results. It was assumed, from studies with individual NNAs, that they had little if any influence on CSC tumorigenicity to mouse skin. Millions of dollars and thousands of hours expended since 1953 in conducting bioassays—particularly mouse-skin-painting studies—did not adequately define the total tumorigenicity of CSC in laboratory animals	
Precursors of NNAs in both tobacco and tobacco smoke are the proteins and amino acids (plus nitrate) for the volatile NNAs [Brunnemann et al. (481, 482), Hoffmann et al. (1694)] and nicotine and nicotine-related alkaloids (plus nitrate) for the TSNAs [Boyland et al. (422, 423), Rathkamp et al. (3080), Hecht et al. (1563, 1565)]. The levels of NNAs in tobacco and its smoke parallel the tobacco nitrate level [Morie and Sloan (2635), Hecht et al. (1576, 1578), Tso et al. (3985)]	
Removal of lipophilic PAH precursors from tobacco by solvent extraction reduces the PAH yield in MSS and the tumorigenicity (mouse-skin painting) of the CSC [Wynder (4294), Wright (4281), Wynder et al. (4355, 4356)]. This led to their recommendations to remove lipophilic components from tobacco. Confirmation of the reduced levels of PAHs in MSS from cigarettes fabricated with organic solvent-extracted tobaccos was provided by Rodgman (3241, 3242, 3246) and Rodgman and Cook (3286)	Personnel from Wynder's laboratory subsequently recommended the addition of lipophilic compounds, e.g., *n*-hentriacontane, to tobacco [Brunnemann and Hoffmann (480)] to reduce the generation during the smoking process of nitrate-derived nitrogen oxide which was postulated as a reactant in the formation of NNAs

TABLE 26.4 (continued)
NNAs in Tobacco Smoke

Assertion	Contradiction
NNA formation in tobacco smoke involves the reaction of methyl nitrite and secondary amines [Rodgman and Cook (3286), Wynder and Hoffmann (4332)].	The proposal by Rodgman and by Wynder and Hoffmann (4332) that NNAs arise by reaction of methyl nitrite with secondary amines was shown to be invalid: Methyl nitrite in MSS is zero initially, but during the period of tobacco smoke generation, collection, and analysis, it is formed artifactually in tobacco smoke [Vilcins and Lephardt (4058)]
NNA formation in tobacco smoke involves reaction among secondary amines, nitrogen oxides, and water	Individual NNAs, particularly the TSNAs, have little or no influence on CSC tumorigenicity in the skin-painting bioassay. Millions of dollars and thousands of hours have been expended since 1953 in conducting bioassays that do not adequately define the total tumorigenicity of CSC in laboratory animals.
Despite the contradictory evidence that precludes the involvement of NNAs either collectively or individually not only in various bioassays with laboratory animals but also in respiratory tract cancer in cigarette smokers, some investigators still maintain that the "tumorigenicity" of cigarette smoke in humans is due to its PAH content and its content of the TSNA, NNK.	Inhalation studies with NNAs at levels comparable to those in cigarette MSS were consistently negative.
In 1991, Hecht and Hoffmann (1571a) wrote "Polynuclear aromatic hydrocarbons and NNK [4-(*N*-methyl-nitrosamino)-1-(3-pyridyl)-1-butanone] are the major carcinogens involved in lung cancer induction by cigarette smoke…"	Lung tumor production by exposure to extremely high inhalation levels of NNAs was classified as "equivocal" by the Registry of Toxic Effects of Chemical Substances (RTECS) (3095)
Hoffmann and Hecht (1727) also noted that NNK had not been tested in laboratory animals for tumorigenicity via inhalation	Bioassay results in lifetime inhalation studies with laboratory animals exposed to various cigarette MSSs show no relationship between tumor production and volatile NNAs and/or TSNA content
On the basis of the following results, nitrate addition or use of high-nitrate tobaccos was proposed: Addition of nitrate to the tobacco blend significantly reduced MSS yields of "tar," PAHs, and phenols. NO generated from nitrate during the smoking process interrupted the free radical mechanism of formation of PAHs [Hoffmann and Wynder (1797, 1798)]. The tumorigenicity (% TBA) of the resulting CSC is also reduced	Later, data showed that increasing the nitrate increases both the volatile NNAs and TSNAs in MSS. Even though an increased level of TSNAs in mainstream CSC was accompanied by decreased tumorigenicity of the CSC to mouse skin, it was subsequently proposed to remove nitrates from the tobacco or use *low*-nitrate tobaccos [Brunnemann and Hoffmann (480)]. However, several of the NNAs and TSNAs were included in the lists of "tumorigenic agents in tobacco and tobacco smoke."
No volatile NNAs is considered a "marker" for other volatile NNAs in MSS; no TSNA is considered a "marker" for other TSNAs, either individual or total, in MSS. No NNAs—either a TSNA, a volatile NNA, or a nonvolatile NNA—is considered a "marker" for the tumorigenicity of CSC in the mouse-skin-painting bioassay	As noted previously, as the level of nitrate in tobacco and subsequently the levels of the TSNAs in CSC increase, the tumorigenicity of CSC to mouse skin decreases [Wynder and Hoffmann (4332), Hoffmann and Wynder (1801, 1802)], but its mutagenicity in the Ames system with *S. typhimurium* increases [Mizusaki et al. (2569)]
The tumorigenicity of NNAs is inhibited by a variety of tobacco smoke components. For example, *D*-limonene is anticarcinogenic to NNK [Wattenberg and Coccia (26A187)]; ethanol, *n*-butanol, and *tert*-butanol are anticarcinogenic to NNN [Waddell and Marlowe (26A178)]; indole [Matsumoto et al. (26A97)], cholesterol [Cohen et al. (26A12)], β-sitosterol [Wattenberg (4149b)], and 3,4,5-trihydroxybenzoic acid (gallic acid) [Mirvish et al. (2559c)] and its esters [Lo and Stich (26A87), Teel and Castonguay (26A172)] are anticarcinogenic to several of the NNAs in tobacco smoke [*cf.* Rodgman (3255, 3255a, 3257)]. Tobacco smoke not only contains other compounds such as long-chained fatty acids [Takeda et al. (26A171)] reported to diminish the tumorigenicity of various NNAs but also contains components structurally similar to compounds [(+)-catechin, esculetin, esculin] [Liu and Castonguay (26A86), Teel and Castonguay (26A172)] that have been reported to act as antitumorigens and/or antimutagens to NNAs	

(*continued*)

TABLE 26.4 (continued)
NNAs in Tobacco Smoke

Assertion	Contradiction
Various tobacco components and other compounds structurally similar to tobacco or smoke components are known to inhibit the *N*-nitrosation of secondary and tertiary amines to NNAs, a reaction known to occur among the nitrogen oxides, amino compounds, and water during the tobacco smoking process. These inhibitors of NNA formation include several primary amines, ascorbic acid and ascorbates [Mirvish et al. (26A112), Mirvish and Shubik (26A111), Archer et al. (26A03a), Mirvish (2559b, 26A104, 26A105)], indole, the tocopherols (particularly α-tocopherol) [Mergens et al. (26A100), Mirvish (2559b)], the carotenes, several phenols, and polyphenolic compounds such as chlorogenic acid [cf. Brunnemann and Hoffmann (484, 486)]. *Note:* The effect of these compounds on the *N*-nitrosation reaction should be differentiated from the effect of some of the same compounds on the tumorigenicity or mutagenicity of various NNAs, e.g., inclusion of ascorbic acid or ascorbate in the reaction substantially reduces the yield of NNAs; administration of ascorbic acid with a tumorigenic NNA such as NNK substantially reduces the tumorigenicity in laboratory animals. Little study has been devoted to determining whether compounds such as those noted earlier would exert a beneficial effect on MSS properties if added to cigarette tobacco because of diminished *N*-nitrosation with resulting lower NNA yield or because of the simultaneous delivery of the antitumorigen or antimutagen together with the NNAs	
Because of the nature of cigarette smoke aerosol, Wynder and Hoffmann (4311) considered selective filtration of a specific smoke component or class of smoke components such as the PAHs to be an "impossibility."	Selective filtration is not "impossible." Wynder and Hoffmann (4314) reversed their view on the impossibility of selective filtration when they found that relatively volatile smoke components, e.g., low-molecular-weight phenols, are selectively removed from MSS by filters incorporating certain plasticizers such as triacetin [cf. Laurene et al. (3211, 2312)]. Some years later, the same phenomenon was observed with volatile NNAs [Fredrickson (1236), Brunnemann et al. (514), Hoffmann et al. (1711)]
Guerin et al. (1445) estimated the exposure to NNAs in ETS-filled rooms to be low: NDMA <10–40 ng/m^3 NDEA 3 ng/m^3 NNN <1–3 ng/m^3 NNK <1–3 ng/m^3	Consumers are exposed daily to NNAs from a variety of nontobacco sources. Many foodstuffs, beverages, and cosmetics contain appreciable levels of some of the volatile NNAs also identified in tobacco and/or tobacco smoke [Magee and Barnes (2442), Sebranek and Cassens (26A142), Preussmann and Eisenbrand (2990), Maga (2438), Bailey and Williams (158a)]. Daily nontobacco exposure (primarily dietary) to NNAs is estimated to exceed 1800 ng/person; daily nontobacco source exposure to NDMA is estimated to exceed 1100 ng/person [Preussmann and Eisenbrand (2990)]. *Note:* These estimates are based on analytical data that may have included values for NNAs artifactually generated during the analytical procedure

26.2 ANTICARCINOGENS, INHIBITORS, AND ANTIMUTAGENS

In preceding publications and earlier chapters, (1) the listing of numerous MSS components as significant toxicants was questioned [Rodgman and Green (3300)], and (2) the assertions that ingredients added to cigarette tobacco adversely affect the chemical and biological properties of MSS were shown to be in error [Rodgman (3266)]. In this chapter, we will discuss the identified MSS components that have been shown in bioassays to significantly diminish the adverse biological effects of a number of the listed MSS toxicants.

The toxicological properties of an MSS component asserted to adversely affect the smoker have generally been defined in one or more bioassays devoted to the study of the effect of the component administered individually to a host. In most cases other than numerous studies of tumorigenesis, the effect on the toxicological property of a specific compound by other compounds such as those in the complex MSS aerosol has not been studied. The toxicological effect of a specific component in MSS is usually derived by extrapolation from the effect observed in one or more bioassays with the individual component.

It is known that the complex MSS aerosol has a significant effect on the chemistry of components in it. For example, (1) the rate of conversion of NO to NO_2 is significantly less in the MSS aerosol than in a system comprising only NO and O_2 (816) and (2) methyl nitrite reported as an MSS component is not formed during the smoking process but is formed during aging of the MSS during the analytical procedure (4058).

TABLE 26.5
Summary of Tumorigenic *N*-Heterocyclic Amines in Tobacco Smoke

Component	MSS Level, ng/cig[a]	IARC Evaluation of Evidence of Tumorigenicity in	
		Laboratory Animals	Humans
A*a*C	25–260	Sufficient	—
MeA*a*C	2–37	Sufficient	—
Glu-P-1	0.37–0.89	Sufficient	—
Glu-P-2	0.25–0.88	Sufficient	—
PhIP	11–23	Sufficient	Possible
IQ	0.26	Sufficient	Probable
MeIQ	0.28–0.75[b]	Sufficient	Probable
Trp-P-1	0.29–0.48	Sufficient	—
Trp-P-2	0.82–1.1	Sufficient	—

[a] See cigarette MSS yields listed in Table 26.1 (1740, 1741, 1743, 1744).
[b] MeIQ was not listed in (1740, 1741, 1743, 1744) but was listed by Smith et al. (3714).

If the chemistry of an MSS aerosol component be altered by the presence of thousands of other aerosol components, then logic dictates that its toxicology will also be altered.

Except for tumorigenic effects, little has been reported on the effect of other components in the complex MSS aerosol on the toxicological properties of an individual component. The tumorigenicity of many MSS components has been discussed frequently and in great detail, but little has been written about the biological activity of nontumorigenic MSS components reported to counteract the tumorigenicity in laboratory animals of the various tumorigens.

Inhibitors of carcinogens or anticarcinogens are compounds which prevent tumor development. Wattenberg (26A186) divided them into three categories based on the time in the carcinogenic process when they are effective: The first category consists of compounds that prevent the formation of carcinogens from precursor substances, e.g., ascorbic acid [Mirvish (26A103, 26A104)], tocopherols [Newmark and Mergens (26A116)], and phenols [Newmark and Mergens (26A116), Kuenzi et al. (2216)] which inhibit the formation of nitroso tumorigens from precursor amine and nitrite both in vivo and in vitro. The second category includes "blocking agents" which inhibit carcinogenesis by preventing carcinogenic compounds from reaching or reacting with critical target sites in the tissues, e.g., disulfiram [Wattenberg (26A183)] which inhibits the metabolism of symmetrical dimethylhydrazine to its carcinogenic metabolites [Fiala et al. (26A34)]. The last category of inhibitors—the "suppressing agents"—works by suppressing the expression of neoplasia in cells exposed to a carcinogenic agent. Retinoids are an example of this category.

In 1941, Shear and Leiter (3627) described in detail the many factors affecting tumorigenicity of a chemical. In the mid-1940s, several nontumorigenic aromatic hydrocarbons (benzene, naphthalene, anthracene) administered with B[*a*]P or DB[*a,h*]A significantly diminished the B[*a*]P and DB[*a,h*]A tumorigenicity (843, 844, 26A17). In recent lists of MSS toxicants, benzene, B[*a*]P, and DB[*a,h*]A are listed as significant tumorigens. Reported many times, however, is the noncarcinogenicity of benzene in the solvent-control group when it was used as the solvent for known or suspect tumorigens in skin-painting bioassays (1544, 3665).

Steiner and Falk (3814) reported that B[*a*]A, categorized as either an extremely weak or an inactive mouse-skin tumorigen (983), significantly diminishes DB[*a,h*]A tumorigenicity when both DB[*a,h*]A and B[*a*]A are administered simultaneously by subcutaneous injection. Despite this and similar bioassay results plus the presence of B[*a*]A and DB[*a,h*]A in MSS, both are repeatedly categorized as significant tumorigens in cigarette MSS! Similar inhibition was reported with mixtures of DMB[*a*]A and several inactive PAHs (1654).

In subsequent studies, other nontumorigenic PAHs (phenanthrene, fluoranthene, pyrene) were reported to be effective antitumorigens against B[*a*]P and DMB[*a*]A (976, 3686). The nontumorigenic hydrocarbons—benzene, naphthalene, anthracene phenanthrene, fluoranthene, pyrene—are MSS components, present at per cigarette delivery levels far in excess of those of B[*a*]P, DB[*a,h*]A, or any of the other PAHs classified as tobacco smoke toxicants.

Much evidence collected since 1932 on the tumorigenicity of PAHs indicates their tumorigenicity is not inherent but depends on specific metabolites that comprise one or more epoxides, dihydroxy compounds, and dihydroxy epoxides. For B[*a*]P, more than a dozen metabolites are known, and they show a range of tumorigenicities (983).

Conversion of B[*a*]P in an inhaled MSS particle to a particular metabolite cannot be a simple process. The more than 500 PAHs in cigarette MSS range from bicyclic to decacyclic structures. In a variety of chemical reactions, the rate of reaction decreases as the molecular weight (number of rings) of the PAH increases. That is, with stoichiometric levels of the PAH and the reactant, bicyclic PAHs react faster than tricyclic PAHs which in turn react faster than tetracyclic PAHs, etc.

Diol, epoxide, and/or diol–epoxide metabolites structurally similar to those described for B[*a*]P have been reported for many PAHs, e.g., naphthalene, anthracene, phenanthrene, B[*a*]A, benzo[*c*]phenanthrene, pyrene, chrysene, DB[*a,h*]A, benzo[*b*]triphenylene, and DMB[*a*]A (983). All of these and structurally similar PAHs have been reported by Snook et al. as cigarette MSS components (3756).

In a situation, such as the formation of metabolites, where an equimolar mixture of bicyclic through hexacyclic PAHs is present, a pentacyclic aromatic hydrocarbon such as B[*a*]P will form little of its metabolite(s) compared to the levels formed by a more reactive bicyclic or tricyclic aromatic hydrocarbon. Numerous in vitro studies have demonstrated that inclusion of equimolar quantities of lower-molecular-weight PAHs, such as phenanthrene or anthracene, inhibits the hydroxylation–epoxidation of B[*a*]P in hepatic microsomes (26A192). However, PAH data from Hoffmann and Wynder (1798) and Rodgman and Cook (3273) indicate the PAH classes (bicyclic, tricyclic, etc.) in MSS are present at

TABLE 26.6
Chronology of *N*-Heterocyclic Amine Studies

Year	Event
1959	Only one fused ring *N*-heterocyclic compound was listed by Johnstone and Plimmer (1971) as a tobacco smoke component: the bicyclic compound, quinoline
1960	Mold et al. (2592) isolated and identified the tricyclic *N*-heterocyclic 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) from CSC and defined its relationship to its precursor in tobacco, proline
1961/1962	Poindexter and Carpenter (2972) reported the isolation and identification of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) from CSC. They reported that the yield of total harmans in burley and flue-cured MSSs was between 15 and 20 μg/g of tobacco smoked, values which were 40–50 times that of the harmans in the unsmoked tobacco. Since the weight of tobacco in cigarettes sold at that time approximated 1 g, the yield of these two compounds was about 15–20 μg/cig. Poindexter and Carpenter concluded from experiments with radiolabeled tryptophan that the harmans (found to be radiolabeled in the MSS) were generated pyrogenetically by a reaction between aldehydes (formaldehyde for norharman, acetaldehyde for harman) and tryptophan in tobacco
1962	Rodgman and Cook (3279) confirmed the presence in CSC of pyrocoll and also reported the identification of indole, carbazole, and several alkylated indoles and carbazoles. Rodgman and Cook (3279) also reviewed the previously reported biological studies on indole, 3-methylindole (skatole), and carbazole: None of the three were reported to be tumorigenic
1964	Schmeltz et al. (3505) reported 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), 9*H*-pyrido[3,4-*b*]indole (norharman), and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) as tobacco smoke components. Testa and Testa (3886, 3887) also identified 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) as components of CSC
1964	The Advisory Committee to the U.S. Surgeon General (3999) briefly discussed only four fused-ring *N*-heterocyclic compounds in tobacco smoke, quinoline and the two dibenzacridines (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine) and the dibenzocarbazole (7*H*-dibenzo[*c,g*]carbazole) reported by Van Duuren et al. (4027)
1968	In his review of tobacco smoke composition, Stedman (3797) discussed the identification of tumorigenic *N*-heterocyclic compounds (dibenz[*a,h*]acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]carbazole) reported by Van Duuren et al. (4027) as well as 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll) reported by Mold et al. (2592) and 9*H*-pyrido[3,4-*b*]indole (norharman), 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), and 9*H*-pyrido[2,3-*b*]indole reported by Poindexter and Carpenter (2972)
1971/1972	Wakeham (4103) noted the reported presence of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) in cigarette MSS and discussed their formation from a reaction product of tryptophan and an aldehyde. As noted by Rodgman (3253a), the structure of the aldehyde reacting with tryptophan ultimately dictated the structure of alkylated norharmans found in CSC
1974	In addition to 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), Izard et al. (1899) reported the identification of methyl-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (methylpyrocoll) in CSC
1974/1975/1977	In a 1974 in-house RJRT report, a 1975 TCRC presentation, and a 1977 publication on their study of the water-soluble portion of CSC, Schumacher et al. (3553) reported the identifications of 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman), 5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (pyrocoll), octahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione (octahydropyrocoll), and 2-ethyl-9*H*-pyrido[2,3-*b*]indole
1977	Sugimura et al. (3829) reported the isolation and identification of the *N*-heterocyclic amines 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-1) and 3-amino-1-methyl-5*H*-pyrido[4,3-*b*]indole (Trp-P-2) from tryptophan pyrolysates
1977	In separate studies, Levitt et al. (2355a) and Nagao et al. (2667b) demonstrated the mutagenicity of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) in the Ames test
1978	Yamamoto et al. (4365a) reported the isolation and identification of Glu-P-1 and Glu-P-2 from glutamic acid pyrolysates
1978/1981	Heckman and Best (1587) reported the identification of 268 previously unidentified and over 150 previously identified *N*-containing components in CSC. These included several components structurally similar to the mutagenic *N*-heterocyclic amine: 9*H*-pyrido[2,3-*b*]indole, 2-methyl-9*H*-pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-9*H*-pyrido[2,3-*b*]indole, 2-pentyl-9*H*-pyrido[2,3-*b*]indole, 1-butyl-9*H*-pyrido[3,4-*b*]indole, 9*H*-1-propenyl-pyrido[3,4-*b*]indole, and a partially characterized norharman isomer
1979	In the 1979 U.S. Surgeon General's report (4005), the aza-arenes dibenz[*a,h*]-acridine, dibenz[*a,j*]acridine, 7*H*-dibenzo[*c,g*]carbazole, quinoline, and alkylated quinolines in CSC were discussed but not the presence or properties of the mutagenic *N*-heterocyclic amines identified in tobacco smoke
1980/1981	Yoshida and Matsumoto (4388) and Matsumoto et al. (2492) reported the identification of A*a*C and MeA*a*C in CSC
1981	Matsukura et al. (2491a) demonstrated the tumorigenicity in mice of Trp-P-1 and Trp-P-2. Hosaka et al. (1835a) demonstrated the tumorigenicity in rats of Trp-P-1 and Trp-P-2
1982	In the 1982 Surgeon General's report (4010), 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) were classified as "toxic and tumorigenic agents of cigarette smoke" in amounts of 3.2–8.1 and 1.1–3.1 μg/cig, respectively, in cigarette MSS. None of the other mutagenic *N*-heterocyclic amines in tobacco smoke were discussed
1982/1984	Snook and Chortyk (3739, 3740) reported the MSS yield of 9*H*-pyrido[3,4-*b*]indole (norharman) to be 1.2–13.4 μg/cig and that for 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman) to be 0.3–3.8 μg/cig. They found a linear relationship between the yield of cigarette MSS "tar" and the yields of 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman). In contrast to the 1962 findings of Poindexter and Carpenter (2972), Snook and Chortyk reported that the MSS yields of these two compounds were not influenced by the tobacco type

TABLE 26.6 (continued)
Chronology of *N*-Heterocyclic Amine Studies

Year	Event
1983	Demarini (933) reviewed the studies on the mutagenicity of CSC. He discussed the studies of Yoshida and Matsumoto (4388) and Matsumoto et al. (2492) on the mutagens A*a*C (80 ng/cig) and MeA*a*C (7 ng/cig)
1984	None of the authors contributing to the Searle-edited 1400-page American Chemical Society's monograph on chemical carcinogens (3568) mentioned the tumorigenic and mutagenic *N*-heterocyclic amines reported in cigarette smoke and numerous cooked foods
1984	Ohgaki et al. (2849b) demonstrated the tumorigenicity in mice, and Takayama et al. (3862b) demonstrated the tumorigenicity in rats of Glu-P-1 and Glu-P-2. Takayama et al. (3862c) demonstrated the tumorigenicity in rats of the tobacco smoke component IQ
1984/1985	Ohgaki et al. (2849, 2849a) demonstrated the tumorigenicity in mice of IQ and MeIQ, found in broiled fish, fried beef, beef extract, and CSC
1985	Takayama et al. (3862d) demonstrated the tumorigenicity in rats of Trp-P-1 and Trp-P-2. Tanaka et al. (3865c) demonstrated the tumorigenicity of IQ
1985/1986	The IARC (1870) listed several tryptophan-derived tobacco smoke isolates including 9*H*-pyrido[3,4-*b*]indole (norharman) and 1-methyl-9*H*-pyrido[3,4-*b*]indole (harman). The levels in cigarette MSS of these two components were listed as 9.5–14.1 and 2.5–5.8 μg/cig, respectively. No mention was made of the mutagenic *N*-heterocyclic amines in CSC or the degree of evidence for their carcinogenicity in animals and humans
1985/1986	Yamashita et al. (4367, 4368) identified and quantitated the following mutagenic *N*-heterocyclic amines in CSC: IQ 0.3 ng/cig Trp-P-1 0.3 ng/cig Trp-P-2 0.2 ng/cig A*a*C 16.9 ng/cig MeA*a*C 1.6 ng/cig
1986	Sugimura (3828c) reviewed the isolation and identification of the mutagenic *N*-heterocyclic amines, their high mutagenicity in the Ames test (*S. typhimurium*) of several of them, their tumorigenicity, and their various sources—including CSC for many. However, Sugimura did write the following about the importance of the mutagenic *N*-heterocyclic amines as human carcinogens: "Taking various factors into consideration, it is probably impractical and not realistic to make risk estimations from the carcinogenicity data on rodents given a single carcinogen. However, for a simple extrapolation of animal data for risk estimation, TD_{50} values, which are the doses needed to develop cancers in 50% of animals fed on carcinogens [IQ, Trp-P-1, Trp-P-2, Glu-P-1, Glu-P-2, A*a*C, and MeA*a*C] for their life time, have been calculated based on mouse experiments… If we assume the average TD_{50} value of heterocyclic amines should be about 8 mg/kg/day, we can roughly estimate the risk of these carcinogenic heterocyclic amines for human beings. The intake of heterocyclic amines was calculated from available data on their quantities in foods. Apparently the human intake is about 0.0002% times the TD_{50} obtained from animal data. This means that heterocyclic amines may not be so serious for human cancer development… On the other hand, it is also true that human beings are being exposed to many heterocyclic amines and many other carcinogens with tumor promoters and/or suppressing factors for carcinogenesis. At this moment, it is honest to state that no solid information on the estimation of risk of heterocyclic amines has been obtained in any direction, either positive or negative."
1990	Felton and Knize (1177d) reviewed the results of numerous studies on the mutagenicity and tumorigenicity of the mutagenic *N*-heterocyclic amines
1994	Lee et al. (2327c) reported that the condensate from cigarette MSS significantly inhibited the mutagenicity of several *N*-heterocyclic aromatic amines as measured in the Ames assay with *S. typhimurium* strain TA 98 in presence of S-9 mix. The mutagenic *N*-heterocyclic amines tested included: IQ MeIQ Glu-P-1 Glu-P-2 Trp-P-1 Trp-P-2 The mutagenic activities of these mutagens were suppressed as much as 80% by addition of 50–100 μg of CSC per plate
1997	Hoffmann and Hoffmann (1740) issued a revised list of tumorigenic components in tobacco and tobacco smoke. Their revision of the Hoffmann–Hecht (1727) list included, in addition to several vapor-phase components, eight of the mutagenic *N*-heterocyclic amines: IQ MeIQ Glu-P-1 Glu-P-2 Trp-P-1 Trp-P-2 A*a*C MeA*a*C

significantly higher molar levels than the pentacyclic PAHs which include B[*a*]P and DB[*a,h*]A.

In an in vitro study, the nontumorigenic PAHs pyrene and fluoranthene significantly inhibited the binding of a tumorigenic PAH to calf thymus DNA (enzyme source—mouse-skin homogenate) [Slaga and Boutwell (3683), Slaga et al. (3688)]. The in vitro inhibition of the hydroxylation reaction is paralleled by a reduction of in vivo tumorigenicity.

Because of their vapor pressure properties, tumorigenic PAHs (B[*a*]P, DB[*a,h*]A, etc.) and aza-arenes are present primarily in the MSS particulate phase. Similarly, many of the reported anticarcinogens or inhibitors occur in the MSS particulate phase (3255, 3255a, 3257), e.g., high-molecular-weight alkanes (1099), β-sitosterol and cholesterol (1099), α-tocopherol (3271, 3347), indole (3279), indole-3-acetonitrile (1898), duvatrienediols (3361), and PAHs (anthracene, phenanthrene, pyrene, fluoranthene, B[*e*]P) [see (3255a)].

Despite the fact that the anticarcinogenicity of certain components of tobacco (1171) and tobacco smoke (1672A, 1824) and of tobacco smoke itself (1824) has been known for over four decades, most discussions are directed at them as toxicants. Seldom is any significant discussion directed at smoke components known to possess anticarcinogenic properties. In a brief 1964 review of the possibility of anticarcinogenic agents in tobacco smoke, Wynder and Hoffmann [see 296, 330 in (4319)] discussed the findings of Steiner and Falk (3814) and Kotin and Falk [see 489–490 in (26A76)] in their studies with potent and weakly tumorigenic PAHs in the subcutaneous injection bioassay as well as their own findings in the mouse-skin-painting bioassay (4314, 4316). Ignored was the discussion by Kotin and Falk (26A76) on the anticarcinogenicity *vs.* B[*a*]P or *vs.* DB[*a,h*]A of nine PAHs (anthracene, benzo[*a*]fluorene, B[*a*]A, chrysene, pyrene, B[*e*]P, benzo[*k*]fluoranthene (B[*k*]A), benzo[*ghi*]fluoranthene, perylene), two aza-arenes (benzo[*a*]carbazole, benz[*c*]acridine), and 2-naphthol. All but the two aza-arenes had been identified in cigarette MSS prior to their 1964 review. Subsequently, the aza-arenes noted were identified as MSS components (3339, 3750).

Earlier, Wynder and Hoffmann (4311) had reported on MSS components that inhibited the action of a "tumorigen" invariably listed as significant. The finding was an outgrowth of their investigation of the effect of organic solvent extraction of tobacco on the PAH content of MSS. Cigarettes fabricated from the extracted tobacco yielded lower quantities of B[*a*]P and DB[*a,h*]A in MSS (3240, 3242, 3262). Skin-painting bioassays with MSS CSCs from the control and extracted tobaccos gave a lower percentage of tumor-bearing animals (% TBA) in the group treated with the extracted tobacco CSC. However, the decrease in % TBA was considerably less than the percent decrease in the level of tumorigenic PAHs in the CSC (4307). One explanation for the difference was that the solvent extracted almost all the alkanes from the tobacco. Thus, the alkanes were absent from the MSS from extracted tobacco cigarettes. This fraction (constituting about 3% of MSS CSC) was reported to significantly inhibit the tumorigenicity of B[*a*]P (4311, 4314, 26A59).

Mouse-skin-painting studies with B[*a*]P and the alkanes *n*-hentriacontane and *n*-pentatriacontane at ratios of alkane/B[*a*]P of 20:1 and 100:1 for each alkane showed they significantly inhibited B[*a*]P tumorigenicity (4311, 4314, 26A59). The MSS of a cigarette delivering 20 mg of CSC contains about 0.6 mg (600,000 ng) of the alkane fraction and 10 ng of B[*a*]P, an alkane fraction/B[*a*]P ratio of 60,000:1, far in excess of the ratios that produced significant inhibition of B[*a*]P tumorigenicity [Wynder and Hoffmann (4311, 4319, see pp. 370–371) in (4332)]. Increasing the long-chained alkane level in CSC by 1% from ~3% (C_{12} to C_{30}) to 4% by addition of crystalline alkanes isolated from CSC resulted in reduction of the tumorigenicity of the CSC from 40% to 24% TBA. This result was dismissed as "not statistically significant."

Wynder and Hoffmann [see 245–247, 628 in (4332)] again discussed anticarcinogenic components of tobacco smoke:

> Any discussion of as complex a carcinogen as tobacco smoke should at least mention the existence of anticarcinogens. These are substances that reduce or "neutralize" the effect of a carcinogen by reacting with the carcinogen or a carcinogenic metabolite, thereby deactivating it, or by competing for reaction with cell constituents, or by interfering with the resorption of a carcinogen … The existence of anticarcinogens, however, must be considered in evaluating any complex mixture such as tobacco smoke condensate … An explanation of the tumorigenic activity of tobacco smoke condensate in terms of single constituents is made more difficult by the presence of substances that may act as anticarcinogens and/or absorption retarders, especially for tumorigenic agents. It is known that structurally related noncarcinogenic hydrocarbons can inhibit the effect of carcinogenic hydrocarbons … Several investigators have noticed some inhibition of tumor growth by tobacco smoke condensate … [including] Hoffman and Griffin [1672a] … Falk et al. [1174] … [and] Homburger and Treger [1823b] … it should not come as a surprise that a material which has been proved to be carcinogenic may also interfere with tumor development, if not with tumor initiation …

They also noted [see pp. 370–371, 628–629 in (4332)]:

> An explanation of the tumorigenic activity of tobacco smoke condensate in terms of single constituents is made more difficult by the presence of substances that may act as anticarcinogens and/or absorption retarders, especially for tumorigenic agents. It is known that structurally related noncarcinogenic hydrocarbons can inhibit the effect of carcinogenic hydrocarbons. The same interrelationship may apply to tumor-promoting and nontumor-promoting phenols.

Numerous compounds demonstrated in various bioassays to be highly effective anticarcinogens against many MSS toxicants have been identified in tobacco smoke at per cigarette delivery levels far in excess of those of the alleged tumorigens. Seldom have these anticarcinogenic MSS components been discussed in the numerous reviews of the biological properties of MSS. Even though some of the earliest data on MSS components, e.g., the alkanes, that inhibit B[*a*]P tumorigenicity in the skin-painting bioassay were provided by Wynder and Hoffmann [4314, see 370–371, 628–629

in (4332)], they more often preferred to discuss alkanes as major precursors of tumorigenic PAHs in MSS [see 496–501 in (4332), 1798, 4314, 4342] rather than inhibitors of B[*a*]P tumorigenicity. MSS components reported to possess significant inhibitory or anticarcinogenic action against various tumorigenic PAHs and NNAs in MSS have been cataloged (3255, 3255a, 3257).

Those opposed to cigarette smoking view the complex mixture MSS differently from other complex mixtures such as raw or cooked foods, gasoline and diesel engine exhausts, and factory effluents [see (1345, 3685)]. Most are reluctant to accept the premise that a nontumorigenic component will offset the tumorigenicity of a tumorigen in animals treated with the complex mixtures CSC, MSS, SSS, or ETS containing the two (1773).

Other MSS components may have also influenced the mouse-skin-painting results obtained with control tobacco and extracted tobacco CSCs. Hexane extraction of tobacco not only removes alkane inhibitors thus making impossible their transfer to MSS but also removes substantial amounts of β-sitosterol (4356), α-tocopherol (3271, 3347), indole (3279), duvatrienediols (3361, 3389), and *D*-limonene (765, 2174), thus eliminating or drastically reducing their transfer to MSS during smoking. Subsequently, it was demonstrated that (1) these smoke components are present by transfer from tobacco to MSS during smoking and to SSS during smolder between puffs, or they are generated during smoking, and (2) the compounds listed are anticarcinogenic *vs*. several of the listed tumorigens, e.g., PAHs, NNAs, ethyl carbamate. However, in the 1950s, neither the identity of several of these tobacco or smoke components nor their anticarcinogenicity was known.

Comparison of identified MSS components (1373) with lists of compounds (1177a, 3685) that possess inhibitory or anticarcinogenic action in tumorigenesis studies reveals not only that MSS contains many anticarcinogens but also that their MSS levels often exceed those of the components listed as significant tumorigens. Previously, we discussed a few inhibitory and anticarcinogenic MSS components, but they represent a small sample of the MSS components reported to exhibit such properties. From the review by Slaga and DiGiovanni (3685) and other reports (1177a), we compiled a list of MSS (and tobacco) components reported to counteract the tumorigenicity of MSS toxicants (Table 26.7).

From the per cigarette MSS deliveries (Table 26.7), it may be calculated that the tumorigenic PAHs listed contribute from 4 to 10 μg/g of mainstream CSC. Nontumorigenic PAHs (naphthalene, anthracene, pyrene, phenanthrene, fluoranthene, benzo[*e*]pyrene, benzo[*b*]triphenylene) total 90–180 μg/g of CSC. The anticarcinogenic effect of nontumorigenic PAHs and weakly tumorigenic or nontumorigenic aza-arenes *vs*. carcinogenic PAHs has been known since the 1940s (3685, 3814).

An interesting aspect of Table 26.7 is that it includes the dioxins as antitumorigens. Slaga and DiGiovanni (3685) summarized the studies in which dioxins were shown to interfere with the enzyme pathways responsible for tumorigenesis of several of the most potent PAHs. The dioxins were not listed as MSS toxicants in previous tabulations similar to Table 26.7 (3255, 3255a, 3257). In fact, only the 2001 Fowles–Bates toxicant list issued since 1990 (1217) included the dioxins even though their presence in MSS was known in 1980 (854). Is the omission of such MSS toxicants related in any way to the fact that dioxins are significant antitumorigens *vs*. some of the most potent mouse-skin tumorigenic PAHs present in MSS? The 1964 advisory committee in Chapter 6 of its 1964 report mentions that 27 nontumorigenic PAHs had been identified in MSS, but none by name [see Chapter 6, p. 55 in (3999)]. Was the omission of their identities related to the fact that several were known to be antitumorigenic to several potent mouse-skin tumorigens such as B[*a*]P?

In Table 26.7 are listed only the two *n*-alkanes (C_{31} and C_{35}) shown experimentally by Wynder and Hoffmann to reduce the tumorigenicity of B[*a*]P to mouse skin. However, the alkane listing in Table 26.7 could logically be increased because the total alkane fraction consisting of *n*-, *iso*-, and *anteiso*-alkanes reduced the tumorigenicity of B[*a*]P, and presumably all of the alkanes could be involved in the tumorigenicity reduction. The number of identified components in the alkane fraction in tobacco smoke approximates 70. The complete list of the identified tobacco smoke alkanes appears in Table 1.10.

The antitumorigens and antimutagens in Table 26.7 are presented in a slightly different way in Table 26.8. Several of the significant PAH, NNA, and *N*-heterocyclic amine tumorigens or mutagens are listed in the same sequence as in Table 26.1, and the tobacco smoke components that reduce or nullify their tumorigenicity or mutagenicity are listed for each. It is interesting to see how many tobacco smoke components have been reported to inhibit or reduce the potent tumorigenicity of B[*a*]P (18 in all) or DB[*a,h*]A or DMB[*a*]A (20 in all). Here again, only 2 of the 70 alkanes examined for their inhibition of B[*a*]P tumorigenicity are included; these are the *n*-hentriacontane ($C_{31}H_{64}$) and *n*-pentatriacontane ($C_{35}H_{72}$) studied in detail by Wynder and Hoffmann (4314, 4319, 4332).

In Table 26.9, references are listed on various aspects (identification, quantitation, tobacco precursors, biological results, etc.) of the tobacco and tobacco smoke components listed in Table 26.7 as known inhibitors, anticarcinogens, and antimutagens. For the reader's benefit, the sequence of the 59 components in Table 26.9 is identical with that in Table 26.7, and the CAS nomenclature has been included in each case.

In a review of antimutagens and inhibitors of mutagenesis, Ramel et al. (26A133) discussed the many antimutagens found naturally occurring in plants. They did not discuss tobacco specifically but did discuss the natural occurrence of the following antimutagens: α-tocopherol, 2*H*-1-benzopyran-2-one, 7-hydroxy-2*H*-1-benzopyran-2-one, and 3-phenyl-2-propenal. All four have been identified as tobacco components; all but 7-hydroxy-2*H*-1-benzopyran-2-one have been identified in MSS.

Lee and Reed (2327d) investigated the antimutagenicity of nicotine *vs*. NDMA and nicotine *vs*. B[*a*]P in the Ames test (*S. typhimurium* TA 100). They observed that nicotine

TABLE 26.7
Inhibitors, Anticarcinogens, and Antimutagens in Tobacco and Tobacco Smoke

CAS No.	Component	Approximate Delivery, µg/g MSS CSC	Effective Against	AT, AM[a]	Representative References to Inhibition, Anticarcinogenicity, and/or Antimutagenicity[a]
Hydrocarbons, Aliphatic					
	Saturated aliphatic hydrocarbons[b]	30,000	B[*a*]P	AT	Wynder and Hoffmann (4314)
630-04-6	Hentriacontane $C_{31}H_{64}$				
630-07-9	Pentatriacontane $C_{35}H_{72}$				
7235-40-7	β,β-Carotene		DMB[*a*]A	AT	Mathews-Roth (2486a)
5989-27-5	*D*-Limonene	15–50	NNK	AT	Wattenberg and Coccia (26A187)
			DB[*a,i*]P	AT	Homburger et al. (26A61)
Hydrocarbons, Aromatic					
71-43-2	Benzene	480–1900	B[*a*]P, DB[*a,h*]A	AT	Crabtree (843, 844, 26A17)
91-20-3	Naphthalene	80–160	B[*a*]P, DB[*a,h*]A	AT	Crabtree (843, 844, 26A17)
120-12-7	Anthracene	4–7	B[*a*]P, DB[*a,h*]A	AT	Crabtree (843, 844, 26A17)
85-01-8	Phenanthrene	2–4	DMB[*a*]A	AT	DiGiovanni et al. (976)
206-44-0	Fluoranthene	3–4	DMB[*a*]A	AT	DiGiovanni et al. (976) Slaga et al. (3686)
129-00-0	Pyrene	3–4	DMB[*a*]A	AT	DiGiovanni et al. (976) Slaga et al. (3686)
56-55-3	B[*a*]A	0.8–2.8	DB[*a,h*]A B[*a*]P	AT	Steiner and Falk (3814) Hoffmann and Wynder [unpublished data cited on pp. 246, 292 in (4332)]
192-97-2	Benzo[*e*]pyrene	0.2	DMB[*a*]A	AT	DiGiovanni et al. (976) Slaga et al. (3686)
215-58-7	Benzo[*b*]triphenylene[c]	0.05	MC, DB[*a,h*]A, DMB[*a*]A	AT	Slaga and Boutwell (3683) Slaga et al. (3686)
Alcohols					
64-17-5	Ethanol		NNN	AT	Waddell and Marlowe (26A178)
			NNN	AM	Farinati et al. (26A32)
71-36-3	1-Butanol		NNN	AT	Waddell and Marlowe (26A178)
75-65-0	2-Propanol, 2-methyl- {*tert*-butanol}		NNN	AT	Waddell and Marlowe (26A178)
57605-80-8	α-4,8,13-Cyclodecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl) {α-4,8,13-duvane-1,3-diol}	8–20	DMB[*a*]A	AT	Saito et al. (3389)
57605-81-9	β-4,8,13-Cyclodecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl) {β-4,8,13-duvane-1,3-diol}	12–25	DMB[*a*]A	AT	Saito et al. (3389)
68-26-8	2,4,6,8-Nonatetraen-1-ol, 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (all-*E*)- {retinol}		DMB[*a*]A	AT	Shamberger (26A158)
83-46-5	β-Sitosterol	400–550	NNA PAH	AT	Wattenberg (4149b) Yasukawa et al. (26A196)
57-88-5	Cholesterol	120–240	NNA	AT	Cohen et al. (26A12)
Acids					
57-10-3	Acids, long-chained aliphatic		NNA	AM	Takeda et al. (26A171)
57-11-4	Palmitic acid $C_{16}H_{32}O_2$ Stearic acid $C_{18}H_{36}O_2$				
149-91-7	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}		NNA	AT	Mirvish et al. (2559c)
499-12-7	1-Propene-1,2,3-tricarboxylic acid {aconitic acid}		B[*a*]P	AT	Kallistratos (26A68) Kallistratos and Fasske (26A17)
331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {cinnamic acid, 3,4-dihydroxy-} {caffeic acid}		B[*a*]P	AT	Wattenberg et al. (4149c)

TABLE 26.7 (continued)
Inhibitors, Anticarcinogens, and Antimutagens in Tobacco and Tobacco Smoke

CAS No.	Component	Approximate Delivery, µg/g MSS CSC	Effective Against	AT, AM	Representative References to Inhibition, Anticarcinogenicity, and/or Antimutagenicity[a]
1135-24-6	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)- {cinnamic acid, 3-hydroxy-4-methoxy-} {ferulic acid}		B[*a*]P	AT	Wattenberg (4149b)
614-60-8	2-Propenoic acid, 3-(2-hydroxyphenyl)- {*o*-coumaric acid}		B[*a*]P	AT	Wattenberg et al. (4149c)
621-82-9	2-Propenoic, 3-phenyl-{cinnamic acid}		NPYR, NNN	AT	Chung et al. (26A07, 26A08)
Lactones					
50-81-7	Ascorbic acid		DMB[*a*]A	AT	DiGiovanni et al. (976) Slaga and Bracken (3684)
91-64-5	2*H*-Benzopyran-2-one {coumarin}		B[*a*]P, DMB[*a*]A	AT	Wattenberg et al. (26A189)
108-29-2	3*H*-2-Furanone, dihydro-5-methyl- {α-angelica lactone}		B[*a*]P	AT	Wattenberg et al. (26A189)
Phenols					
117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)- 3,5,7-trihydroxy- {quercetin}		DMB[*a*]A	AT	Kato et al. (2046a)
327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)- 1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid}		B[*a*]P	AT	Lesca (2351a)
108-95-2	Phenol	1000–7000	B[*a*]P NNN, NPYR	AT	Van Duuren et al. (4035) Chung et al. (26A07, 26A08)
88-18-6	Phenol, 2-(1,1-dimethylethyl)-		B[*a*]P	AT	Lam et al. (26A79)
128-37-0	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-		B[*a*]P, DMB[*a*]A NDEA 12-DMH	AT	Slaga and Bracken (3684) Slaga et al. (3687) Wattenberg (26A182) Clapp et al. (26A11) Clapp et al. (26A10)
150-76-5	Phenol, 4-methoxy-		B[*a*]P DMB[*a*]A	AT	Wattenberg et al. (4149c) Slaga et al. (3687)
59-02-9	α-Tocopherol {vitamin E}	400–600	MC, DMB[*a*]A DB[*a,i*]P 1,2-DMH NNA CSC	AT AT AM	Shklar (3655a) Slaga and Bracken (3684) Viaje et al. (4049a) Weerapradist and Shklar (4159c) Thompson (26A175) Rosin (26A136)
305-01-1	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}		NNK	AT	Teel and Castonguay (26A172)
520-18-3	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy- 2-(4-hydroxyphenyl)- {kaempferol}		AHR	AT	Puppala et al. (26A132)
N-Containing Components					
120-72-9	Indole	400–600	NNA NNN, NPYR NNK	AT	Matsumoto et al. (26A97) Chung et al. (26A07, 26A08) Chung et al. (26A09)
771-51-7	Indole-3-acetonitrile		B[*a*]P	AT	Wattenberg and Loub (26A190)
83-67-0	1*H*-Purine-2,6-dione, 3,7-dihydro- 3,7-dimethyl- {theobromine}		EC	AT	Nomura (26A119)
58-08-2	1*H*-Purine-2,6-dione, 3,7-dihydro- 1,3,7-trimethyl- {caffeine}		EC DMB[*a*]A NNA, NMOR	AT	Nomura (26A119) Perchellet and Boutwell (26A126) Mirvish et al. (2559c)
54-11-5	Nicotine		NNK NDMA NNAL	AT AM AM	Schüller et al. (26A141) Lee et al. (2327b) Brown et al. (437)

(*continued*)

TABLE 26.7 (continued)
Inhibitors, Anticarcinogens, and Antimutagens in Tobacco and Tobacco Smoke

CAS No.	Component	Approximate Delivery, µg/g MSS CSC	Effective Against	AT, AM	Representative References to Inhibition, Anticarcinogenicity, and/or Antimutagenicity[a]
494-97-3	Nornicotine		NDMA	AM	Lee et al. (2327b)
			NNAL	AM	Brown et al. (437)
486-56-6	Cotinine		NDMA	AM	Lee et al. (2327b)
			NNAL	AM	Brown et al. (437)
Miscellaneous Components					
622-78-6	Benzene, (isothiocyanatomethyl)-		DMB[*a*]A	AT	Wattenberg (26A184, 26A185)
121-79-4	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}		NNK	AT	Lo and Stich (26A87) Teel and Castonguay (26A172)
75-15-0	Carbon disulfide		1,2-DMH	AT	Wattenberg and Fiala (26A188)
52-90-4	Cysteine		NDMA	AT	Lo and Stich (26A87)
	Dioxin		DMB[*a*]A, MC, B[*a*]P, 7-MB[*a*]A, 12-MB[*a*]A, 5-MeC, DB[*a,h*]A	AT	Berry et al. (26A06) Cohen et al. (26A13) DiGiovanni et al. (26A23)
108-31-6	Maleic anhydride		PAH, DMB[*a*]A	AT	Klein (26A74)
7439-96-5	Manganese		B[*a*]P	AT	Sunderman et al. (3836a)
7782-49-2	Selenium		DMB[*a*]A	AT	Shamberger (26A157)
			NNA	AT	Thompson (26A175)
	CSC		Glu-P-1, Glu-P-2, Trp-P-1, Trp-P-2, IQ, MeIQ[d]	AM	Lee et al. (2327c)

B[*a*]P, Benzo[*a*]pyrene; DB[*a,h*]A, Dibenz[*a,h*]anthracene; DB[*a,i*]P, Dibenzo[*a,i*]pyrene = benzo[*rst*]pentaphene; DMB[*a*]A, 7,12-Dimethylbenz[*a*]anthracene1; 2-DMH, 1,2-Dimethylhydrazine; 7-MB[*a*]A, 7-Methylbenz[*a*]anthracene; 12-MB[*a*]A, 12-Methylbenz[*a*]anthracene; 5-MeC, 5-Methylchrysene; EC, Ethyl carbamate; Glu-P-1, 2-Amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole; Glu-P-2, 2-Aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole; PhIP, 2-Amino-1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridine; IQ, 2-Amino-3-methyl-3*H*-imidazo[4,5-*f*]quinoline; MC, 3-Methylcholanthrene = 1,2-dihydro-3-methylbenz[*j*]aceanthrylene; NDMA, *N*-Nitrosodimethylamine; NNA, *N*-Nitrosamine; NNAL, 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol; NNN, *N*′-Nitrosonornicotine; NNK; 4-(*N*-Methylnitrosamino)-1-(3-pyridinyl)-1-butanone; NPYR, *N*-Nitrosopyrrolidine; PAH, Polycyclic aromatic hydrocarbon; AHR, Aryl hydrocarbon receptor; MeIQ, 2-Amino-3,4-dimethyl-3*H*-imidazo[4,5-*f*]quinoline; Trp-P-1, 3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole; Trp-P-2, 3-Amino-1-methyl-5*H*-pyrido[4,3-*b*]indole.

[a] AT, test for antitumorigenicity; AM, test for antimutagenicity.

[b] This fraction consists primarily of the *n*-, *iso*- (2-methyl-), and *anteiso*- (3-methyl-) alkanes from C_{15} to C_{40}.

[c] Benzo[*b*]triphenylene was formerly known as dibenz[*a,c*]anthracene.

[d] Several of the highly mutagenic *N*-heterocyclic amines identified in cigarette smoke (and foods) by Sugimura et al. (see Section 17.6).

inhibits the mutagenicity of NDMA but not that of B[*a*]P. Although the mechanism of this antimutagenicity was not elucidated, the report by Murphy and Heilbrun (26A115) on the inhibition of NNN metabolism by nicotine suggests nicotine inhibition of NNA activation may be involved. Lee et al. (2327b) repeated their earlier experiment and not only confirmed the antimutagenic effect of nicotine on NDMA but also demonstrated the similar activity of nornicotine and cotinine. Brown et al. (437) reported the antimutagenicity of nicotine and cotinine *vs.* 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL).

Lee et al. (2327c) reported that CSC inhibits the mutagenic activity of several *N*-heterocyclic amines when tested in the Ames assay with *S. typhimurium* TA 98 in the presence of the S-9 activation system. The mutagenic *N*-heterocyclic amines tested included Glu-P-1, Glu-P-2, Trp-P-1, Trp-P-2, IQ, and MeIQ. These compounds are among the most potent mutagens known (3828c, 3829. 3829a, 4365a, 4357, 4368). Several have also been reported to be tumorigenic in mammalian bioassays (1177d). In one of the first demonstrations of antimutagens in tobacco smoke, Lee et al. (2327c) reported that 50–100 µg of CSC per plate suppresses the mutagenic activity of these compounds by as much as 80%. Enzymatic studies indicate that CSC is a potent inhibitor of cytochrome P-450-dependent monooxygenase. Therefore, it appears that CSC exerts its antimutagenicity by inhibiting the P-450 system.

TABLE 26.8
Inhibitors, Anticarcinogens, and Antimutagens in Tobacco and Tobacco Smoke

Component Affected	Anticarcinogen, Inhibitor, Antimutagen	Reference
PAHs	Maleic anhydride	Klein (26A74)
	β-Sitosterol	Wattenberg (4149b)
		Yasukawa et al. (26A196)
Benz[*j*] aceanthrylene, 1,2-dihydro-3-methyl-[a]	Dioxin	Berry et al. (26A06)
		Cohen et al. (26A13)
		DiGiovanni et al. (26A23)
	α-Tocopherol {vitamin E}	Shklar (3655a)
		Slaga and Bracken (3684)
		Viaje et al. (4049a)
		Weerapradist and Shklar (4159c)
B[*a*]A, 7,12-dimethyl-[b]	Ascorbic acid	DiGiovanni et al. (976)
		Slaga and Bracken (3684)
	Benzene, (isothiocyanatomethyl)-	Wattenberg (26A184, 26A185)
	Benzo[*e*]pyrene	DiGiovanni et al. (976) Slaga et al. (3686)
	2*H*-Benzopyran-2-one {coumarin}	Wattenberg et al. (26A189)
	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin}	Kato et al. (2046a)
	Benzo[*b*]triphenylene	Slaga and Boutwell (3683)
		Slaga et al. (3686)
	β,β-Carotene	Mathews-Roth (2486a)
	α-4,8,13-Cyclodecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl) {α-4,8,13-duvane-1,3-diol}	Saito et al. (3389)
	β-4,8,13-Cyclodecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl) {β-4,8,13-duvane-1,3-diol}	Saito et al. (3389)
	Dioxin	Berry et al. (26A06)
		Cohen et al. (26A13)
		DiGiovanni et al. (26A23)
	Fluoranthene	DiGiovanni et al. (976)
		Slaga et al. (3686)
	Maleic anhydride	Klein (26A74)
	2,4,6,8-Nonatetraen-1-ol, 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (all-*E*)- {retinol}	Shamberger (26A158)
	Phenanthrene	
	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	Slaga and Bracken (3684)
		Slaga et al. (3687)
		Wattenberg (26A182)
	Phenol, 4-methoxy-	Wattenberg et al. (4149c)
		Slaga et al. (3687)
	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine}	Nomura (26A119)
		Perchellet and Boutwell (26A126)
		Mirvish et al. (2559c)
	Pyrene	DiGiovanni et al. (976)
		Slaga et al. (3686)
	Selenium	Shamberger (26A157)
	α-Tocopherol {vitamin E}	Shklar (3655a)
		Slaga and Bracken (3684)
		Viaje et al. (4049a)
		Weerapradist and Shklar (4159c)
B[*rst*]P	*D*-Limonene	Homburger et al. (26A61)
B[*a*]P	Anthracene	Crabtree (843, 844, 26A17)
	B[*a*]A	Hoffmann and Wynder [unpublished data cited on pp. 246, 292 in (4332)]

(*continued*)

TABLE 26.8 (continued)
Inhibitors, Anticarcinogens, and Antimutagens in Tobacco and Tobacco Smoke

Component Affected	Anticarcinogen, Inhibitor, Antimutagen	Reference
	Benzene	Crabtree (843, 844, 26A17)
	2*H*-Benzopyran-2-one {coumarin}	Wattenberg et al. (26A189)
	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid}	Lesca (2351a)
	Dioxin	Berry et al. (26A06) Cohen et al. (26A13) DiGiovanni et al. (26A23)
	3*H*-2-Furanone, dihydro-5-methyl- {α-angelica lactone}	Wattenberg et al. (26A189)
	Hentriacontane $C_{31}H_{64}$	Wynder and Hoffmann (4314)
	Manganese	Sunderman et al. (3836a)
	Naphthalene	Crabtree (843, 844, 26A17)
	Pentatriacontane $C_{35}H_{72}$	Wynder and Hoffmann (4314)
	Phenol	Van Duuren et al. (4035)
	Phenol, 2-(1,1-dimethylethyl)-	Lam et al. (26A79)
	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	Slaga and Bracken (3684) Slaga et al. (3687) Wattenberg (26A182)
	1-Propene-1,2,3-tricarboxylic acid {aconitic acid}	Kallistratos (26A68) Kallistratos and Fasske (26A69)
	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {cinnamic acid, 3,4-dihydroxy-, caffeic acid}	Wattenberg et al. (4149c)
	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)- {cinnamic acid, 3-hydroxy-4-methoxy-, ferulic acid}	Wattenberg (4149b)
	2-Propenoic acid, 3-(2-hydroxyphenyl)- {*o*-coumaric acid}	Wattenberg et al. (4149c)
DB[*a,h*]A	Anthracene	Crabtree (843, 844, 26A17)
	B[*a*]A	Steiner and Falk (3814)
	Benzene	Crabtree (843, 844, 26A17)
	Benzo[*b*]triphenylene	Slaga and Boutwell (3683) Slaga et al. (3686)
	Dioxin	Berry et al. (26A06) Cohen et al. (26A13) DiGiovanni et al. (26A23)
	Naphthalene	Crabtree (843, 844, 26A17)
	Phenol, 4-methoxy-	Wattenberg et al. (4149c) Slaga et al. (3687)
NNAs	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}	Mirvish et al. (2559c)
	Cholesterol	Cohen et al. (26A12)
	Indole	Matsumoto et al. (26A97)
	Palmitic acid $C_{16}H_{32}O_2$	Takeda et al. (26A171)
	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-Trimethyl- {caffeine}	Nomura (26A119) Perchellet and Boutwell (26A126) Mirvish et al. (2559c)
	Stearic acid $C_{18}H_{36}O_2$	Takeda et al. (26A171)
	Selenium	Thompson (26A175)
	β-Sitosterol	Wattenberg (4149b) Yasukawa et al. (26A196)
NDMA	Cotinine	Lee et al. (2327b)
	Cysteine	Lo and Stich (26A87)
	Nicotine	Schüller et al. (26A141)
	Nornicotine	Lee et al. (2327b)
NDEA	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	Clapp et al. (26A11)

TABLE 26.8 (continued)
Inhibitors, Anticarcinogens, and Antimutagens in Tobacco and Tobacco Smoke

Component Affected	Anticarcinogen, Inhibitor, Antimutagen	Reference
NPYR	2-Propenoic, 3-phenyl- {cinnamic acid}	Chung et al. (26A07, 26A08)
	Phenol	Chung et al. (26A07, 26A08)
	Indole	Chung et al. (26A07, 26A08)
NNN	1-Butanol	Waddell and Marlowe (26A178)
	Ethanol	Waddell and Marlowe (26A178)
		Farinati et al. (26A32)
	Indole	Chung et al. (26A07, 26A08)
	Phenol	Chung et al. (26A07, 26A08)
	2-Propanol, 2-methyl- {*tert*-butanol}	Waddell and Marlowe (26A178)
	2-Propenoic, 3-phenyl- {cinnamic acid}	Chung et al. (26A07, 26A08)
NNK	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}	Lo and Stich (26A87)
		Teel and Castonguay (26A172)
	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}	Teel and Castonguay (26A172)
	Indole	Chung et al. (26A09)
	D-Limonene	Wattenberg and Coccia (26A187)
	Nicotine	Schüller et al. (26A141)
NMOR	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine}	Mirvish et al. (2559c)
N-Heterocyclic Amines		
Glu-P-1	CSC	Lee et al. (2327c)
Glu-P-2	CSC	Lee et al. (2327c)
IQ	CSC	Lee et al. (2327c)
MeIQ	CSC	Lee et al. (2327c)
Trp-P-1	CSC	Lee et al. (2327c)
Trp-P-2	CSC	Lee et al. (2327c)

[a] 1,2-Dihydro-3-methylbenz[*j*]aceanthrylene = 3-methylcholanthrene is regarded as one of the most potent tumorigens to mouse skin known. Although it does not appear in any of the lists in Table 26.1 by Hoffmann et al., it is a tobacco smoke component.

[b] DMB[*a*]A is regarded as one of the most potent tumorigens to mouse skin known. Although it does not appear in any of the lists in Table 26.1 by Hoffmann et al., it is a tobacco smoke component.

Lee et al. (2327c) subsequently reported that fractionation of CSC gave fractions that showed low mutagenicity themselves but were significantly antimutagenic.

Only a few of the listed MSS tumorigens have ever been tested for tumorigenicity to lung tissue by exposure of animals via inhalation. The results with all but one of the four MSS components [B[*a*]P, NDMA, NDEA, ^{210}Po], tested via inhalation at dose levels substantially exceeding those in MSS, were rated "equivocal" (3095). Only ^{210}Po, administered via inhalation at massive dose levels to rats, produced squamous cell carcinoma, the lung tumor type similar to that associated statistically with cigarette smoking. However, the U.S. Surgeon General (4005, 4010) and Hoffmann and Hecht (1727) discounted the effect of ^{210}Po in MSS in lung cancer causation in active smokers. From the type of evidence available presently, it is doubtful that many of the toxicants should be included in the various lists. Examination of data and reports on the tobacco smoke components present in one or more of the many lists sustains the premise that it is inappropriate to use such lists as evidence of any relationship between exposure to MSS and lung cancer induction in smokers or exposure to ETS and lung cancer induction in nonsmokers.

Several specific components could and should be excluded from the toxicant lists for reasons other than the failure to induce lung tumors via inhalation:

1. By the early 1960s, dibenzo[*a,l*]pyrene had been reported in MSS by several groups [see account in (3262)]. For its identification, the investigators relied on a published UV spectrum purportedly that of synthetic dibenzo[*a,l*]pyrene (dibenzo[*def,p*]chrysene). However, in 1966, it was demonstrated that the published spectrum was that of an isomer, dibenz[*a,e*]aceanthrylene (dibenzo[*a,e*]fluoranthene) (2314).
2. Previously was noted the failure by many research groups between 1963 and 2000 to confirm the presence in MSS of the tumorigenic aza-arenes reported by Van Duuren et al. (4027). Dibenz[*a,j*]acridine was reported recently by Rustemeier et al. (3370).
3. The precursors of arsenic and NDELA in MSS have been banned from U.S. tobacco agronomy since 1952 and 1981, respectively.

TABLE 26.9
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

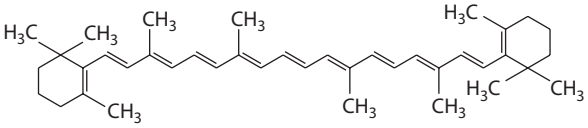
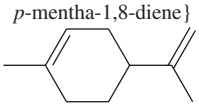
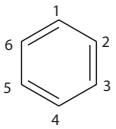
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Hydrocarbons, Aliphatic					
1.	630-04-6	Hentriacontane $H_3C\text{-}(CH_2)_{29}\text{-}CH_3$	14, 18, 239, 613, 619, 625, 727, 765, 767, 776, 883, 966, 1099, 1100, 1360, 1375, 1375a, 1375b, 1437, 1444, 1445, 1586, 1651, 1744, 1842, 2079, 2100, 2102, 2170, 2172, 2176, 2177, 2570, 2601a, 2761, 2762, 2765–2767, 2777, 2799a, 2857, 2939, 3240, 3247, 3251, 3255, 3265, 3308, 3431, 3457, 3557, 3562, 3608, 3768, 3797, 3876, 3966, 4184, 4193, 4194, 4249, 4284, 4320, 4333, 4354, 4406, 5079, 5512, 5811b	120, 181, 182, 480, 613, 619, 647, 701, 727, 832, 840, 876, 877, 883, 908, 1308, 1480, 1591, 1651, 1848, 1893b, 1978, 2079, 2101, 2270, 2283, 2595, 2939, 3194, 3604, 3605, 3607–3609, 3613a, 3616, 3679, 3703, 3755, 3797, 3964, 3965, 4249, 4337, 5079, 5189, 5345, 5657, 5682, 5811b	1360, 1375a
2.	630-07-9	Pentatriacontane $H_3C\text{-}(CH_2)_{33}\text{-}CH_3$	625, 727, 1375, 1375b, 1586, 2176, 2767, 2939, 3265, 3557, 3797, 4249, 4320, 4333, 5811b	727, 1893b, 1978, 2939, 3607, 3609, 3613a, 3616, 3679, 3755, 3797, 4249, 4320, 5811b	
3.	7235-40-7	β,β-Carotene {β-carotene, all-*trans*} 	3257	120, 367, 433, 543a, 585, 830a, 832, 835, 838, 922b, 943, 971, 972, 1053, 1063–1066, 1068–1074, 1110, 1156, 1254, 1256, 1927a, 1941, 1956, 2079, 2270, 2283, 2338, 2339b, 2543, 2545, 2611, 2761, 2762, 2765, 2766, 2939, 3059, 3194, 3218, 3266, 3616, 3645, 3797, 3971, 3973, 3974a, 4090, 4159, 4222, 4249, 4286, 5079, 5189, 5300, 5811b	
4.	5989-27-5	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- {*D*-limonene}	2543, 2601a, 3300, 4249, 4570a		

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

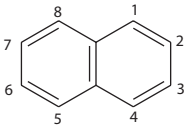
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		The following includes reports on limonene in which its stereochemistry was not defined:			
5.	138-86-3	Cyclohexene, 1-methyl-4-(1-methylethenyl)- {limonene, *p*-mentha-1,8-diene} 	111, 112, 156, 157, 172, 199, 239, 299, 314, 315, 462, 568b, 765, 900, 1063–1066, 1068–1074, 1099, 1140, 1153, 1154, 1262a, 1286, 1313, 1338, 1348–1350, 1354, 1364, 1365, 1371, 1373–1375, 1375a, 1375b, 1377, 1416–1419, 1427, 1431, 1432, 1437, 1445, 1586, 1589, 1634, 1637, 1638, 1663, 1842, 1882, 1947, 1971, 1974, 1975, 2002, 2003, 2173, 2174, 2387, 2493, 2506, 2507, 2508, 2543, 2545, 2570, 2597, 2628, 2629, 2636, 2722, 2765, 2767, 2777, 2799a, 2857, 2870, 2874, 2939, 3255, 3257, 3265, 3302, 3308, 3397, 3410, 3451, 3508, 3530, 3557, 3797, 3826, 4068, 4121, 4249, 4259, 4570a, 5034, 5512, 5770, 5811b	404, 568b, 909, 984, 2282, 2339a, 2611, 2917a, 3186, 3188, 3905, 4249, 5811b	1354, 1375a, 1377, 2387, 2506, 2507
Hydrocarbons, Aromatic					
6.	71-43-2	Benzene 	73, 111, 112, 126, 126a, 126b, 141–143, 147, 151, 156, 157, 167, 172, 173a, 174a, 174b, 174c, 174e, 199, 203, 222–224, 237, 239, 299, 314, 315, 402, 414, 462, 493–495, 544–546, 566, 568, 568b, 603, 605, 643, 645, 688, 705, 902, 966, 1026, 1050, 1063–1074, 1139, 1140, 1148, 1153, 1154, 1168, 1217, 1243, 1262a, 1313, 1348–1351,	568b, 984, 4249, 5811b	1228, 1354, 1375a, 1377, 1378, 2244, 3401, 4052, 4056

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
	Benzene (cont.)	1354, 1365, 1373–1375, 1375a, 1375b, 1377, 1378, 1386, 1412–1414, 1416, 1418, 1423, 1443, 1445, 1472, 1485, 1571a, 1586, 1589, 1634, 1637, 1639, 1643, 1649, 1673, 1674, 1701, 1727, 1740, 1741, 1743, 1744, 1751, 1760, 1773, 1842, 1849–1852, 1868, 1870, 1871, 1873, 1947, 1966, 1975, 2002, 2063, 2079, 2088, 2090, 2096, 2114, 2133, 2142, 2256, 2270, 2293, 2310, 2313a, 2354, 2520, 2543, 2545, 2570, 2589, 2601b, 2634, 2644, 2645, 2765, 2767, 2777, 2782, 2799a, 2800, 2804, 2822, 2825, 2857, 2870, 2939, 2942, 3003, 3007, 3059, 3106, 3135–3137, 3190, 3251, 3254, 3255, 3257, 3260, 3265, 3300, 3302, 3308, 3370, 3368, 3441a, 3410, 3418, 3464–3470, 3482, 3493, 3498, 3500, 3530, 3557, 3692, 3711, 3729, 3794, 3797, 3876, 3897, 3901, 3992, 4005–4007, 4052, 4056, 4078, 4104, 4111,4135, 4151, 4162, 4166, 4249, 4257, 4259, 4319, 4360, 5034, 5049, 5070, 5508, 5512, 5531, 5547, 5554, 5692a, 5770, 5811b, 5869a, 5960		

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
7.	91-20-3	Naphthalene 	84, 104, 141–144, 147, 151, 156, 157, 167, 172, 174e, 239, 291, 299, 329, 394, 397, 568b, 603, 624, 710, 746a, 798, 869, 966, 1094, 1099, 1100, 1135, 1139, 1287, 1288, 1313, 1360, 1371, 1375, 1375a, 1375b, 1377, 1378, 1427, 1435a, 1437, 1442, 1445, 1447, 1462, 1472, 1485, 1649, 1650, 1652, 1744, 1760, 1767, 1781, 1842, 1959, 1972, 1981, 2013, 2079, 2113, 2114, 2133, 2134, 2142, 2195, 2255, 2270, 2313a, 2428, 2438, 2479, 2506, 2507, 2508, 2543, 2545, 2557, 2570, 2722, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2784, 2939, 2961, 2962, 3003, 3081, 3082, 3176, 3191, 3240, 3241, 3249, 3251, 3255, 3257, 3262, 3263, 3265, 3269, 3273, 3286, 3292, 3300, 3302, 3307, 3308, 3370, 3397, 3410, 3441a, 3452, 3464–3470, 3472, 3492, 3498, 3509, 3557, 3559, 3578, 3616, 3618–3620, 3647, 3729, 3732, 3741, 3757–3759, 3787, 3797, 3847, 4009, 4010, 4249, 4282, 4319, 4325, 4342, 4355, 4570a, 4966, 5010, 5034, 5077, 5512, 5539, 5811b, 5869a, 5960	84, 172, 568b, 2339a, 2784, 4249, 5533, 5567, 5636, 5811b	1360, 1375a, 1377, 1378, 2506, 2507, 3401, 3402

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

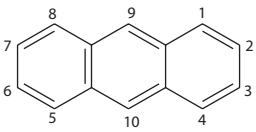
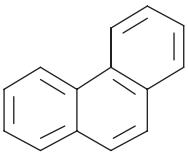
	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
8.	120-12-7	Anthracene 	39, 49, 50, 84, 104, 126a, 128, 141–143, 147, 151, 172, 245, 290, 291, 329, 394, 397, 398, 443, 568b, 583, 584, 603, 624, 646a, 710, 726, 746a, 785, 818–820, 869, 878, 885, 966, 1099, 1100, 1136, 1139, 1172, 1211, 1287–1289, 1360, 1371, 1373, 1375a, 1378, 1388–1390, 1406, 1408, 1409, 1427, 1435a, 1445, 1462, 1471, 1485, 1649, 1744, 1767, 1842, 1870, 1871, 1873, 1933, 2013, 2037a, 2079, 2088, 2099, 2113, 2114, 2116, 2120, 2121, 2126, 2127, 2130, 2134, 2170, 2194–2196, 2200, 2203, 2210, 2255, 2256, 2270, 2313a, 2352, 2365–2367, 2370, 2425, 2501, 2543, 2557, 2570, 2596a, 2648–2650, 2710, 2713–2715, 2717, 2761, 2762, 2765–2767, 2773, 2777, 2799a, 2893, 2894, 2939, 2961, 2962, 2964, 3003, 3032, 3046, 3176, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3265, 3273–3275, 3286, 3291, 3292, 3300, 3302, 3307, 3308, 3323, 3324, 3340a, 3370, 3410, 3415, 3421–3424, 3437, 3452, 3465–3470, 3472, 3514, 3557, 3578, 3616, 3618–3620, 3741,	84, 172, 568b, 903, 2079, 2939, 2995, 3059, 3194, 3547, 4249, 4332, 5567, 5811b	50, 1360, 1375a, 1378, 2210

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Anthracene (cont.)	3758, 3759, 3787, 3788, 3797, 3863, 3876, 3973, 3999, 4001, 4248, 4249, 4282, 4284, 4296, 4300, 4311, 4342, 4352–4355, 4399, 4404, 5010, 5077, 5079, 5359, 5512, 5539, 5811b		
9.	85-01-8	Phenanthrene 	39, 50, 84, 104, 126a, 128, 141–143, 151, 147, 172, 239, 291, 329, 394, 397, 443, 584, 603, 646a, 710, 726, 746a, 798, 819, 820, 869, 966, 1099, 1136, 1139, 1172, 1287, 1288, 1329, 1330, 1360, 1375, 1375a, 1375b, 1377, 1388–1390, 1406, 1408, 1409, 1427, 1435a, 1437, 1445, 1462, 1471, 1485, 1644, 1645, 1647–1649, 1744, 1767, 1842, 1981, 2013, 2037a, 2079, 2099, 2113, 2130, 2134, 2142, 2170, 2191, 2195, 2200, 2210, 2215, 2238, 2256, 2270, 2313a, 2365, 2438, 2537, 2543, 2557, 2596a, 2570, 2710, 2722, 2731, 2735, 2761, 2762, 2765–2767, 2773, 2777, 2799a, 2822, 2858, 2894, 2939, 2961–2964, 3003, 3024, 3030, 3032, 3033, 3047, 3049, 3081, 3082, 3149, 3176, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3265, 3273, 3292, 3300, 3302, 3307, 3308, 3323,	84, 172, 1660, 2339a, 2917a, 3059, 3194, 3205, 4249, 5567, 5811b	50, 1330, 1360, 1375a, 1375a, 1377, 2210

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

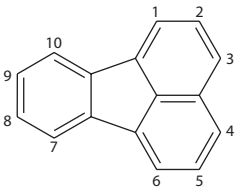
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Phenanthrene (cont.)	3325, 3370, 3410, 3421–3424, 3437, 3441a, 3452, 3465–3470, 3472, 3514, 3557, 3616, 3618–3620, 3685, 3729, 3741, 3758, 3759, 3787, 3797, 3876, 4248, 4249, 4282, 4284, 4300, 4311, 4342, 4355, 4400, 5010, 5027, 5077, 5079, 5359, 5510, 5512, 5539, 5811b		
10.	206-44-0	Fluoranthene 	39, 49, 50, 104, 117, 126a, 126b, 128, 141–143, 151, 172, 216, 239, 244, 291, 329, 583, 584, 603, 646a, 726, 746a, 798, 804, 818–820, 966, 869, 1019, 1099, 1100, 1136, 1139, 1172, 1235, 1236, 1287–1289, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408, 1409, 1437, 1445, 1462, 1471, 1649, 1712, 1744, 1763, 1781, 1787, 1788, 1800, 1842, 1870, 1871, 1873, 1971, 2013, 2037a, 2079, 2099, 2130, 2134, 2191, 2196, 2200, 2203, 2210, 2238, 2256, 2270, 2313a, 2365–2367, 2430, 2438, 2473, 2474, 2501, 2557, 2596a, 2722, 2777, 2799a, 2893, 2939, 2961, 2962, 2964, 3083, 3141, 3149, 3176, 3191, 3240–3243, 3246, 3249–3251, 3255, 3257, 3262, 3265, 3273–3275, 3286, 3291, 3292,	903, 2079, 2939, 3059, 3194, 3205, 4249, 5567, 5811b	50, 1375a, 1377, 1378, 2210

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

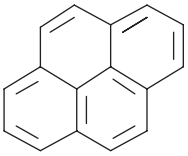
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Fluoranthene (cont.)	3300, 3302, 3307, 3308, 3370, 3421–3424, 3437, 3452, 3465–3467, 3469, 3493, 3514, 3610, 3616, 3618, 3685, 3686, 3756, 3758–3759, 3787, 3788, 3797, 3820, 3876, 3952, 4005, 4009–4011, 4018, 4019, 4020, 4022, 4031, 4110, 4249, 4282, 4284, 4300, 4307, 4308, 4311, 4315, 4319, 4323, 4324, 4354, 4355, 4404, 5077, 5512, 5539, 5732, 5811b		
11.	129-00-0	Pyrene {benzo[*def*]phenanthrene} 	39, 49, 50, 104, 126a, 126b, 128, 141–143, 151, 154, 172, 239, 245, 290, 291, 329, 394, 397–399, 583, 584, 588, 589, 603, 646a, 710, 726, 746a, 785, 804, 818–820, 878, 885, 966, 869, 1019, 1099, 1100, 1136, 1139, 1172, 1211, 1287–1289, 1373, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408, 1409, 1437, 1445, 1462, 1471, 1475, 1644, 1645, 1647–1649, 1744, 1781, 1787, 1788, 1800, 1842, 1870, 1871, 1873, 2013, 2037a, 2099, 2113, 2116, 2130, 2134, 2142, 2195, 2203, 2238, 2255, 2256, 2270, 2313a, 2352, 2353, 2365–2367, 2425, 2426, 2428, 2430, 2438, 2473, 2479, 2501, 2557, 2596a, 2648–2650,	172, 903, 2079, 2939, 3059, 3194, 3205, 3973, 4249, 5567, 5811b	50, 1375a, 1377, 1378

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TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

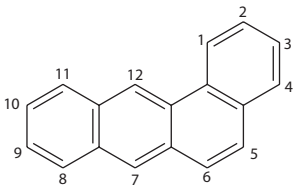
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyrene {benzo[def]phenanthrene} (cont.)	2709, 2710, 2713–2715, 2717, 2799a, 2865, 2893, 2894, 2939, 2960–2962, 2964, 3003, 3024, 3030, 3032, 3033, 3046, 3047, 3049, 3149, 3176, 3191, 3240–3243, 3246, 3249, 3251, 3255, 3257, 3262, 3265, 3269, 3273, 3286, 3291, 3292, 3300, 3302, 3307, 3308, 3370, 3415, 3421–3424, 3437, 3452, 3465–3467, 3469, 3470, 3472, 3514, 3610, 3616, 3618–3620, 3685, 3686, 3756, 3758, 3759, 3787, 3788, 3797, 3820, 3863, 3876, 3952, 3999–4001, 4005–4007, 4009–4011, 4018, 4019, 4020, 4031, 4110, 4248, 4249, 4282, 4284, 4300, 4307, 4308, 4311, 4315, 4319, 4354, 4355, 4399, 4404, 5010, 5027, 5077, 5079, 5486, 5512, 5539, 5811b		
12.	56-55-3	Benz[*a*]anthracene {B*a*A or B[*a*]A} 	39, 104, 126, 126a, 126b, 128, 139, 141–143, 147, 151, 203, 216, 237, 239, 290, 291, 329, 394, 397–399, 603, 624, 646a, 726, 746a, 797, 869, 1025, 1136, 1139, 1148, 1211, 1217, 1287–1289, 1329, 1330, 1332, 1333, 1373, 1375a, 1377, 1378, 1388–1390, 1397, 1405, 1406, 1408,	903, 3205, 4249, 4332, 5567, 5811b	1330, 1332, 1375a, 1377, 1378

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References		
		Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Benz[a]anthracene {BaA or B[a]A} (cont.)	1409, 1445, 1462, 1471, 1492, 1674, 1709, 1727, 1740, 1741, 1743, 1744, 1760, 1767a, 1773, 1781, 1787, 1788, 1792, 1798, 1800, 1802, 1803, 1808, 1842, 1870, 1871, 1873, 1933b, 1971, 2013, 2037a, 2078, 2079, 2099, 2113, 2116, 2121, 2126, 2127, 2130, 2133, 2134, 2142, 2195, 2199, 2215, 2238, 2256, 2313a, 2352, 2366, 2367, 2425, 2426, 2430, 2438, 2524a, 2537, 2596a, 2710, 2799a, 2825, 2893, 2939, 2960–2962, 2964, 3003, 3007, 3024, 3030, 3032, 3033, 3047, 3049, 3081, 3082, 3087, 3088, 3131, 3158, 3162, 3176, 3190, 3191, 3240–3242, 3249, 3251, 3255, 3257, 3262, 3264, 3265, 3272–3275, 3286, 3292, 3300, 3302, 3307, 3308, 3370, 3437, 3470, 3472, 3493, 3616, 3618–3620, 3713, 3741, 3756–3759, 3878, 3788, 3797, 3814, 3847, 3952, 3973, 3975, 3984, 3992, 4001, 4005–4007, 4009–4011, 4248, 4249, 4282, 4300, 4307, 4308, 4311, 4315, 4316, 4319, 4322, 4324, 4332, 4355, 5010, 5077, 5512, 5531, 5539, 5732, 5811b, 5869a, 5960		

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

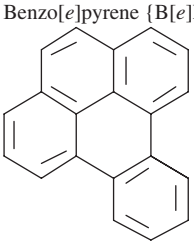
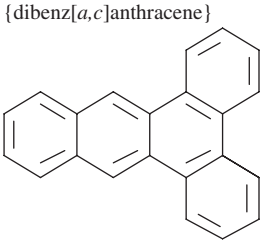
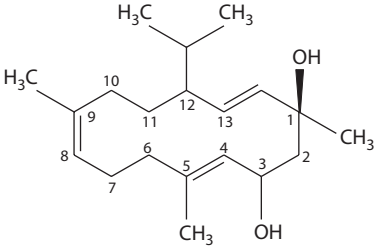
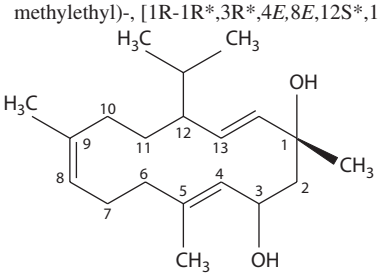
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
13.	192-97-2	Benzo[*e*]pyrene {B[*e*]P} 	39, 50, 104, 126a, 126b, 141–143, 151, 216, 290, 291, 329, 432, 646a, 726, 797, 1025, 1099, 1136, 1139, 1172, 1211, 1289, 1373, 1388–1390, 1397, 1406–1409, 1445, 1462, 1471, 1475, 1781, 1786, 1787, 1788, 1800, 1870, 1871, 1873, 2013, 2037a, 2060, 2099, 2116, 2130, 2134, 2210, 2238, 2255, 2256, 2260, 2313a, 2327, 2352, 2374, 2426, 2438, 2479, 2557, 2596a, 2744, 2799a, 2865, 2893, 2939, 2961, 2962, 2964, 3003, 3033, 3176, 3191, 3251, 3255, 3257, 3262, 3265, 3273, 3286, 3292, 3300, 3302, 3308, 3365, 3437, 3470, 3472, 3514, 3572, 3610, 3616, 3618–3620, 3685, 3686, 3741, 3756, 3758, 3759, 3787, 3788, 3797, 3952, 4005–4007, 4009–4011, 4018, 4019, 4031, 4036, 4110, 4249, 4300, 4307, 4308, 4315, 4317, 4319, 4323, 4324, 4332, 4355, 5010, 5077, 5732	903, 3205, 4249	50, 2210
14.	215-58-7	Benzo[*b*]triphenylene {dibenz[*a,c*]anthracene} 	1373, 1781, 2037a, 2438, 3003, 3255, 3257, 3265, 3300, 3365, 3683, 3685, 3686, 3688, 3756, 3787, 3788, 4005–4007, 4010, 4011, 4036, 4249, 5811b		

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Alcohols					
15.	64-17-5	Ethanol {ethyl alcohol}	37, 38, 172, 222–224, 314, 568b, 605, 916, 1140, 1375a, 1377, 1378, 1412–1414, 1416, 1419, 1422, 1449, 1481, 1905, 1907, 2088, 2270, 2634, 2858, 2939, 3224, 3255, 3257, 3265, 3302, 3308, 3530, 3692, 3797, 3882, 3901, 4005–4007, 4052, 4056, 4162, 4249, 4319, 4570a, 5811b	120, 172a, 174b, 568b, 1053, 1481, 1550, 2702a, 2339a, 2861a, 2939, 3266, 3328, 3370, 3797, 3973, 3974a, 4249, 5079, 5811b	1375a, 1377, 1378, 4052, 4056
16.	71-36-3	1-Butanol {*n*-butyl alcohol} $H_3C\text{-}(CH_2)_2\text{-}CH_2OH$	172, 568b, 1140, 1218, 1373, 1375a, 1377, 1378, 1416, 2559, 2559a, 3255, 3257, 3265, 3266, 3302, 3559, 3797, 4249, 5811b	568b, 1053, 1550, 2339a, 3186, 3188, 3266, 3328, 3905, 3973, 4249	1375a, 1377, 1378
17.	75-65-0	2-Propanol, 2-methyl- {*tert*-butanol}	3265	2386, 4249	
18.	57605-80-8	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]- 	1063–1066, 1068–1075, 1373, 2543, 2570, 2601a, 2726, 2761, 2762, 2765, 2766, 3255, 3257, 3265, 3971, 4249	9, 227, 297, 404, 675, 676, 909, 943, 1149, 1149a, 1591, 2054, 2338, 2341a, 2786, 2914, 2939, 3195, 3197, 3215, 3219, 3221, 3329, 3389, 3613a, 3621, 3703, 3704, 3706, 3797, 3971, 3973, 3974a, 4089, 4249, 5811b	
19.	57605-81-9	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-1R*,3R*,4*E*,8*E*,12S*,13*E*]- 	1373, 2726, 3255, 3257, 3265, 4249	9, 227, 675, 676, 909, 943, 1149, 1149a, 1591, 2054, 2338, 2341a, 2786, 2914, 2939, 3195, 3197, 3215, 3219, 3221, 3389, 3607, 3613a, 3621, 3703, 3704, 3706, 3778, 3797, 3971, 3973, 3974a, 4089, 4249, 5811b	
20.	68-26-8	2,4,6,8-Nonatetraen-1-ol, 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (all-*E*)- {retinol}		2917a	

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

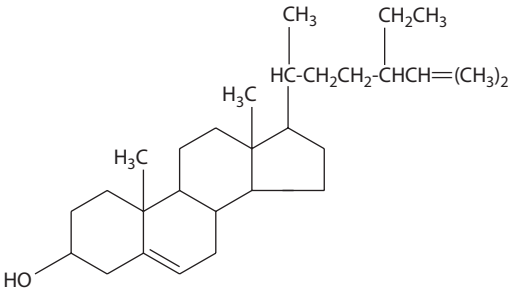
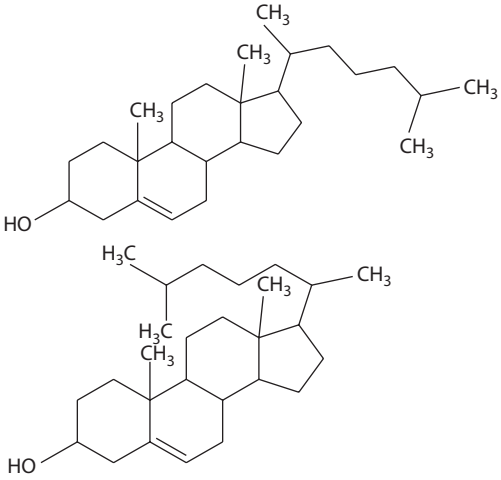
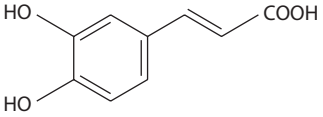
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
21.	83-46-5	Stigmast-5-en-3-ol, (3β)- {β-sitosterol} 	172, 278, 705, 765, 1099, 1100, 1352, 1360, 1375, 1375a, 1375b, 1586, 1651, 1744, 1842, 1933, 2176, 2570, 2767, 2939, 3059, 3251, 3255, 3257, 3265, 3268, 3302, 3308, 3391, 3423, 3484, 3557, 3608, 3741, 3797, 3999, 4249, 4319, 5512, 5811b	114, 116, 120, 722, 832, 838, 907a, 214, 1291,1329, 1352, 1647, 1651, 2338, 2400, 2939, 3059, 3072, 3219, 3263, 3268, 3269, 3291, 3346, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3604, 3605, 3608, 3611, 3616, 3755, 3797, 3867, 3920, 3924, 3974a, 4249, 5628, 5811b, 5860	1360, 1375a
22.	57-88-5	Cholest-5-en-3-ol (3β)- {cholesterol} 	126a, 126b, 172, 237, 1099, 1100, 1171, 1352, 1360, 1373, 1375a, 1434, 1445, 1586, 1651, 1674, 1744, 1842, 1933, 2080, 2570, 2601a, 2767, 2939, 3255, 3257, 3265, 3484, 3557, 3608, 3741, 4249, 5079, 5108, 5109, 5189, 5300, 5413, 5512, 5811b	832, 840, 907a, 1076a, 1171, 1329, 1352, 1651, 1933a, 2080, 2338, 2400, 2939, 3072, 3263, 3435, 3470, 3472, 3476, 3484, 3493, 3511, 3608, 3755, 3797, 3867, 3920, 3973, 3974a, 4249, 5079, 5242, 5811b, 4A03, 4A04, 4A05, 25A54, 25A58	1360, 1375a
Acids					
23.	57-10-3	Hexadecanoic acid {palmitic acid} H_3C-$(CH_2)_{14}$-COOH	60, 101, 172, 239, 257, 258, 722, 723, 765, 809, 966, 1132, 1063–1066, 1068–1074, 1231, 1329, 1330, 1332, 1333, 1348, 1364, 1365, 1371, 1373, 1375, 1375a, 1375b, 1377, 1388–1390, 1437, 1448, 1449, 1582, 1586, 1651, 1744, 1785, 1944, 2387, 2418, 2529, 2543, 2545, 2570, 2601a, 2683, 2761, 2762, 2766, 2767, 2773, 2775, 2777,	60, 101, 120, 172a, 174b, 404, 634, 637, 722, 835, 836, 838, 891, 908, 1053, 1329, 1330, 1332, 1333, 1388–1390, 1590a, 1651, 1785, 1848, 1893a, 1893b, 1982, 2079, 2270, 2283, 2338, 2339a, 2356, 2386, 2389, 2529, 2544, 2570, 2593, 2862, 2917a, 2939, 3155, 3194, 3219, 3266, 3328, 3329, 3332, 3349, 3430, 3511, 3543, 3545, 3547, 3549, 3550,	1330 (0), 1332 (0), 1375a, 1377, 2387

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Hexadecanoic acid {palmitic acid} (cont.)	2799a, 2857, 2939, 3265, 3266, 3293, 3302, 3308, 3384, 3410, 3447, 3454, 3457, 3496, 3553, 3555, 3557, 3608, 3876, 4005–4007, 4030, 4249, 4280, 4319, 4354, 4570a, 5512, 5552, 5811b	3555, 3560, 3561, 3608, 3755, 3812, 3973, 3974a, 4042c, 4131, 4249, 4280, 5079, 5189, 5367, 5380, 5388, 5695, 5811b	
24.	57-11-4	Octadecanoic acid {stearic acid} $H_3C\text{-}(CH_2)_{16}\text{-}COOH$	60, 101, 172, 257, 258, 722, 765, 809, 966, 1063–1066, 1068–1074, 1132, 1329, 1330, 1332, 1333, 1348, 1360, 1364, 1373, 1375, 1375a, 1375b, 1388–1390, 1448, 1582, 1586, 1651, 1744, 1785, 1842, 1944, 2418, 2529, 2570, 2601a, 2683, 2767, 2777, 2939, 3265, 3293, 3302, 3308, 3384, 3447, 3457, 3557, 3608, 3876, 4005–4007, 4030, 4249, 4280, 4319, 5512, 5552, 5811b	60, 101, 120, 404, 634, 835, 836, 838, 908, 1329, 1330, 1332, 1333, 1388–1390, 1472, 1651, 1785, 2092, 2270, 2283, 2338, 2339a, 2356, 2389, 2529, 2544, 2570, 2593, 2649, 2917a, 2939, 3155, 3219, 3329, 3332, 3349, 3461, 3511, 3545, 3547, 3560, 3561, 3608, 3755, 3812, 3876, 3974a, 4131, 4042c, 4249, 4280, 5079, 5189, 5367, 5811b	1330, 1332, 1360, 1375a
25.	149-91-7	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}	1373, 1842, 2195, 3219, 3265, 3308, 3712, 4249	3655b, 5079	
26.	499-12-7	1-Propene-1,2,3-tricarboxylic acid {aconitic acid}	2572, 3255, 3257, 3265, 4249	1053, 3266, 3370	
27.	331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid} 	1626, 1743, 1744, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3300, 3308, 3712, 3714, 3797, 4036, 4113, 4163, 4249, 4376, 5079, 5389, 5512, 5811b, 4A01	72, 120, 722, 835, 890, 1102, 1626, 1981, 2154, 2216, 2270, 2514, 2939, 2954, 3029, 3103, 3161, 3462, 3476, 3655b, 3660, 3700, 3748, 3749, 3751, 3973, 3974a, 4249, 4999, 5079, 5126, 5385, 5389, 5591, 5652, 5672. 5673, 5705, 5713, 5722, 5809, 5810, 5811b, 5830, 5831, 5900, 5908, 4A01	

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

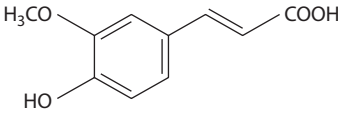
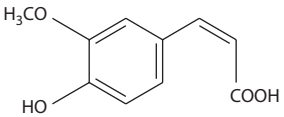
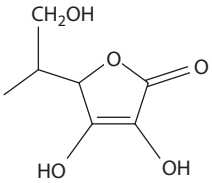
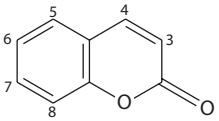
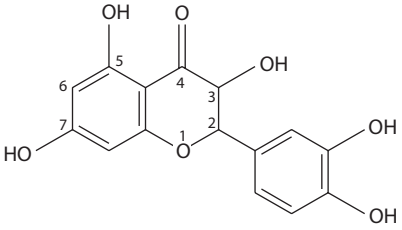
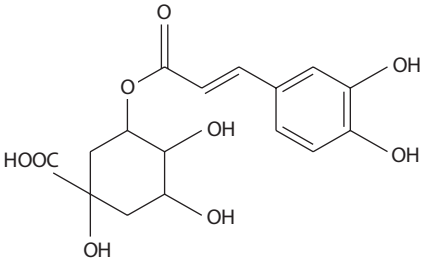
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
28.	1135-24-6	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)- {cinnamic acid, 3-hydroxy-4-methoxy-, ferulic acid} The following numerous reports describe the identification of the *cis*- or *trans*- isomers of ferulic acid:	3712, 5811b	5811b	
29.	537-98-4	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid} 	1626, 1842, 1884, 2216, 2939, 3255, 3257, 3265, 3555, 3749, 3797, 4249, 4377, 5811b	404, 1102, 1626, 1884, 2216, 2389, 2544, 2939, 2954, 3103, 3161, 3555, 3748, 3749, 3751, 3797, 3973, 3974a, 4249, 4377	
30.	1014-83-1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid} 	1626, 1842, 2216, 2939, 3255, 3257, 3302, 3712, 3741, 3743, 3749, 4249, 4377	1102, 1626, 2216, 2389, 2544, 2939, 2954 3103, 3161, 3748, 3749, 3751, 3797, 3973, 3974a	
31.	614-60-8 583-17-6	2-Propenoic acid, 3-(2-hydroxyphenyl)- {*o*-coumaric acid}	3265, 3741, 3743, 4113, 4249, 5811b	3109, 4249, 5811b	
32.	621-82-9	2-Propenoic acid, 3-phenyl- {cinnamic acid} C_6H_5-CH═CH-COOH	2767, 3265, 3266, 3557, 4159, 4249, 5811b	172a, 174b, 722, 1053, 1102, 1983, 2389, 2544, 2914, 3266, 3370, 3973, 4249, 5811b	
Lactones					
33.	50-81-7	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-} 	3257, 3266, 3685, 4249, 4751a	120, 174b, 379, 486, 557, 1053, 1971, 2079, 2270, 2489, 2532, 2939, 3266, 3707, 3922, 4236, 4249, 5079, 5267a, 5811b	
34.	91-64-5	2*H*-1-Benzopyran-2-one {coumarin} 	239, 568b, 966, 1364, 1371, 1373, 1427, 1599, 1649, 1842, 2209, 2413, 2543, 2757, 2759, 2767, 2773, 2939, 3193, 3255, 3257, 3263, 3265, 3300, 3302, 3308, 3410, 3474, 3557, 3685, 3753, 3876, 3995, 4025, 4050, 4249, 4354, 5811b	568b, 633, 729, 774, 1156, 1256, 1578, 1649, 1785, 2280, 2543, 2545, 2611, 2699, 2757, 2759, 2761, 2762, 2765, 2766, 3263, 3328, 3329, 3536, 3560, 3643, 3676, 4050, 4090, 4249, 5591, 5711, 5811b	
35.	108-29-2	2(3*H*)-Furanone, dihydro-5-methyl- {α-angelica lactone, γ-valerolactone}	1360, 1371, 1375a, 1883, 2731, 2735, 2775, 3266, 4249	172a, 174b, 404, 1053, 2389, 2544, 2917a, 3219, 3266, 3370, 4249, 5811b	1360, 1375a

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
Phenols					
36.	117-39-5	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin, 3,3a,4a,5,7-pentahydroxyflavone} 	3096, 3555, 5652, 5750, 5758, 5811b, 5904	72, 120, 970, 1077b, 1837a, 2270, 2379, 2704a, 2939, 3059, 3462, 3555, 3685, 3794, 3797, 3974a, 4036, 4403, 4999, 5079, 5255, 5641, 5652, 5750, 5758, 5811b, 5904	
37.	327-97-9 93451-46-8	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid} 	172, 602, 1884, 3257, 3302, 3792, 3797, 4249, 5811b	69, 72, 120, 254, 385, 486, 598, 602, 657, 665, 677b, 718, 830a, 831, 834, 835, 838, 840, 890, 917, 970, 1040, 1063–1066, 1068–1074, 1077b, 1309, 1329, 1333, 1352, 1485, 1625, 1626, 1923, 2014, 2056a, 2079, 2154, 2250a, 2270, 2283, 2313a, 2338, 2361, 2395, 2514, 2531, 2529, 2557a, 2810–2812, 2911c, 2911d, 2914, 2939, 2954, 3029, 3059, 3096, 3161, 3302, 3366a, 3367a, 3400, 3459–3462, 3551, 3616, 3628, 3631, 3641, 3646, 3655b, 3700, 3705, 3738, 3748, 3749, 3751, 3754, 3792, 3794, 3797, 3806, 3973, 3974a, 3974b, 3984, 3999, 4005–4007, 4156, 4221, 4249, 4275, 4279, 4372, 4402, 4403, 4421, 4999, 5079, 5189, 5200, 5246, 5353, 5389, 5576, 5592–5594, 5596, 5604, 5652, 5665, 5672, 5673, 5681, 5697,	

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

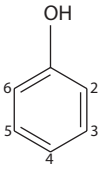
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-O-caffeoylquinic acid} (cont.)		5698, 5700, 5705, 5713, 5722, 5737, 5761, 5782, 5784, 5788, 5808–5810, 5811b, 5812, 5827, 5831, 5834, 5839, 5850, 5856, 5889, 3890, 5896, 5900, 5908	
38.	108-95-2	Phenol 	37, 38, 50, 83, 100, 126a, 126b, 155, 157, 167, 172, 173a, 174a, 174b, 174c, 174e, 213, 237, 239, 248, 269, 270, 274–277, 293, 295, 337, 351, 359, 392, 396, 397, 402, 414, 520, 521, 532, 539, 568b, 603, 615, 616, 636, 640, 663, 664, 688, 722, 723, 765, 789, 789a, 804, 828, 830a, 851, 859, 884, 891a, 912, 922c, 1051, 1063–1074, 1091, 1099, 1115, 1129, 1132, 1138, 1140, 1153, 1158, 1213, 1215, 1232, 1236, 1283, 1284, 1292, 1303, 1329, 1330, 1332, 1333, 1336, 1339, 1348–1350, 1354, 1360, 1361,1364, 1365, 1369, 1371, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1423, 1426, 1427, 1437, 1442, 1445, 1449, 1450, 1492, 1494, 1502, 1589, 1647, 1648, 1649, 1673, 1674, 1699, 1709, 1741, 1744, 1751, 1760, 1764, 1766, 1789, 1791, 1797, 1803, 1807a, 1827, 1842, 1857, 1879, 1881, 1882 1884,	100, 120, 404, 568b, 937, 984, 1085, 1590a, 1825, 1876, 1877a, 1980, 2014, 2338, 2339a, 2379a, 2386, 2389, 2544, 2607, 2862, 2917a, 2939, 3090, 3194, 3350, 3430, 3547, 3549, 3973, 3974a, 4064, 4202, 4249, 5079, 5093, 5811b	50, 1330, 1332, 1354, 1360, 1375a, 1377, 1378, 2387, 2506, 2507, 3395, 3401, 3402, 3405

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Phenol (cont.)	1906, 1928, 1966, 1981, 1995, 1999, 2042–2045, 2062, 2079, 2082–2086, 2088, 2089, 2114, 2125, 2133, 2142, 2170, 2190, 2191, 2195, 2230, 2245, 2253, 2254, 2261, 2262a, 2270, 2274, 2295, 2306, 2307, 2311, 2312, 2313a, 2327c, 2351, 2374, 2376–2378, 2379a, 2387, 2397, 2399, 2400d, 2408, 2476, 2480, 2493, 2506, 2507, 2508, 2526, 2543, 2545, 2570, 2577, 2578, 2582, 2583, 2598, 2601a, 2605, 2607, 2628–2631, 2636, 2653, 2681, 2683, 2691–2695, 2719, 2731, 2735, 2737, 2739, 2740, 2747, 2761, 2762, 2775, 2777, 2799a, 2800, 2820, 2857, 2858, 2876, 2899, 2927, 2939, 2983, 3007, 3043, 3059, 3–65, 3087, 3088, 3090, 3093, 3095, 3105, 3111, 3121a, 3131, 3132, 3165, 3166, 3171–3175, 3187, 3190, 3228, 3251, 3255, 3257, 3263–3265, 3277, 3286, 3291, 3300, 3302, 3305, 3306, 3308, 3314, 3370, 3373, 3394, 3397, 3410, 3447, 3451–3453, 3454, 3457, 3462, 3468, 3470, 3476, 3482, 3486, 3488, 3493,		

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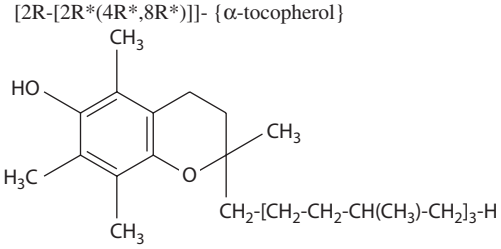
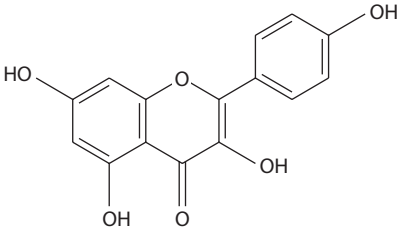
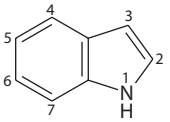
TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Phenol (cont.)	3497, 3500, 3551, 3553, 3555, 3557, 3559, 3572, 3576, 3577, 3616, 3625, 3650, 3671, 3712, 3716–3720, 3746, 3747, 3764, 3765, 3767, 3795, 3797, 3800, 3826, 3844, 3884, 3892, 3912a,3939, 3952, 3984, 3990a, 3992, 4005–4007, 4009, 4036, 4064, 4065, 4067, 4113, 4118, 4121, 4122, 4159, 4228, 4232, 4248, 4249, 4259, 4268, 4269a, 4290, 4301, 4304, 4311, 4314, 4317, 4319, 4322, 4328–4330, 4338, 4349, 4350, 4407, 4418, 4636, 4796, 4965, 5011, 5031, 5034, 5079, 5093, 5140, 5207, 5500, 5512, 5531, 5532, 5546, 5555, 5564, 5576, 5588, 5643a, 5811b, 5835, 5838, 5865a, 5960		
39.	88-18-6	Phenol, 2-(1,1-dimethylethyl)-	2554, 3746, 3747, 4249, 5811b		
40.	128-37-0	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-	568b, 1063–1066, 1068–1074, 1364, 1365, 1825, 1884, 2327c, 2767, 3410, 3553, 3557, 3712, 4159, 4249, 4570a	568b, 1825, 2386, 2917a, 3186, 3188, 3549, 3550, 4249	
41.	150-76-5	Phenol, 4-methoxy-	414, 1586, 1626, 2387, 2570, 2598, 2767, 3255, 3257, 3265, 3555, 3712, 3764, 3797, 4319, 4414, 4796, 5011, 5811b	1876, 1877a, 2389, 2544, 3555, 5811b	2387, 3395
42.	1406-66-2	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl) {tocopherol}		5811	

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
43.	59-02-9	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- {α-tocopherol} 	1360, 1373, 1375a, 1842, 1884, 2601a, 2939, 3059, 3170, 3251, 3255, 3257, 3265, 3266, 3271, 3286, 3295, 3300, 3302, 3655a, 3684, 3685, 3797, 3875, 4159c, 4249	120, 174b, 486, 557, 667, 840, 1053, 1651, 2270, 2939, 3059, 3155, 3156, 3170, 3266, 3295, 3347, 3349, 3357, 3484, 3493, 3616, 3655a, 3707, 3755, 3797, 3811, 3875, 3971, 3973, 3974a, 4098a, 4236, 4249, 5079, 5811b	1360, 1375a
44.	305-01-1	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}	969, 1572, 1626, 1884, 2939, 3059, 3257, 3265, 3302, 3797, 4249, 5811b	969, 970, 1626, 2939, 2954, 3103, 3059, 3194, 3797, 3973, 3974a, 4249, 5711, 5811b, 5888	
45.	520-18-3	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(4-hydroxyphenyl)- {kaempferol, 3,4a,5,7-tetrahydroxyflavone} 	2767, 3095a, 3555, 3794, 4249, 5652, 5758	1626, 1971, 2939, 3059, 3555, 3794, 4249, 5652, 5758, 5811b	
N-Containing Components					
46.	120-72-9	1*H*-Indole {2,3-benzopyrrole} 	127, 172, 239, 568b, 722, 884, 918a, 1063–1066, 1068–1074, 1099, 1329, 1330, 1332, 1333, 1360, 1361, 1364, 1365, 1371, 1375, 1375a, 1375b, 1388–1390, 1423, 1426, 1427, 1437, 1580, 1586, 1649, 1744, 1765, 1767, 1778, 1842, 1881, 1898, 2005, 2060, 2387, 2493, 2506–2508, 2510, 2524a, 2537, 2543, 2545, 2552, 2553, 2570, 2601a, 2630, 2683, 2724–2727, 2731, 2735, 2596a,	172, 404, 543a, 568b, 937, 984, 1063–1066, 1068–1074, 1256, 1590a, 2093, 2282, 2339a, 2386, 2389, 2544, 2611, 2917a, 3198, 3219, 3430, 3491, 3547, 3549, 3550, 3555, 3973, 4249, 5811b	1330, 1332, 1360, 1375a, 2387, 2506 (0), 2507 (0)

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

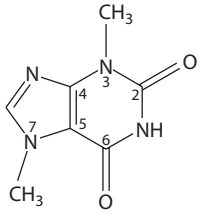
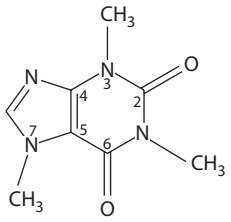
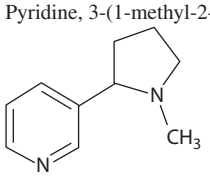
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		1*H*-Indole {2,3-benzopyrrole} (cont.)	2761, 2762, 2765–2767, 2773, 2775, 2799a, 2857, 2939, 3081, 3082, 3251, 3255–3257, 3265, 3279, 3286, 3300, 3302, 3308, 3386, 3397, 3410, 3491, 3493, 3504, 3506, 3555, 3557, 3559, 3729, 3733, 3741, 3750, 3752, 3797, 3886, 3887, 3890, 4249, 5034, 5512, 5811b		
47.	771-51-7	1*H*-Indole-3-acetonitrile	1842, 1898, 3219, 3255, 3257, 3265, 3308, 3685, 4249, 5811b		
48.	83-67-0	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- {theobromine} 	568b, 1375, 1375b, 2601a, 3255, 3257, 3265, 3553, 4249, 5811b	568b, 1204, 2313, 4249a	
49.	58-08-2	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine} 	568b, 1365, 1842, 3255, 3257, 3265, 3266, 3553, 4249, 5811b	568b, 1053, 3266, 4249	
50.	54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} 	14, 29–31, 41–43, 50, 83, 85a, 86–89, 95, 96, 106, 107, 117, 119, 123, 126, 126a, 126b, 126c, 160, 171, 172, 173a, 174b, 174c, 175, 178, 187, 188, 196–198, 207, 209, 211, 218, 222–224, 237, 239, 270, 274–276, 282, 288, 292b, 293, 294, 302, 306, 308, 337–339, 352, 353,	29, 64, 69, 120, 174c, 207, 212, 256, 261, 262, 306, 308, 324, 337, 339, 374, 404, 410, 427–429, 429e, 468, 480, 499, 504, 506- 508, 515, 548–550, 555, 555a, 557, 559, 568b, 647, 654, 660, 667, 677b, 678, 679, 685, 687, 689, 722, 792, 830a, 856, 866, 867, 888, 910, 914, 915a, 915b,	50 (0), 1330 (0), 1332 (0), 1354, 1360, 1375a (0), 1377 (0), 1378 (0), 2387, 2506 (0), 2507 (0)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	355, 357a, 357b, 362–365, 375, 376, 378, 382, 388, 395, 409, 410, 413, 424, 427–429, 429e, 437, 438, 441, 442, 445, 446, 456, 462, 469a, 473, 480, 488, 489, 491, 492, 499, 521, 527, 559, 568b, 575, 576, 578, 590, 603, 636, 638, 677b, 678, 679, 681, 686, 688, 723, 761, 765, 767, 768, 804, 824, 830a, 849, 850, 852, 866, 887, 888, 916, 918a, 919, 921, 953, 959, 962, 966, 973, 975, 988a, 989, 998, 999, 1006a, 1007, 1011, 1016, 1022, 1031, 1051, 1063–1075, 1078, 1083, 1084, 1088, 1089a, 1097, 1099, 1100, 1107, 1112, 1118, 1128b, 1129, 1134, 1137, 1138, 1162, 1166–1170, 1177b, 1187, 1188, 1199, 1203, 1215, 1225, 1232, 1263, 1271, 1275, 1283, 1284, 1293, 1301, 1314, 1317–1319, 1320, 1323, 1329–1334, 1334a, 1336, 1338, 1339, 1341, 1348–1350, 1354, 1360–1363, 1366, 1368, 1371–1375, 1375a, 1375b, 1376, 1377, 1378, 1380, 1384–1386, 1388–1390, 1423, 1427, 1437, 1442–1445, 1449, 1450, 1464, 1466, 1469, 1483, 1484, 1491, 1492, 1497,	959, 963, 984–986, 989, 995, 997, 998, 1003, 1004, 1007, 1015, 1020, 1033, 1035, 1036, 1063–1066, 1068–1074, 1086, 1088, 1090, 1101, 1107, 1113, 1114, 1118, 1176, 1189, 1193–1199, 1203, 1220–1226, 1276, 1324, 1327, 1329, 1330, 1332, 1333, 1361, 1384, 1385, 1388–1390, 1393, 1464, 1492, 1546, 1549, 1550, 1564, 1567a, 1568, 1575, 1577, 1580, 1584, 1606, 1608–1613, 1615, 1624, 1676, 1686, 1702, 1709, 1712, 1719, 1725, 1730, 1746, 1749, 1774, 1811, 1812, 1814, 1836, 1837, 1848, 1853b, 1860a, 1927, 1933a, 1962a, 1990, 2006, 2079, 2104–2111, 2118, 2139, 2146–2150, 2152, 2153, 2164, 2166, 2167, 2191, 2212, 2226, 2263, 2270, 2272, 2273, 2282, 2283, 2290, 2294, 2331a, 2332, 2334, 2337, 2338, 2339a, 2349, 2359, 2372, 2374, 2389, 2417, 2446, 2488, 2503, 2504, 2528, 2529, 2532, 2534, 2543–2545, 2557a, 2606, 2611, 2682, 2688, 2689, 2724, 2761, 2762, 2765, 2766, 2786, 2792, 2841, 2844, 2913, 2914, 2917a, 2919, 2920, 2921,	

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	Name (per CA Collective Index)	References: Tobacco Smoke	References: Tobacco	References: Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	1502, 1519, 1523, 1536, 1542, 1546, 1567a, 1568, 1580, 1584, 1586, 1589, 1606, 1607, 1614, 1615, 1637, 1639, 1642, 1673, 1674, 1686, 1687, 1692, 1695, 1696, 1700, 1702, 1709, 1719, 1725, 1730, 1736, 1738, 1741, 1743, 1744, 1749, 1760, 1761, 1764, 1766, 1797, 1807a, 1810–1812, 1814, 1818, 1827, 1836, 1837, 1842, 1848, 1860a, 1878, 1882, 1887a, 1890, 1891, 1901, 1908, 1909, 1912, 1913, 1921, 1928, 1933, 1942, 1950, 1966, 1984–1996, 1989, 1990, 2006, 2007, 2012, 2055, 2061, 2062, 2079, 2088, 2097, 2100, 2103, 2110, 2111, 2133, 2134a, 2142, 2144, 2146–2153, 2164, 2166, 2167, 2170, 2171, 2181, 2191, 2211, 2212, 2223, 2225–2229, 2231, 2247, 2254, 2261, 2263, 2267, 2269, 2270–2272, 2294, 2303, 2313, 2313b, 2324, 2327c, 2337, 2338, 2349, 2353a, 2371, 2372, 2374–2378, 2400d, 2401, 2408, 2410, 2412, 2416, 2417, 2446, 2451, 2458, 2459, 2482, 2488, 2493, 2503, 2504, 2506, 2507, 2517, 2523, 2524, 2524a,	2924–2926, 2938, 2939, 2954, 2979–2982, 2989, 3016, 3019, 3022, 3024, 3027, 3028, 3034, 3035, 3041, 3044, 3056, 3059, 3063, 3073, 3074, 3087, 3155, 3188, 3214, 3219, 3254, 3329, 3333, 3375, 3420, 3430, 3444, 3459, 3460, 3476, 3477, 3482, 3491, 3499, 3511, 3512, 3517, 3543, 3549, 3560, 3561, 3570, 3571, 3608a, 3614, 3633, 3634, 3670a, 3705, 3707, 3767a, 3797, 3816, 3905, 3925, 3926, 3928, 3942, 3943b, 3950, 3961, 3972–3974, 3974a, 3974b, 3976, 3980, 3983a, 3999, 4009–4011, 4016, 4017, 4043, 4045, 4047, 4051, 4071, 4073, 4103, 4127, 4159, 4169–4173, 4189, 4207, 4210, 4213, 4218, 4236, 4249, 4266a, 4267, 4370, 4418, 4420, 4529, 4744, 4745, 4817, 4885, 4921, 5000, 5001, 5005, 5018, 5020, 5024, 5033, 5040, 5053, 5079, 5083, 5106, 5107, 5112, 5121, 5122, 5126, 5131, 5133, 5140, 5144, 5146, 5150, 5159, 5161, 5162, 5165, 5171, 5172, 5174, 5189, 5198, 5209, 5213, 5214, 5223, 5229, 5244, 5247, 5258, 5259, 5263, 5267, 5294, 5324, 5331, 5335, 5336, 5339, 5349, 5351, 5366, 5382, 5389, 5390, 5390a, 5391, 5404, 5405, 5416, 5419, 5427, 5430, 5439a, 5444, 5445, 5451–5453, 5463, 5469, 5474, 5477, 5481, 5482, 5487, 5488, 5498, 5499, 5508, 5512, 5528, 5535, 5536, 5542,	

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

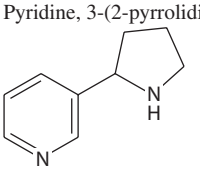
		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	2528, 2535, 2543, 2545, 2546, 2549, 2557a, 2570, 2601a, 2603, 2606, 2610, 2612, 2613, 2622, 2628, 2632, 2635, 2652, 2653, 2658, 2668–2673, 2683, 2688, 2690–2695, 2696, 2717, 2719, 2724, 2737, 2739, 2740, 2744, 2761, 2762, 2767, 2774, 2777, 2792, 2793, 2799a, 2800, 2827–2829, 2831, 2832, 2835–2837, 2839, 2840, 2842–2845, 2848, 2857, 2863, 2869, 2874, 2877, 2878a, 2879, 2880, 2899, 2912, 2919, 2920, 2921, 2924–2927, 2936–2939, 2947, 2951, 2958, 2959, 2966, 2967a, 2969, 2970, 2973–2976, 2980, 2982, 2984–2986, 2998, 3008–3016, 3019, 3021, 3022, 3024, 3025, 3027- 3029, 3035, 3040, 3041, 3044, 3045, 3054, 3056, 3057, 3059, 3072b, 3078, 3087–3089, 3116, 3121a, 3133, 3137, 3139, 3140, 3142, 3143, 3148a, 3156, 3190, 3214, 3227, 3228, 3254, 3255, 3257, 3258, 3265, 3274, 3300, 3302, 3308, 3333, 3370, 3373, 3375, 3378, 3386, 3397, 3398, 3406, 3407, 3410, 3415, 3426, 3443–3446, 3457,	5561, 5573, 5582, 5622, 5623, 5634, 5652, 5654–5656, 5663, 5664, 5667, 5676, 5681, 5685, 5701, 5702, 5712, 5725, 5726, 5734, 5735, 5765, 5771, 5772, 5774, 5775, 5790, 5803, 5811b, 5824, 5828, 5848, 5853, 5884, 5886, 5895, 5896, 5901, 5905, 17B05, 17B06, 17B08, 17B11, 17B14, 17B18, 17B20, 17B29, 17B42, 17B43, 17B44, 17B48, 17B61, 17B62, 17B64, 21A07, 21A08, 21A40–21A42,	

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

		References		
CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	3461, 3454, 3477, 3482, 3491, 3493, 3499, 3505, 3516, 3517, 3521, 3548, 3553, 3557–3559, 3562, 3563, 3570–3572, 3576, 3577, 3585, 3623, 3640, 3658, 3659, 3662, 3670–3672, 3682, 3722, 3731, 3739–3742, 3782–3784, 3790, 3796, 3797, 3803, 3822, 3826, 3833, 3844, 3876, 3884, 3896, 3909, 3910, 3921, 3926, 3928, 3930, 3934, 3936–3939, 3942, 3943, 3952, 3955–3959, 3961, 3972, 3980, 3984, 3990, 3992, 3999, 4009–4011, 4016, 4017, 4039, 4045, 4064, 4065, 4072, 4075, 4076, 4078, 4082, 4103, 4116, 4119–4122, 4127, 4132, 4134, 4137, 4138, 4140–4143, 4162, 4167–4176, 4178–4183, 4189–4191, 4194, 4197, 4198, 4202–4207, 4210, 4211, 4213, 4240, 4248, 4249, 4259, 4264, 4267, 4268, 4273, 4275a, 4285, 4291, 4309, 4310, 4319, 4330, 4363, 4366, 4370, 4385, 4398, 4418, 4529, 4570a, 4636, 4745, 4921, 4994, 5000, 5008, 5013, 5017, 5034, 5035, 5041, 5045, 5047, 5052., 5065, 5068, 5069, 5071, 5079, 5082,		

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine} (cont.)	5084, 5099, 5100, 5104, 5112, 5118, 5124, 5129, 5130, 5140, 5159, 5163, 5175, 5166, 5179, 5183, 5189, 5207, 5210, 5211, 5219, 5225, 5226, 5236, 5258, 5259, 5263, 5325, 5343, 5346, 5351, 5390, 5401, 5412, 5414, 5427, 5431, 5443, 5452, 5458–5461, 5470–5472, 5473, 5475, 5476, 5480, 5489, 5507, 5508, 5512, 5520, 5529, 5531, 5532, 5544-5546, 5554, 5558, 5563, 5565, 5643a, 5679, 5706, 5770, 5811b, 5836, 25A84, 25A85		
51.	494-97-3	Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine} 	126, 174b, 237, 239, 429e, 480, 568b, 761, 830a, 1078, 1084, 1222, 1315–1317, 1373, 1375, 1375b, 1437, 1567a, 1568, 1584, 1696, 1702, 1744, 1751, 1842, 2079, 2228, 2482, 2647, 2724, 2734, 2767, 2844, 2845, 2921, 2922, 2939, 3044, 3056, 3057, 3059, 3126c, 3265, 3302, 3308, 3444, 3477, 3491, 3499, 3553, 3557, 3559, 3742, 3797, 3972, 3999, 4103, 4249, 4350, 5008, 5079, 5258, 5259, 5512, 5531, 5811b	64, 120, 174b, 324, 429e, 480, 504, 548–550, 555a, 557, 568b, 654, 660, 667, 687, 792, 830a, 856, 915b, 995, 1005, 1010, 1015, 1087, 689, 867, 1101, 1114, 1221, 1311, 1315–1317, 1324, 1327, 1564, 1567a, 1568, 1584, 1696, 1702, 1712, 1916a, 1927, 1962a, 2079, 2139, 2224, 2283, 2331a, 2334, 2349, 2359, 2532, 2543, 2647, 2724, 2746, 2761, 2762, 2765, 2766, 2844, 2914, 2921, 2922, 2939, 3044, 3050, 3056, 3059, 3063, 3126c, 3444, 3459, 3460, 3477, 3482, 3491, 3499, 3260a, 3511, 3608a, 3670a,	

(*continued*)

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

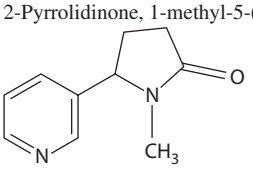
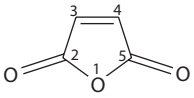
			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine} (cont.)		3767a, 3797, 3943b, 3972–3974, 3974a, 3974b, 3983a, 3999, 4073, 4103, 4161, 4218, 4236, 4249, 4683, 4885, 4974, 5005, 5008, 5023, 5033, 5038, 5079, 5189, 5258, 5259, 5382, 5390, 5406, 5408, 5409, 5416, 5455, 5463, 5477, 5488, 5497, 5561, 5573, 5582, 5620, 5676, 5685, 5701, 5702, 5727, 5771, 5804, 5811b, 5820, 5853, 5864, 5884, 5895, 5896, 5901, 5905, 17B06, 17B18, 17B38, 17B55	
52.	486-56-6	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, (S)- {cotinine} 	353, 437, 469a, 568b, 761, 830a, 1078, 1063–1066, 1068–1074, 1084, 1099, 1100, 1360, 1365, 1375a, 1567a, 1568, 1580, 1586, 1673, 1695, 1700, 1702, 1719, 1751, 2228, 2482, 2543, 2601a, 2724, 2761, 2762, 2765, 2767, 2773, 2775, 2799a, 2839, 2939, 3054, 3056, 3057, 3059, 3190, 3255, 3257, 3265, 3302, 3308, 3386, 3398, 3410, 3491, 3553, 3559, 3739–3742, 3972, 3992, 4249, 4407, 5035, 5508, 5565, 5811b	64, 120, 504, 553, 568b, 689, 830a, 984, 995, 998, 1012, 1226a, 1385, 1567a, 1568, 1702, 1712, 2338, 2359, 2724, 2917a, 2939, 2995, 3056, 3059, 3444, 3477, 3491, 3549, 3550, 3797, 3972–3974, 3974a, 4236, 4249, 4921, 5011, 5508, 5685, 5735, 5811b	1360, 1375a
Miscellaneous Components					
53.	622-78-6	Benzene, (isothiocyanatomethyl)-		4249	
54.	121-79-9	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}	3265	5811b	

TABLE 26.9 (continued)
Anticarcinogens, Antitumorigens, Inhibitors, and Antimutagens in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
55.	75-15-0	Carbon disulfide	237, 722, 1140, 1373, 1420, 1422, 1741,1831, 2310, 2313a, 2799a, 2939, 2940, 2945, 3255, 3257, 3265, 3300, 3302, 3729, 3797, 4249, 4319, 4332, 5039, 5811b, 5869a	5079, 5189, 21A05	
56.	52-90-4	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto- (R)} $HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	1274, 3265, 3266, 4249	120, 158, 172, 342, 722, 927, 1053, 1128b, 1305a, 1351, 1918, 2049, 2337, 2939, 3266, 3491, 3729, 3797, 3974a, 3978, 4224, 4249, 4398c, 5079, 5189, 5376, 5811b, 5874, 5881	
57.		Dioxin {various polychloro derivatives of benzo[*b,e*-][1,4] dioxin}	177, 854, 1217, 2160, 2391, 2490, 2491,3265, 3300, 4249, 5811b		
58.	108-31-6	2,5-Furandione {maleic anhydride} 	239, 568b, 1233, 1375, 1375b, 1375a, 1377, 1586, 2543, 2570, 2767, 3029, 3255, 3257, 3265, 3300, 3553, 3557, 4249, 5811b	568b, 2917a, 4249, 5605, 5642, 5667, 5686, 5687, 5717, 5774	1375a, 1377
59.	7439-96-5	Manganese	50, 160, 273, 344, 769, 966, 1445, 1933, 1933b, 1934, 2079, 2270, 2393, 2524a, 2633, 2799a, 2939, 3302, 3308, 4005–4007, 4134, 4229, 4230, 4242, 4249, 4319, 5079, 5811b, 5869a	193, 250, 769, 1127b, 1333, 1933, 1934, 2079, 2270, 2283, 2338, 2489, 2529, 2939, 3797, 3973, 3974a, 3974b, 4249, 4357, 5079, 5137, 5189, 5268, 5285, 5448, 5514, 5654, 5811b, 5666, 5896, 20A02, 20A26	50, 641, 4249
60.	7782-49-2	Selenium	50, 174b, 174c, 273, 641, 688,724, 1273, 1386, 1445, 1455, 1456, 1842, 2468, 2667, 2799a, 3007, 3257, 3265, 3300, 3685, 3775, 4005–4007, 4230, 4249, 5541, 5811b, 5869a	174c, 374, 721, 724, 1445, 1455, 1456, 2468, 2667, 3707, 3775, 3797, 3895, 3973, 3974a, 4249, 5018, 5053, 5079, 5094, 5274, 5541, 5811b	50, 641, 4249

Note: The symbol (0) indicates the component identified in tobacco substitute smoke was not detected in tobacco smoke or vice versa.

26.2.1 Alternate Exposures to Carcinogens, Tumorigens, and Mutagens

Examination of the tumorigens listed in Table 26.1 logically leads to the questions: What, if any, are the human exposures to the listed tumorigens other than MSS and/or ETS? Is the exposure to a given tumorigen less, more, or equal to that from cigarette smoke? A detailed account of such alternate exposures requires many pages and tables. Most tumorigens in Table 26.1 have many alternate sources. The one obvious exception is the TSNAs which, by definition, being tobacco specific, have no alternate.

Table 26.10 is a brief list, with references, of alternate exposures to the major classes of tumorigens in tobacco smoke. The cited references provide tabulated details of the human exposures to them. Subsequent to Table 26.10 are discussions and tables in which the alternate exposures to the four major tumorigen classes in tobacco smoke are presented in more detail.

26.2.1.1 Alternate Exposures to Polycyclic Aromatic Hydrocarbons

Despite the ubiquity of PAHs in modern society, their presence in and their contribution to the alleged hazard of tobacco smoke have been repeatedly emphasized for over half a century, but seldom are the other many sources and/or levels of exposure to PAHs currently acknowledged as they were in the 1930–1950 period. Daily exposure to PAHs by inhalation (MSS, ETS, air pollutants) may represent only a small part of the total daily exposure; other exposures to PAHs often substantially exceed exposure via inhalation. Exposures to various PAHs are summarized in two different forms in Tables 26.11 and 26.12.

Results from many studies have been reported on the types and levels of PAHs, with particular emphasis on B[*a*]P, B[*a*]A, chrysene, benz[*e*]acephenanthrylene (B[*e*]A) (benzo[*b*]fluoranthene), B[*k*]A, indeno[1,2,3-*cd*]pyrene, DB[*a,h*]A, and benzo[*ghi*]perylene. As noted by Menzie et al. (2533), all of these PAHs have been identified in exhausts or effluents from fossil fuel combustion sources; in soils, sediments, and water; and in a variety of commonly used foodstuffs.

Although concern about PAHs in foodstuffs, particularly those arising pyrogenetically during cooking (grilling, broiling, roasting, etc.), predates the major concern of their presence in tobacco smoke, efforts to identify them in foodstuffs have been much less than the tobacco smoke effort: The number of PAHs identified in tobacco smoke exceeds 500, including several hundred derivatives where the positions of the alkyl groups have not been precisely defined (3757, 3758). PAHs identified in foodstuffs, both cooked and uncooked, number fewer than 150. Whether one considers the overall composition in general or the PAH fraction in particular, no other commercial product has been examined as extensively as tobacco or tobacco smoke.

Many PAHs are components of foodstuffs in the average diet (see Tables 26.11 and 26.12). Except for 5-MeC, PAHs listed in the many reports by Hoffmann et al. (1727, 1740,

TABLE 26.10
Exposures to Tumorigens and Mutagens from Sources Other than Mainstream and ETS

Alternate Exposure	References
PAHs	
Foodstuffs	Bailey and Williams (158a) Grasso (1345) Lijinsky and Shubik (2364a, 2364b) Maga (2438) Neukomm and Bonnet (2715) Vaessen et al. (4014) Waldman et al. (4106)
Beverages (coffee, tea, cocoa, etc.)	Kuratsune (2237) Kuratsune and Hueper (2238) Maga (2438)
Vehicle engine exhaust	Grimmer (1399–1402, 1405, 1406a, 1406b) Lyons (2428) Mauderly et al. (2505) Strach (3821) Sawicki et al. (3419b, 3419c) Williams et al. (4247a) Wynder and Hoffmann (4315, 4316)
Furnace effluents	Mumford et al. (26A114)
Aza-Arenes	
Vehicle engine exhaust	Grimmer (1407a)
Furnace effluents	Grimmer (1407b)
NNAs	
Foodstuffs	Bailey and Williams (158a) Grasso (1345) Kröller (2205, 2206) Preussmann and Eisenbrand (2990)
Beverages (coffee, tea, cocoa, water, etc.)	Preussmann and Eisenbrand (2990) Mitch et al. (26A112a)
Cosmetics	Preussmann and Eisenbrand (2990)
Industrial exposure (rubber, leather, metal, and pharmaceutical industries)	Preussmann and Eisenbrand (2990)
N-Heterocyclic Amines	
Foodstuffs	Bailey and Williams (158a) Jägerstad et al. (1916b) Matsumoto et al. (2492) Nagao et al. (2667f) Sugimura (3828b, 3828c, 3828e, 3828f) Sugimura and Nagao (3829b) Sugimura et al. (3829a) Tanaka et al. (3865c) Yasuda et al. (4382a)
Beverages (coffee, tea, cocoa, etc.)	Aeschbacher and Würzner (38a) Kosugi et al. (2178b) Nagao et al. (2667d, 2667e)
Metals	
Foodstuffs	Grasso (1345)

TABLE 26.11
Personal Exposure to Tobacco Smoke PAHs Listed as Tumorigens

Exposure Source	B[α]A[a]	B[e]A	B[*j*]F	B[*k*]F	B[*a*]P	Chr	Chr, me	DB[*a,h*]A	NC	DB[*b*]C	B[rst]P	DB[*d*]P	IP
Fish													
Raw	x	x	—	x	x	—	—	—	—	—	—	—	—
Cooked	x	x	—	x	x	—	—	—	—	—	—	—	—
Smoked	—	—	—	—	x	—	—	—	—	—	—	—	—
Oysters	x	—	—	—	x	—	—	—	—	—	—	—	—
Mussels	—	—	—	—	x	—	—	—	—	—	—	—	—
Meat													
Frankfurters	—	—	—	—	x	—	—	—	—	—	—	—	—
Hamburgers	x	x	—	x	x	—	—	x	x	x	—	—	x
Bacon	—	—	—	—	x	—	—	—	—	—	—	—	—
Ham, smoked	—	—	—	—	x	—	—	—	—	—	—	—	—
Bologna	—	—	—	—	x	—	—	—	—	—	—	—	—
Sausage	x	—	—	—	x	—	—	—	—	—	—	—	—
Beef, broiled	x	—	—	—	x	—	—	—	—	—	—	—	—
Beef, roasted	x	—	—	—	x	—	—	—	—	—	—	—	—
Beef, barbecued	—	—	—	—	x	—	—	—	—	—	—	—	—
Poultry	—	—	—	—	x	—	—	—	—	—	—	—	—
Cholesterol, heated	—	—	—	—	—	x	—	—	—	—	—	—	—
Dairy Products													
Milk	—	—	—	—	x	—	—	—	—	—	—	—	—
Cheese	—	—	—	—	x	—	—	—	—	—	—	—	—
Cereals													
Puffed corn	—	x	—	x	x	—	—	—	—	—	—	—	—
Puffed oats	x	x	—	—	—	—	—	—	—	—	—	—	—
Puffed wheat		x	—	x	x	—	—	—	—	—	—	—	—
Barley malt	x	x	—	—	x	—	—	x	—	—	—	—	x
Bran	x	x	—	x	x	—	—	—	—	—	—	—	—
Bread													
Untoasted	—	—	—	—	x	—	—	—	—	—	—	—	—
Toasted	—	—	—	—	x	—	—	—	—	—	—	—	—
Beverages													
Tea	—	—	—	—	x	—	—	—	—	—	—	—	—
Coffee, regular	—	—	—	—	x	—	—	—	—	—	—	—	—
Coffee, instant	—	—	—	—	x	—	—	—	—	—	—	—	—
Water	—	x	—	—	x	—	—	—	—	—	—	—	—
Bourbon	—	—	—	—	x	—	—	—	—	—	—	—	—
Scotch	—	—	—	—	x	—	—	—	—	—	—	—	—
Fruits, Vegetables													
Fresh	x	—	—	—	x	—	—	—	—	—	—	—	—
Potatoes, cooked	—	—	—	—	x	—	—	—	—	—	—	—	—
Potatoes, French fried	—	—	—	—	x	—	—	—	—	—	—	—	—
Endive	—	—	—	—	x	—	—	—	—	—	—	—	—
Spinach	—	—	—	—	x	—	—	—	—	—	—	—	—
Soybeans	—	—	—	—	x	—	—	—	—	—	—	—	—
Kale	—	—	—	—	x	—	—	—	—	—	—	—	—
Tomatoes	—	—	—	—	x	—	—	—	—	—	—	—	—
Apples	—	—	—	—	x	—	—	—	—	—	—	—	—
Prunes	—	—	—	—	x	—	—	—	—	—	—	—	—
Oils, Cooking													
Coconut oil	x	—	—	—	x	—	—	—	—	—	—	—	—
Vegetable oil	x	—	—	—	x	—	—	—	—	—	—	—	—
Mayonnaise	x	—	—	—	x	—	—	—	—	—	—	—	—

(*continued*)

TABLE 26.11 (continued)
Personal Exposure to Tobacco Smoke PAHs Listed as Tumorigens

Exposure Source	B[*a*]A[a]	B[e]A	B[*j*]F	B[*k*]F	B[*a*]P	Chr	Chr, me	DB[*a,h*]A	NC	DB[*b*]C	B[rst]P	DB[*d*]P	IP
Margarine	x	—	—	—	x	—	—	—	—	—	—	—	—
MSS, SSS, ETS	x	x	x	x	x	x	x	x	x	x	x	x	x
Engine Exhausts[b–d]	x	x	x	x	x	x	x	x	—	—	—	—	x
Tars, Soots, Oils, excluding ETS[c]	x	x	—	x	x	x	—	x	—	—	—	—	x
Oils, Catalytically Cracked	—	—	—	—	x	x	x	—	—	—	—	—	—
Vehicle Tire Carbon Blacks	x	—	—	—	x	x	—	—	—	—	—	—	—
Open Fire, Coal Combustion[e]	x	x	x	x	x	x	—	x	x	—	x	x	x
Urban Atmospheres	x	—	—	—	x	x	x	—	—	—	—	—	—

B[*a*]A, Benz[*a*]anthracene; B[*e*]A, Benz[*e*]acephenanthrylene = benzo[*b*]fluoranthene; B[*j*]A, Benzo[*j*]fluoranthene; B[*k*]A, Benzo[*k*]fluoranthene; B[*a*]P, Benzo[*a*]pyrene; Chr, Chrysene; Chr, me, Chrysene, 5-methyl-; DB[*a,h*]A, Dibenz[*a,h*]anthracene; NC, Naphtho[1,2,3,4-*def*]chrysene = dibenzo[*a,e*]pyrene; DB[*b*]C, Dibenzo[*b,def*]chrysene = dibenzo[*a,h*]pyrene; B[*rst*]P, Benzo[*rst*]pentaphene = dibenzo[*a,i*]pyrene; DB[*d*]P, Dibenzo[*def,p*]chrysene = dibenzo[*a,l*]pyrene; IP, Indeno[1,2,3-*cd*]pyrene.

[a] The PAHs listed also occur in MSS, SSS, and ETS.
[b] Wynder and Hoffmann (4315).
[c] Williams et al. (4247a).
[d] Grimmer et al. (1405).
[e] Mumford et al. (26A114).

1741, 1743, 1744, 1773, 1808) and OSHA (2825) as tobacco and tobacco smoke "tumorigens" have been identified in many foodstuffs. Grasso discussed the PAHs in foods and their significance as follows [see p. 1213 in (1345)]:

> The significance of these low levels of PAH carcinogens in food is difficult to assess. Undoubtedly, they are among the most potent carcinogens known, and every effort should be made to reduce their concentration in food. There are no clear indications, however, that they cause human cancer… Furthermore, there are indications that low levels of [benzo[a] pyrene], probably one of the most potent of the PAH found in food, do not produce tumors in experimental animals. The repeated application of 1.25 µg of [benzo[a]pyrene] in acetone to the skin of mice for 68 weeks failed to produce tumors [Roe (3310, 3311)]; dietary intake of 100 ppm of [benzo[a]pyrene] or less also had no effect in mice [Neal and Rigdon (2687)].

His comments on the carcinogenicity to humans of PAHs in ingested foods are equally applicable to the carcinogenicity to humans of the PAHs in inhaled cigarette MSS or ETS. Grasso noted that the following five PAHs were commonly found in foods: B[*a*]A, B[*a*]P, DB[*a,h*]A, B[*e*]A (benzo[*b*]-fluoranthene), and B[*k*]A; all listed by Hofmann et al. (1727, 1740, 1741, 1743, 1744, 1773, 1808) and OSHA (2825) as "tobacco smoke tumorigens." Grasso also listed the ranges of B[*a*]A and B[*a*]P levels found in a variety of commonly consumed foodstuffs.

Maga (2438) listed 65 common PAHs-containing foodstuffs. These, as did the list compiled by Grasso, included fruits and vegetables, dairy products, cereal products, legumes, beverages (including water), cooking oils, meat products, seafood products, and miscellaneous foodstuffs such as eggs, sugar, and olives. When many foodstuffs are heated during preparation, their PAH content increased dramatically, e.g., a single serving of charcoal-broiled meat contains more than 600 times the B[*a*]P level in the MSS from one cigarette [Lijinsky and Shubik (2364a, 2364b)].

Estimates such as this one are usually based on the Federal Trade Commission's (FTC) listing of TPM, "tar," nicotine, and CO deliveries plus an average value for the level of the B[*a*]P in the MSS TPM. Such comparisons between cigarettes and foodstuffs may yield estimates that are actually too low. For a given cigarette brand, the FTC numbers are obtained via precisely defined smoking regime and analytical methods (preconditioned cigarettes [25°C; relative humidity, 60%; conditioning time, 24 h]; smoking parameters—35 mL puff volume, 2 s puff duration, 1 puff/min; 25°C, 60% relative humidity, cigarette smoked to a defined butt length). On the other hand,

- Few smokers, if any, in the smoking of a cigarette take in the TPM amount found in the FTC determination.
- Few smokers smoke their cigarettes to as short a butt length as in the FTC procedure.
- Because of involvement in other tasks, smokers often place their cigarette in an ash tray for a brief time, thus missing one or more puffs on the cigarette. Few smokers take the number of puffs obtained for a given cigarette brand in the FTC procedure.

TABLE 26.12
PAH Sources

PAH	Tobacco Smoke	Gasoline Engine Exhaust[a]	Cooked Fish[b]	Broiled Hamburger[b]	Barley Malt[b,c]	Puffed Cereals[b]	Common Foods[b]
Benz[*j*]aceanthrylene, 1,2-dihydro-[d]	x	—	—	—	—	—	x
Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl-[e]	x	—	—	—	—	—	x
B[*e*]A[f]	x		x	x	—	x	x
B[*a*]A	x	x	x	x	x	x	x
B[*a*]A, 7,12-dimethyl-	x	—	—	—	—	x	x
B[*j*]A	x	x	—	—	—	—	x
B[*k*]A	x	x	x	x	—	x	x
11*H*-Benzo[*b*]fluorene	x	x		—	—	—	x
Benzo[*rst*]pentaphene[g]	x	—	—	—	—	—	x
Benzo[*ghi*]perylene	x	x	x	—	—	—	x
Benzo[*c*]phenanthrene	x	—	—	—	—	—	x
B[*a*]P	x	x	x		x	x	x
B[*e*]P	x	x	x	—	—	—	x
Benzo[*b*]triphenylene[h]	x	—	—	x	x	—	x
Chrysene	x	x	—	x		—	x
DB[*a,h*]A	x	x	—	x	x	—	x
Dibenz[*a,j*]anthracene	x	x	—	—	—	—	x
Dibenzo[*e,l*]pyrene[i]	x	—	—	x		—	x
Indeno[1,2,3-*cd*]fluoranthene	x	x	—	—	—	—	x
Indeno[1,2,3-*cd*]pyrene	x	x	—	—	—	—	x

[a] Wynder and Hoffmann (4315), Hoffmann and Wynder (1790. 5943, 26A59), Hoffmann et al. (5942).
[b] Maga (2438).
[c] Also contains a high level of NDMA.
[d] Previously known as cholanthrene.
[e] Previously known as 3-methylcholanthrene.
[f] Previously known as benzo[*b*]fluoranthene.
[g] Previously known as dibenzo[*a,i*]pyrene (DB[*a,i*]P).
[h] Previously known as dibenz[*a,c*]anthracene.
[i] Also known as dibenzo[*fg,op*]naphthacene.

The smoking machine used in the method never misses a puff on the cigarette under test!

- The smoking machine used in the FTC procedure does not "exhale" as do smokers. It has been determined in numerous studies that cigarette smokers exhale between 10% and 50% of the TPM inspired during the puffs needed to consume the cigarette, thus retaining between 50% and 90% of the inspired TPM.

All of these factors, if taken into account for a foodstuff–cigarette comparison such as the one noted previously, will increase the calculated number of cigarettes in the B[*a*]P comparison.

Analysis of a foodstuff as elementary as bread reveals a B[*a*]P level of 0.23 ng/g (mainly in the crust); light toasting raised the B[*a*]P level to 0.39 ng/g; darker toasting raised it to 0.56 ng/g. For an average slice of bread (weight one ounce or approximately 30 g), these values would be about 7, 12, and 17 ng/slice. Maga also reported the dietary intake of B[*a*]P (charcoal-broiled meat excluded) averaged about 500 ng/day. From their analysis of human exposure to B[*a*]P, Waldman et al. (4106) reported in 1991 that "the range and magnitude of dietary exposures to benzo[*a*]pyrene" ranged from 2 to 500 ng/day and "were much greater than for inhalation (10–50 ng/[day])." For some subjects, however, they found a dietary maximum of 1149 ng/day, despite omission of the contribution of B[*a*]P-containing beverages such as coffee. These B[*a*]P-intake estimates [Maga (2438), Waldman et al. (4106)] were lower than that reported by Hattemeyer-Frey and Travis (1551): 2200 ng/day (97% from diet, 3% from inhalation and water contamination). If B[*a*]P were tumorigenic in man and its threshold limit value were "zero," the incidence of digestive tract cancer would be substantially higher than it is.

The data tabulated in Table 26.13 on B[*a*]P and B[*a*]A from Maga, Grasso, and other investigators of the PAHs in frequently consumed foodstuffs have been expanded in Table 26.14 to include the cigarette equivalents of various dietary items consumed at estimated per meal levels. The inhaled cigarette MSS particulate phase from one cigarette is assumed to deliver 10 ng of B[*a*]P and 12.5 ng of B[*a*]A to the smoker. The following situation, known to be contrary

TABLE 26.13
Levels of B[*a*]P and B[*a*]A in Common Foodstuffs

Foodstuff	B[a]P, ng/g	B[a]A, ng/g
Fresh vegetables	2.85–24.5	0.3–43.6
Vegetable oils	0.4–1.4	0.8–1.1
Coconut oil	43.7	98.0
Margarine	0.4–0.5	1.4–3.0
Mayonnaise	0.4	2.2
Coffee	0.3–1.3	1.3–3.0
Tea	3.9	2.9–4.6
Grain	0.19–4.13	0.40–6.85
Oysters and mussels	1.5–9.0	…
Smoked ham	3.2	2.8
Smoked fish	0.83	1.9
Smoked bonito	37	189
Cooked sausage	12.5–18.8	17.5–26.2
Singed meat	35–99	28–79
Broiled meat	0.17–0.63	0.2–0.4
Charcoal-broiled steak	8.0	4.5
Broiled mackerel	0.9	2.9
Barbecued beef	3.3	13.2
Barbecued ribs	10.5	3.6
Cigarette MSS[a]	20–25	20–35

[a] The total MSS (particulate phase plus vapor phase) from an 85 mm filtered cigarette smoked under FTC conditions approximates 0.5 g.

to experimentally determined fact, is also assumed: None of the MSS particulate phase, nor its B[*a*]P content, nor its B[*a*]A content is exhaled by the smoker.

How do these exposures to B[*a*]P in the diet, etc., compare to the exposure to B[*a*]P in ETS? It is obvious that dietary intake of B[*a*]P far outweighs the intake of B[*a*]P via inhalation, including that inhaled in ETS. Guerin et al. (1445) of the Oak Ridge National Laboratory discussed the contribution of ETS to indoor air PAH concentrations and tabulated their assessments of the situation. They noted:

> The data suggest that ETS contributes between 0.5 and 1 ng/m^3 of BaP to indoor environments containing measurable ETS-contamination … Excursions in BaP concentrations due to ETS in such environments reach approximately 2.5 ng/m^3 … The magnitude of ETS-contribution [to PAH and BaP concentration] is generally small and is often difficult to consistently detect in most environments.

The daily intake of B[*a*]P from ETS may be estimated if the following assumptions are made:

- The average hourly intake of air is independent of whether the host is awake or asleep and is 1 m^3.
- The B[*a*]P level due to ETS is at the high end of the range estimated by Guerin et al. (1992) to be 0.5–1 ng/m^3.
- None of the daily intake of B[*a*]P, whether from diet, ETS, and the like, is eliminated by exhalation, etc.

Table 26.15 shows a comparison of the intake of B[*a*]P from ETS *vs.* the other B[*a*]P intakes discussed previously.

26.2.1.2 Alternate Exposures to Aza-Arenes

Even though, as indicated in Table 26.3 and the text accompanying it, the presence of the three pentacyclic *N*-heterocyclic compounds in tobacco smoke is equivocal, the alternate exposure to them and similar components is discussed later.

In their 1956 review of angular benzacridines and dibenzacridines and their tumorigenicity, Lacassagne et al. (2247a) made the following interesting observation, pertinent to the alleged "carcinogenicity" of benzene, frequently used as a solvent in tumorigenicity studies in the 1930s, 1940s, and 1950s:

> These molecules [the angular benzacridines] are very soluble in benzene and acetone (two solvents currently used for the investigations of carcinogenic activity) …

In addition to the exposure to acridines and benzacridines in tobacco smoke, other exposures to various acridines and benzacridines have been cataloged in the scientific literature. Many of the sources (Table 26.16) comprise environmental pollutants.

Unlike the PAHs and the NNAs, nontobacco smoke exposure to the acridines/benzacridines does not include foods. However, exposures other than tobacco smoke to polycyclic nitrogen compounds include exposures to the mutagenic *N*-heterocyclic amines in a variety of foods.

26.2.1.3 Alternate Exposures to *N*-Nitrosamines

Among several groups who have been involved in research on NNAs since soon after their tumorigenicity in laboratory animals was first reported by Magee and Barnes (2441a) are Barnes, Magee, and Schoental in the United Kingdom and Dontenwill, Druckrey, Preussmann, and Schmähl in Germany. From the German group, Preussmann has been a key contributor to our knowledge of NNAs. He has authored/coauthored research results and review articles continuously on NNAs since 1959. Initially, Preussmann was involved with the investigation of the relationship between the structure of a NNA and its tumorigenicity [Druckrey et al. (1059)]. In 1962, Druckrey and Preussmann (1057) proposed the possibility of the formation of NNAs in tobacco smoke from the secondary amines, nitrogen oxides, and water present. For the next two decades, Preussmann investigated methods of NNA analysis [Preussmann et al. (26A129), Egan et al. (1112a)], tumorigenicity of various NNAs [Druckrey et al. (1056a, 1058), Habs et al. (1469a), Magee et al. (2443), Janzowski et al. (1921a, 1921b), Ketkar et al. (2086c, 2086d), Zerban et al. (26A197)], the involvement of nitrate and nitrite in NNA formation [Spiegelhalder et al. (26A165)], NNAs in foods [Spiegelhalder et al. (26A167)], beverages [Spiegelhalder et al. (26A166, 26A168)], and toiletries [Spiegelhalder and Preussmann (26A169)].

In the late 1980s, Preussmann returned to the study of NNAs in tobacco and tobacco smoke and the question of the

TABLE 26.14
Cigarette Equivalents of B[*a*]P and B[*a*]A in Common Foodstuffs

	B[*a*]P			B[*a*]A		
Foodstuff	**ng/g**	**ng/Serving[a]**	**Cigarette Equivalent[b]**	**ng/g**	**ng/Serving[a]**	**Cigarette Equivalent[b]**
Fresh vegetables	2.85–24.5	325–2,800 (4)	32–280	0.3–43.6	34–4,970 (4)	3–400
Vegetable oils	0.4–1.4	46–160 (4)	5–16	0.8–1.1	91–125 (40)	7–10
Coconut oil	43.7	1,245 (1)	125	98.0	2,800 (1)	225
Margarine	0.4–0.5	11–14 (1)	1	1.4–3.0	40–85 (1)	3–7
Mayonnaise	0.4	23 (2)	2	2.2	125 (2)	10
Coffee	0.3–1.3	17–74 (2)	2–7	1.3–3.0	74–171 (2)	6–14
Tea	3.9	222 (2)	22	2.9–4.6	165–262 (2)	13–21
Grain	0.19–4.13	22–471 (4)	2–47	0.40–6.85	46–780 (4)	4–62
Bread, untoasted	0.23	20 (3)	2	—	—	—
Bread, light toast (3 min)	0.39	33 (3)	3	—	—	—
Bread, dark toast (5 min)	0.56	48 (3)	5	—	—	—
Oysters and mussels	1.5–9.0	171–1,026 (4)	17–103	—	—	—
Smoked fish	0.83	95 (4)	10	1.9	217 (4)	17
Smoked bonito	37	4,218 (4)	422	189	21,500 (4)	1,720
Smoked whiting	6.9	787 (4)	79	—	—	—
Broiled mackerel	0.9	103 (4)	10	2.9	330 (4)	26
Smoked ham	3.2	370 (4)	37	2.8	319 (4)	25
Cooked sausage	12.5–18.8	1,425–2,143 (4)	143–214	17.5–26.2	2,000–2,900 (4)	160–232
Singed meat	35–99	3,990–11,290 (4)	400–1,130	28–79	3,200–9,000 (4)	256–720
Broiled meat	0.17–0.63	19–72 (4)	2–7	0.2–0.4	23–46 (4)	2–4
Broiled hamburger, fatty	2.6	296 (4)	30	—	—	—
Broiled hamburger, lean	0	0 (4)	0	—	—	—
Charcoal-broiled steak	8.0	912 (4) 1,824 (8)	9(4) 182 (8)	4.5	513 (4) 1,026 (8)	41 82
Charcoal-broiled T-bone	50	5,700 (4) 11,400 (8)	570 1,140	—	—	—
Barbecued beef	3.3	376 (4)	38	13.2	1,500 (4)	120
Barbecued pork	4.5	513 (4)	51	…	…	…
Barbecued ribs	10.5	1,197 (4)	120	3.6	410 (4)	33
Cigarette MSS[c]	*20–25*			*20–35*		

[a] Number in parentheses indicates number of ounces consumed. B[*a*]P and B[*a*]A content calculated at level per ounce (28.5 g) consumed.

[b] Inhaled cigarette MSS particulate phase from one cigarette is assumed to deliver 10 ng of B[*a*]P and 12.5 ng of B[*a*]A to the smoker. The following, contrary to experimental fact, is also assumed: none of the MSS particulate phase, nor its B[*a*]P content, nor its B[*a*]A content is exhaled by the smoker.

[c] The weight of the total MSS (vapor phase + particulate phase) from an 85 mm filtered cigarette smoked under FTC conditions approximates 0.5 g.

TABLE 26.15
Comparison of Daily Dietary and Inhalation Intake of B[*a*]P[a]

Study	**Type**	**B[*a*]P from Diet, ng/Day**	**B[*a*]P via Inhalation, ng/Day**	**Total B[*a*]P Intake, ng/Day**
Maga (2438)	Estimated	—	—	500
Hattemeyer-Frey and Travis (1551)	Measured	2130	70	2200
Waldman et al. (4106)	Measured	2–500[b]	10–50	12–550[b]
From inhaled ETS	Estimated	—	24[c]	

[a] Based on assumptions listed earlier.

[b] Dietary intakes as high as 1149 ng/day were noted.

[c] Even if intake was at the excursion value of 2.5 ng/m^3, the daily intake from ETS would be 60 ng.

TABLE 26.16
Aza-Arenes Sources Other than Tobacco Smoke

Acridine/Benzacridine Source	Reference
Automobile exhaust	Sawicki et al. (3419b), Williams et al. (4247a)
Coal-fired residential furnace emission	Grimmer et al. (1407b)
Coal distillate	Graebe and Caro (1334f), Kruber (2210a)
Coal tar	Lang and Eigen (2261a), Merli et al. (2534a)
Crude oil	Schmitter et al. (3519b), Grimmer et al. (1407a)
High boiling petroleum distillate	McKay et al. (2519a), Later et al. (26A80)
Industrial stack effluent	Sawicki et al. (3419a)
Urban suspended particulate matter	Sawicki et al. (3419c), Cautreels and van Cauwenberghe (636a), Dong et al. (1040a), Adams et al. (35)

possible endogenous formation of TSNAs in smokers [Tricker et al. (3944. 3945, 3953, 3954), Tricker and Preussmann (3946–3951), Fischer et al. (1191–1200); Spiegelhalder et al. (3773, 3774), Kumar et al. (2235)].

Discussing the escalation in publications on *N*-nitroso compounds, Preussmann (2989a) wrote:

> At present (1981), more than 1400 papers are published annually on the analysis, formation, chemistry, biochemistry, metabolism and biological effects of *N*-nitroso compounds.
>
> There is no equivocal and convincing evidence of carcinogenicity in humans of *N*-nitroso compounds. Therefore, an answer is needed to the question whether exposure to traces of these compounds from the general environment … poses a risk to human health. In this situation animal data must be extrapolated to man, with all the inherent uncertainties.

Preussmann and Stewart (2991) noted the exponential increase in publications on NNAs between 1972 and 1984 and estimated that about three papers were published daily on this topic in the scientific literature in 1983. They also cautioned:

> Patterns of investigations established with nitroso compounds are being extended to more structurally complex carcinogens. Yet the contribution of nitroso compounds to the burden of environmentally determined neoplasia in humans remains to be determined … The priority that might reasonably be placed on reducing human exposure to nitroso compounds could be better judged if the number of cancers likely to be affected by such measures were known.

Discussions in this chapter are limited primarily to the NNAs common to tobacco/tobacco smoke and the other exposures (foodstuffs, beverages, cosmetics, drugs, etc.). As described by Preussmann and Stewart (2991), various bioassays on laboratory animals have been conducted on over 220 different NNAs and 110 *N*-nitrosamides, over 330 in all. Fewer than 60 of these *N*-nitroso compounds have been identified in tobacco and/or tobacco smoke.

Historically, the search for tumorigenic compounds in foodstuffs and beverages began in the early 1930s, shortly after the demonstration that the synthetic PAH DB[*a*,*h*]A [Kennaway and Hieger (2078)] and the coal tar isolate B[*a*]P [Cook et al. (796a, 797), Barry et al. (194)] were carcinogenic when painted on mouse skin and sarcogenic when injected subcutaneously. The initial investigations were limited to attempts to demonstrate the presence of these and similar PAHs in heated foodstuffs (meat, fish, etc.), particularly those containing cholesterol and its derivatives.

Subsequent to the demonstration of the tumorigenicity in laboratory animals of NNAs such as NDMA [Barnes and Magee (192), Magee and Barnes (2441a)], the search for NNAs in commonly used foods and beverages began. Despite nearly half a century of study of food components tumorigenic to laboratory animals, caution was recommended as recently as 1984 in the interpretation of the laboratory findings, e.g., Grasso (1345) in his review of carcinogens in food noted:

> Carcinogens occur at very low concentrations in food so that if any type of tumors result at all, the number is expected to be very low indeed. At present much thought is being given to the relative hazards of these levels and how they can be assessed. Certainly no firm association has been established between any human cancer and the low levels of carcinogens in food, but this problem may only reflect the imperfect state of current epidemiological investigations.

Despite hundreds of publications on the presence of NNAs in foods and beverages and the results of bioassays with NNAs in laboratory animals, Grasso also wrote:

> Despite intensive experimental investigations, however, the hazard to humans from small doses of nitrosamines present in our food and water are difficult to assess, and until further experimental evidence is available, no firm opinion can be given.

This opinion is almost identical with that of Preussmann and Stewart (2991) who reviewed not only the human exposure to NNAs in foods, beverages, water, drugs, cosmetics, etc., but also exposure to the NNAs (volatile, nonvolatile, and tobacco-specific) in tobacco products:

> Although estimates of the total human burden caused by exposure to nitroso carcinogens have been attempted … , we do not think that sufficient data exist for meaningful evaluation; therefore, estimation of nitrosamine contribution to human cancer risk is largely speculative. Premature calculations are liable to be misinterpreted by those who are not thoroughly familiar with the multitude of uncertainties and difficulties inherent in such calculations, especially when estimates of lifetime risks are based on such figures.

Table 26.17 lists the levels (ng/g) of several NNAs identified in commonly used foods and beverages. Table 26.18

TABLE 26.17
NNAs in Foods and Beverages (ng/g)

Food or Beverage	NDMA	NDEA	NPYR	NPIP
Meat				
Bacon, uncooked	1–9.5	1–4	≤17	0
Bacon, fried	0.1–28	≤40	3–44	1
Cured meats	1–80		10–105[a]	≤60[a]
Fish				
Fresh or frozen	3–18	1–2	…	…
Salted or pickled	1–35	50–108	0–37	…
Smoked, baked, or processed	6–177	≤147	…	…
Vegetables/Vegetable Oils				
Beans	0	0–0.2	…	…
Vegetables[b]	0	0	…	…
Soybean oil[c]	0–20	0–4	…	…
Cheeses	0.1–68	…	…	2–11
Beverages				
Water	0.8–3.3	0.1–1.83	…	…
Alcohol beverages	≤10	≤0.1		
Cigarette MSS (ng/cig)[d]	0.1–180	ND–25	30–60	ND–9

NDMA, *N*-nitrosodimethylamine; NDEA, *N*-nitrosodiethylamine; NPYR, *N*-nitrosopyrrolidine; NPIP, *N*-nitrosopiperidine.

[a] Levels in sausage.

[b] Sixteen different vegetable species tested.

[c] Freshly refined.

[d] See Table 26.1.

summarizes the studies in which various NNAs were identified in foods and beverages. One of the earliest investigators of NNAs in foodstuffs was Kröller (2205) who identified NDMA in cheese. Kröller's studies were not limited to possible tumorigens in foodstuffs. From 1963 through 1966, he also investigated the pyrosynthesis of PAHs, particularly B[*a*]P, in cigarette smoke and from various materials used in cigarette fabrication, e.g., cigarette paper, adhesives, humectants, dyes, inks, flavorants, tobaccos [see summary in Wynder and Hoffmann (4332)].

Also included in Table 26.17 are data for the per cigarette deliveries of several NNAs identified in foods and beverages. From these data, comparisons of the relative exposures from foods, etc., and cigarette smoke are possible, e.g., the per cigarette MSS range for NDMA has been reported as 0.1–180 ng (see Table 26.1). Since one ounce is approximately 30 g, a person eating 1 oz of fried bacon would be exposed to 30 (0.1–28) or 3–840 ng of NDMA. Similarly for cured meat, the per cigarette exposure of 0.1–180 ng should be compared to the dietary exposure of 30–2400 ng from eating 1 oz of cured meat. Also, compare the exposure to 30–60 ng/cig of NPYR *vs*. 300–3150 ng NPYR from eating 1 oz of sausage!

Over the years, numerous reports [cf. Neurath et al. (2751), Fredrickson (1236), Krull et al. (26A77), Eisenbrand et al. (26A27), Caldwell and Conner (573)] on the artifactual formation of NNAs during the collection and analysis of tobacco smoke and the various remedial procedures taken to minimize this problem have been published. Similar problems were noted by Wolff and Wasserman (26A195) on inflated levels of NNAs reported in foodstuffs and beverages. They expressed reservations about the validity of pre-1972 analytical methodology since later studies demonstrated that the earlier procedures introduced both artifact and error. Thus, the levels of NNAs reported in foodstuffs were actually lower than those reported prior to 1972. In 1986, Sen et al. (26A150) proposed improvements in analytical methodology to prevent artifactual formation and subsequent inflated levels of NNAs in rubber products; propyl gallate was demonstrated to be an effective inhibitor of *N*-nitrosation during the analytical procedure.

A variety of investigations have been conducted during the past decade on exposures to NNAs, and a few will be cited here. Okieimen et al. (26A120) reported on the total NNAs content of beer, dairy products, bouillon cubes, and tobacco products. They reported that dairy products showed the lowest total value; bouillon cubes, the highest. Mandagere (2450a) reported on the high NNA levels in a variety of meats cured via a smoking process.

Coker et al. (26A16) tested some 200 commercial foodstuffs for NNAs and noted the values for beverages were high, those for dairy products low. Craddock (26A18) and Sen (26A143) found NNA levels in Canadian foodstuffs and beverages to be similar to those of U.S. products. Since the review by Preussmann and Stewart (2991) on the tumorigenicity of NNAs and that by Preussmann and Eisenbrand (2990) on exposure to NNA tumorigens in the environment, numerous detailed reviews of NNA exposures (alcoholic beverages, meats, seafood, cosmetics, tobacco, rubber goods, metal cutting oils, pharmaceuticals, environment, water) have been presented by Mejstrik et al. (26A99), Tricker and Preussmann (3946), Tricker et al. (3954), Ellen (26A30), and Matsui and Kaya (26A95).

The daily intake of NNAs from ETS may be estimated if the following assumptions are made:

- The average hourly intake of air is independent of whether the host is awake or asleep and is 1 m^3.
- The NNA level due to ETS is at the high end of the range estimated by Guerin et al. (1445) for the various NNAs, i.e., 40 ng/m^3 for NDMA, 3 ng/m^3 for NDEA, NPYR, NNN, and NNK.
- None of the daily intake of the NNAs, whether from diet, ETS, and the like, is eliminated by exhalation, etc.
- The measured values reported for NNAs in diet, ETS, etc.

From the dietary NNA data of Preussmann and Eisenbrand (2990), Preussmann et al. (26A130), and Spiegelhalder et al. (26A167) and ETS NNA data summarized by Guerin et al. (1445), the comparison in Table 26.19 was developed.

It is obvious that the estimated exposure to the NNAs in diet *vs*. ETS differs from the B[*a*]P exposure case. Whereas the dietary exposure to B[*a*]P was between 20 and 90 times

TABLE 26.18
Volatile and Nonvolatile NNAs in Foodstuffs and Beverages

NNAs: Foodstuff/ Beverage	Reference
Acetic acid, 2-methylnitrosamino-NSAR	
Meat	Hamburg and Kann (26A49)
Beer (and malt)	Pollock, (26A128), Sen et al. (26A156)
1-Butanamine, N-butyl-N-nitroso-NDBA	
Fish	Huang et al. (26A63)
Ethanamine, N-ethyl-N-nitroso-NDEA	
Bacon	Crosby et al. (26A19), Wasserman et al. (26A181)
Fish	Sen et al. (26A155), Crosby et al. (26A19), Wasserman et al. (26A181), Fong and Chan (26A39, 26A40), Huang et al. (26A63)
Cheese	Crosby et al. (26A19), Wasserman et al. (26A181)
Powdered milk	Maduagwu and Bassir (26A88)
Beer (and malt)	Spiegelhalder et al. (26A166), Scanlan et al. (26A139), Kawabata et al. (2058)
Gastric juices + nitrite	Sen et al. (26A154)
Methanamine, N-methyl-N-nitroso-NDMA	
Meat, cured meat	Wasserman et al. (26A181), Panalaks et al. (26A121, 26A122), Sen (26A142a), Spiegelhalder et al. (26A167), Eisenbrand (26A26), Helgason et al. (26A58)
Bacon	Crosby et al. (26A19), Wasserman et al. (26A181), Vecchio et al. (26A177), Sen et al. (26A152)
Fish	Sen et al. (26A155), Crosby et al. (26A19), Wasserman et al. (26A181), Fong and Chan (26A39, 26A40), Iyengar et al. (26A64), Havery and Fazio (26A51), Kawabata et al. (26A71), Maki et al. (26A90), Josefsson and Nygren (26A67), Matsui et al. (26A96), Huang et al. (26A63), Pedersen and Meyland (26A123) Nieper and Etzel (26A117), Röper (26A134), Röper et al. (26A135),
Squid	Kawabata et al. (26A71),Matsui et al. (26A96)
Cheese	Kröller (2205), Crosby et al. (26A19), Wasserman et al. (26A181), Goodhead et al. (26A42), Havery et al., (26A55), Gough et al. (26A44), Eisenbrand et al. (26B16), Elgersma et al. (26A29); Danish Institute of Protein Chemistry (26A21), Spiegelhalder et al. (26A167), Eisenbrand (26A26)
Powdered milk	Maduagwu and Bassir (26A88), Libbey et al. (26A84), Lakritz and Pensabene (26A78), Havery et al. (26A52), Sen and Seaman (26A147)
Wheat flour	Hedler and Marquardt (26A57)
Beer (and malt)	Sen and Dalpe (26A144), Goff and Fine (26A41), Spiegelhalder et al. (26A166, 26A167), Walker et al. (26A109), USFDA (26A176), Maki et al. (26A91, 26A92), Preussmann et al. (26A130, 26A131), Scanlan et al. (26A138, 26A139), Sen et al. (26A151), Stephany and Schüller (26A170), Eisenbrand (26A26), Havery et al. (26A54), Hotchkiss et al. (26A62), Sen and Seaman (26A146, 26A148), Slack and Wainwright (26A160), Kann et al. (26A70), Kawabata et al. (2058), Mangino et al. (26A93), Spiegelhalder (26A162), Jasinski (26A66), Scanlan et al. (26A139), Scanlan and Barbour (26A138)
Scotch whiskey	Goff and Fine (26A41)
Brandy (French)	Walker et al. (26A179)
Other alcohol beverages	Sen and Dalpe (26A144), Gough (26A43), Bassir and Maduagwu (26A05)
Water	Fine et al. (26A37, 26A38), Kimoto et al. (26A72), Mitch et al. (26A112a)
Morpholine, 4-nitroso-NMOR	
Fish	Fong and Chan (26A39, 26A40)
Piperidine, 1-nitroso-NPIP	
Meat, cured meat	Spiegelhalder et al. (26A167), Eisenbrand (26A26)
Bacon	Crosby et al. (26A19), Wasserman et al. (26A181), Vecchio et al. (26A177)
Fish	Crosby et al. (26A19), Wasserman et al. (26A181)
Squid	Kawabata et al. (26A71), Matsui et al. (26A96)
Cheese	Crosby et al. (26A19), Wasserman et al. (26A181)
1-Propanamine, N-nitroso-N-propyl-NDPA	
Fish	Sen et al. (26A155), Huang et al. (26A63)
Pyrrolidine, N-nitroso-NPYR	
Meat, cured meat	Pensabene et al. (26A124), Spiegelhalder et al. (26A167), Eisenbrand (26A26), Theiler et al.(26A173), Alldrick et al. (26A01)
Bacon	Hansen et al. (26A50), Sen et al. (26A145, 26A153), Gough et al. (26A45), Havery et al. (26A53), Janzowski et al. (26A65), Cross and Bharucha (26A20), Gray and Randall (26A47), American Meat Institute (26A03), Nitrite Safety Council (26A118), Webb and Gough (26A191), Josefsson and Nygren (26A67), Fazio et al. (26A33), Gray (26A46), Pensabene et al. (26A125), Alldrick et al. (26A01), Vecchio et al. (26A177)

TABLE 26.18 (continued)
Volatile and Nonvolatile NNAs in Foodstuffs and Beverages

NNAs: Foodstuff/ Beverage	Reference
Fish	Crosby et al. (26A19), Wasserman et al. (26A181), Kawabata et al. (26A71), Matsui et al. (26A96)
Cheese	Crosby et al. (26A19), Wasserman et al. (26A181)
Beer (and malt)	Spiegelhalder et al. (26A166), Scanlan et al. (26A139), Kawabata et al. (2058), Jasinski (26A66)
2-Pyrrolidinecarboxylic acid, 1-nitroso-NPRO	
Meat	Pensabene et al. (26A124), Hamburg and Hamburg (26A48), Dennis et al. (26A22), Dunn and Stich (26A25), Helgason et al. (26A58), Sen and Seaman (26A148)
Bacon	Hansen et al. (26A50), Brunnemann et al. (509); Sen and Seaman (26A148), Massey et al. (26A94)
Chicken	Brunnemann et al. (509)
Ham	Brunnemann et al. (509)
Toast	Brunnemann et al. (509)
Biscuits	Brunnemann et al. (509)
Cornflakes	Brunnemann et al. (509)
Beer (and malt)	Pollock (26A128), Sen et al. (26A156), Brunnemann et al. (509)
Diethanolamine, N-nitroso-NDELA	
Meat, cured	Coker et al. (26A15)

TABLE 26.19
Comparison of Dietary and ETS

	Dietary Intake, ng/day				
Country	**NDMA**	**NDEA**	**NPYR**	**NPIP**	**Total**
Federal Republic of Germany	1100[a]		100–150	10	1210–1260
United Kingdom					530
Japan					1780
The Netherlands					1100

	Intake from ETS[b], ng/day					
	NDMA	**NDEA**	**NPYR**	**NPIP**	**NNN + NNK**	**Total**
Estimated from German, Japanese, and American ETS studies[c]	960	72	72		144	1248

[a] Because of the reduction in NDMA level in beer after 1979, this number is now probably closer to 700 ng/day.
[b] On basis of the assumptions listed previously.
[c] Brunnemann et al. (457), Stehlik et al. (3812), Matsushita and Mori (2495), Klus et al. (26A75); unfortunately, the TSNAs results from a more recent study on ETS by Brunnemann et al. (1992) were not included in the assessment by Guerin et al. (1445) or Holcomb (26A60).

the exposure to B[*a*]P in ETS, the dietary exposure to NNAs is essentially the same as the exposure to NNAs in ETS.

Previously, the review by Holcomb (26A60), his proportioning of male and female respiration rates during the day, his use of 11% particle retention, and his comments on the contribution of ETS to PAH exposure were discussed. His summary of the NNA situation was as follows:

> Two studies [Stehlik et al. (3812), Hoffmann et al. (1678)] have reported the presence of … (NDEA) and … (NDMA) in smoke-filled rooms … These are not tobacco-specific nitrosamines. The lack of reported background levels and the unusually high level of smoking prevents the evaluation of ETS contribution of these substances. Other nitrosamines reported to be found in tobacco smoke have either not been monitored or not been reported in ambient air where ETS is present.

Unlike the volatile NNAs which are found primarily in the vapor phase, TSNAs are predominantly particulate-phase components.* Thus, their intake and retention should be proportional to the intake and retention of ETS particles. If Holcomb's assigned values for respiration rates during the day and his use of 11% retention are applied to the TSNA

* Although data are sparse, there is some evidence to indicate that TSNAs in ETS may be distributed between the vapor and particulate phases.

TABLE 26.20
TSNAs in Indoor Air

	TSNAs in Indoor Air, ng/m³			
Reference	NNN	NAT	NNK	Total of Three TSNAs
Brunnemann et al. (460)	ND[a]–22.8	ND[a]–9.5	1.4–29.3	1.4–61.6
Hoffmann et al. (1702)	1.8–23	1.5–10	1–29	4.3–62

ND, not detected.

[a] Not detected in 5 of the 10 sites monitored (a restaurant, both trains, the office, smoker's residence).

values in the preceding summary, the intake of NNN plus NNK will be much less than the 144 ng/day indicated. It probably would be less than 10 ng/day. If the more recent data of McAughey et al. (26A98) for the % retention of particulates from aged and diluted SSS be used in the calculations (17%–41%, depending on analytical procedure and subjects' gender), the estimated exposure to NNN plus NNK will not be as low as if the 11% retention from the Hiller et al. (1654a, 1654b) study be used.

Brunnemann et al. (460) determined the levels of several TSNAs in bars (3), restaurants (2), a car, trains (2), an office, and a smoker's private residence. The values reported and the subsequent descriptions of the values found are shown in Table 26.20.

In their discussion of exposure to TSNAs in ETS at various sites, Hoffmann et al. (1702)—perhaps to embellish the situation—apparently disregarded the fact that no NNN nor *N′*-anatabine was detected in half the test sites! Hoffmann et al. (1702) list total TSNAs in the MSS from two different U.S. cigarettes at 979 and 670 ng/cig. Thus, at an exposure level of 62 ng/m³ and a respiration rate of 1 m³/h, it would require a nonsmoker to remain for nearly 16 and 11 h in such an atmosphere to be exposed to similar levels of TSNAs as a smoker who inhales MSS from the two cigarettes, respectively. Such a period surely exceeds the "several hours" noted by Hoffmann et al. (1702).

Analysis of 68 commercially available drug preparations containing aminopyrine indicated that all contained NDMA [Schoenhard et al. (26A140)]. The following ranges for the NDMA levels were reported: 35 samples, 1–10 ppb; 27 samples, 11–50 ppb; 5 samples, 51–100 ppb; 1 sample, 370 ppb. More recently, Preussmann and Eisenbrand (2990), Mejstrik et al. (26A99), Lijinsky (26A85), Ellen (26A30), and Matsui and Kaya (26A95) have reviewed the studies on the detection of NNAs in pharmaceuticals as well as in other consumer products.

Examination by Fan et al. (26A31) of a series of cosmetics widely used in the United States revealed that 27 of 29 samples contained NDELA at levels varying from 1 to 48,000 ppb. From a similar study conducted several years later, Klein et al. (26A73) reported that 5 of 10 cosmetic samples contained NDELA at levels ranging from 20 to 4113 ppb. Despite the concern about the possible tumorigenicity of NDELA, its use in cosmetics has continued since its ban as an agricultural chemical in the United States in 1981 (1147). Although none of the three have been identified in tobacco or tobacco smoke to date, *N*-nitrosomethyldodecylamine (in six of seven products tested), *N*-nitrosomethyloctadecylamine, and *N*-nitrosobenzylmethylamine were identified in 1981 by Hecht (26A56) in various commonly used cosmetics. Fan et al. (26A31) described an analytical method to determine NDELA in various cosmetics and shampoos; this procedure was updated by Fine (26A36). Erickson et al. (1159) reported the presence of NDELA and similar compounds in cosmetics. Preussmann and Eisenbrand (2990) commented on the rapid absorption of NDELA in rats when administered by a variety of routes (subcutaneous, oral, intratracheal).

Preussmann and Eisenbrand (2990), Mejstrik et al. (26A99), Ellen (26A30), Lijinsky (26A85), and Matsui and Kaya (26A95) have reviewed the findings on the detection of NNAs in cosmetics. Spiegelhalder and Preussmann (26A169) described the volatile and nonvolatile NNAs found in many samples of toiletries and cosmetics. Eisenbrand et al. (26B15) reported a series of *N*-nitrosodialkylamines in cosmetics.

Investigations [Spiegelhalder and Eisenbrand (26A164), Spiegelhalder (26A163)] of various rubber products that come in frequent contact with human tissue revealed the presence of several NNAs. Baby-bottle nipples and pacifiers contained appreciable levels of NDMA, NDEA, *N*-nitrosodibutylamine (NDBA) [Thompson et al. (26A174)], and NPIP. NDMA and NDEA were found in various rubber toys. These two NNAs plus NPIP were also found in rubber gloves. In their study of NNAs in rubber products, Sen et al. (26A149), in their analysis of 30 samples, reported the detection of NMOR in various rubber products in addition to NDMA, NDEA, NDBA, and NPIP. Solenova et al. (26A161) reported the presence of NDMA and NDEA.

Several NNAs have been identified in pesticides used on various vegetable crops, e.g., NDMA [Ross et al. (26A137)] and *N*-nitrosodipropylamine (NDPA) [Zweig et al. (26A198)].

Most water supplies show little evidence of volatile or nonvolatile NNAs. However, water deionized by passage through various anion-exchange resins containing trialkylammonium compounds were reported to show NDMA levels ranging from 0.03 to 0.34 mg/L [Fiddler et al. (26A35), Fine et al. (26A37, 26A38), Gough et al. (26A44), Cohen and Bachman (26A14), Kimoto et al. (26A72), Mitch et al. (26A112a)].

On the subject of industrial and occupational exposures to NNAs, Preussmann and Eisenbrand (2990) wrote:

> Data on occupational exposure to different nitrosamines are recent and not yet representative or complete. Nevertheless, the data indicate that certain industries have a serious nitrosamine problem and that the highest known concentrations of preformed *N*-nitrosamines occur in the workplace, especially in the rubber and leather industries … Exposures have been shown to vary considerably in regard to amount and type of nitrosamine found in different working places in several industries and occupations.

Preussmann and Eisenbrand (2990) summarized the following situations: In the rubber industry, workers were exposed to NDMA, NDEA, NMOR, and NPIP. In their study of the atmospheres in 132 sites in 12 rubber-processing plants in France, Ducos and Gaudin (26A24) reported the detection of NDMA, NDEA, and NMOR in 93%, 27%, and 13% of the sites surveyed, respectively. In the leather-tanning industry, exposures to NDMA occur [Bailey et al. (26A04), Skrabs (26A159), Wolf et al. (26A194)] and to NDEA [Skrabs, (26A159), Wolf (26A193)], and NMOR [Wolf (26A193)]. Exposures to NDELA [Erickson et al. (1159)] in the cutting oils used in machine shops and to NDMA and NDEA [Wolf et al. (26A194), Wolf (26A193)] in foundries have been reported. In a plant-producing rocket fuels, including 1,1-dimethylhydrazine by reduction of NDMA, workers were exposed to extremely high levels of NDMA. Shortly after this high exposure was recorded, the factory ceased manufacture of 1,1-dimethylhydrazine. In chemical and pharmaceutical factories where amines are used in production, exposures to NDMA and NDEA have been reported.

In Table 26.21 is presented a simplified summary of the possible exposures to non-TSNAs that are known components of tobacco smoke. All 10 NNAs listed are found not only in tobacco smoke but also in a great variety of commonly consumed foodstuffs and beverages.

26.2.1.4 Alternate Exposures to *N*-Heterocyclic Amines

Because of their concerns about the mutagenicity of commonly consumed heated foods, many of the studies of the isolation, identification, and estimation of *N*-heterocyclic amine in heated foodstuffs or heated food components, particularly amine-containing components such as amino acids, proteins, and peptides, were conducted by Japanese investigators. This becomes obvious from examination of the authors and coauthors of the references listed in Table 26.22.

With the advent of the Ames mutagenicity test with *S. typhimurium* in the mid-1970s and the demonstration of its utility, the number of studies on potential mutagenic systems and the mutagenicity–tumorigenicity relationship virtually exploded. By highly competent application of up-to-date isolation and characterization techniques plus utilization of the Ames test, Sugimura and his staff at the Japanese National Cancer Research Institute contributed significantly to our knowledge of the structures, properties, and precursors in foods of the mutagenic *N*-heterocyclic amines. While the methodologies differed, the 1977 isolation/identification of the mutagenic *N*-heterocyclic amines (Trp-P-1, Trp-P-2) from a tryptophan pyrolysate paralleled the historic 1932 isolation and identification of PAHs (B[*a*]P, B[*e*]P, B[*a*]A, perylene) from coal tar. In the 1930s, the Kennaway group in the United Kingdom used ultraviolet spectrophotometry [Hieger (1631)] to monitor coal-tar PAHs during their concentration and purification by repeated precipitations and recrystallizations of PAH–picric acid complexes [Cook et al. (796a, 797)]. In the mid-1970s, Sugimura et al. (3829) used the Ames test (*S. typhimurium*, TA 98 strain/S-9) to monitor tryptophan pyrolysate mutagens (Trp-P-1, Trp-P-2) during their concentration and purification by sequential chromatography on silicic acid, alumina, and CM-Sephadex® columns.

References to several early studies on the identification of biologically active compounds in heated foodstuffs are included in Table 26.22, e.g., the 1956 study of PAHs such

TABLE 26.21
Nontobacco Exposures to Tobacco/Tobacco Smoke NNAs

Consumer Good or Environment	NNAs									
	NDMA	NDEA	NDPA	NDBA	NDELA	NPIP	NPYR	NPRO	NMOR	NSAR
Tobacco and/or tobacco smoke[a]	x	x	x	x	x	x	x	x	x	x
Food, beverages	x	x	x	x	x	x	x	x	x	x
Rubber goods	x	x	—	x		x	—	—	x	—
Cosmetics	—	—	—	—	x	—	—	—	—	—
Pharmaceuticals[b]	x	—	—	—	—	—	—	—	—	—
Pesticides[b]	x	—	x	—	—	—	—	—	—	—
Water	x	—	—	—	—	—	—	—	—	—
Industrial environments	—	—	—	—	—	—	—	—	—	—
Rubber-processing plants	x	x	—	—	—	x	—	—	—	x
Leather tanneries	x	x	—	—	—	—	—	—	—	x
Foundries	x	x	—	—	—	—	—	—	—	—
Machine shops	—	—	—	—	x	—	—	—	—	—

NDMA, *N*-nitrosodimethylamine; NDEA, *N*-nitrosodiethylamine; NDPA, *N*-nitrosodipropylamine; NDBA, *N*-nitrosodibutylamine; NDELA, *N*-nitrosodiethanolamine; NPIP, *N*-nitrosopiperidine; NPYR, *N*-nitrosopyrrolidine; NPRO, *N*-nitrosoproline; NMOR, *N*-nitrosomorpholine; NSAR, *N*-nitrososarcosine.

[a] In addition to the NNAs listed, tobacco and tobacco smoke contain a variety of TSNAs and *N*-nitrosamino acids other than *N*-nitrososarcosine.

[b] NNAs other than those determined in tobacco and/or tobacco smoke have also been detected in various consumer goods.

TABLE 26.22
Mutagenicity of Beverages, Heated Foods, and Heated Food Components

Food or Food Component	References
Foods, heated (grilled, broiled, etc.)	Sugimura et al. (3829a), Sugimura and Nagao (3829b), Matsumoto et al. (2492), Sugimura (3828a, 3828c, 3828f), Nagao et al. (2667a), Tanaka et al. (2667a), Felton and Knize (1177d)
Beef, extract	Commoner et al. (790a), Hargraves and Pariza (1501a), Hayatsu et al. (1555b), Turesky et al. (3988b), Ohgaki et al. (2849a), Takayama et al. (3862c)
Beef, broiled, fried, and/or charred	Lijinsky and Shubik[a] (2364a, 2364b), Nagao et al. (2667c), Commoner et al. (790a), Yasuda et al. (4382a), Hayatsu et al. (1555a, 1555b), Kasai et al. (2037a), Jägerstad et al. (1916b), Felton et al. (1177d), Ohgaki et al. (2849a), Takayama et al. (3862c)
Cuttlefish, broiled	Yamaguchi et al. (4361a), Ohgaki et al. (2849a)
Eggs; fish; meat Flour; rice Soy beans	Sugimura and Nagao (3829b)
Fish, broiled, charred	Nagao et al. (2667c), Yasuda et al. (4382a), Kasai et al. (2037c, 2037d), Yamaizumi et al. (4361b)
Herring, broiled Mackerel, broiled Pike, broiled Sardine, broiled	Nagao et al. (2667c, 2667f)
Sardine, broiled	Ohgaki et al. (2949a), Takayama et al. (3862c)
Protein pyrolysates	Nagao et al. (2667f), Yoshida and Matsumoto (4387b), Nebert et al. (2688a), Yoshida et al. (4390)
Albumin	Yasuda et al. (4382a)
Soybean globulin	Yoshida et al. (4389a), Ohgaki et al. (2849b)
Calf thymus Egg white Serum albumin	Nagao et al. (2667b)
Casein; collagen Gluten; histone Insulin; lysozyme Ovalbumin; zein Tobacco protein	Matsumoto et al. (2491c)
Peptide pyrolysates	
Polypeptides	Johnson et al. (1968)
Carnosine Glycyl glycine[b] Glycyl glutamic acid Glycyl proline Glycyl tryptophan Leucyl glycyl phenylalanine Tryptophanyl alanine Tryptophanyl glycine Tryptophanyl tryptophan Tryptophanyl tyrosine	Matsumoto et al. (2491c)
Amino acid pyrolysates	Masuda et al. (2486), Kato et al. (2048, 2049), Kosuge et al. (2178a), Nebert et al. (2688a)
Phenylalanine	Sugimura et al. (3829)
Lysine	Wakabayashi et al. (4102a)
Tryptophan	Sugimura et al. (3829), Yoshida and Matsumoto (4387a), Negishi and Hayatsu (2689a), Yamazoe et al. (4379a), Hosaka et al. (1835a), Matsukura et al. (2491a), Takayama et al. (3862d)
Glutamic acid	Sugimura (3828a, 4365a), Takeda et al. (3863a), Yamamoto et al. (4365a), Ohgaki et al. (2849b), Takayama et al. (3862b)
Histidine 3-Methylhistidine	Smith et al. (3722a)

TABLE 26.22 (continued)
Mutagenicity of Beverages, Heated Foods, and Heated Food Components

Food or Food Component	References
Alanine[c]; arginine Asparagine; citrulline Cysteine; cystine Glutamic acid Glutamine; histidine Lysine; methionine Ornithine Phenylalanine; serine Threonine; tryptophan Tyrosine; valine	Matsumoto et al. (2491b)
Beverages	
Coffee, roasted	Kuratsune[b] (2237), Nagao et al. (2667d, 2667e), Sugimura (3828b), Aeschbacher and Würzner (38a)
Coffee, instant	Aeschbacher and Würzner (38a), Kosugi et al. (2178b)
Tea	Nagao et al. (2667e), Sugimura (3828d)
Brandy	Sugimura (3828d)
Sake	Takase and Murakami (3862a)
CSC	Sugimura (3828d), Yoshida and Matsumoto (4388), Matsumoto et al, (2492), DeMarini (930, 9329, 933)

[a] This was a PAH study, with emphasis on the generation of B[*a*]P.
[b] No mutagens detected in glycylglycine pyrolysate.
[c] The pyrolysates from the various amino acids studied showed mutagenicities (Ames test) in the following sequence (revertant/mg of pyrolysate), the amino acid yielding the highest mutagenic pyrolysate listed first: tryptophan, serine, glutamic acid, ornithine, lysine, arginine, citrulline, threonine, alanine, cystine, glutamine, methionine, cysteine, tyrosine, phenylalanine, histidine, asparagine, valine.

as B[*a*]P in roasted coffee [Kuratsune (2237)] and the similar mid-1960s studies of PAHs in broiled meat [Lijinsky and Shubik (2364a, 2364b)]. PAHs such as B[*a*]P were identified in both studies. The major concern of the early investigators was the possible presence of tumorigenic PAHs, particularly B[*a*]P, in the heated foodstuff. Another PAH of concern was the potent tumorigen 3-methylcholanthrene because of its possible pyrosynthesis during cooking from cholesterol, a component of many meats. Of course, it was subsequently demonstrated that B[*a*]P, in addition to its tumorigenicity to mouse skin, is also mutagenic in the Ames test. However, its specific mutagenicity is insignificant compared to that of many *N*-heterocyclic amines.

From their studies of heated foods or food pyrolysates (30 different foods, including rice, flour, soy beans, fish, meat, eggs), Sugimura and Nagao (3828b) reported

- Mutagenicity was proportional to the protein content.
- Mutagenicity was proportional to the levels of specific amino acids (tryptophan, glutamic acid, etc.) in the constituent protein.
- Mutagenicity was dependent on water content and heating temperature, e.g., for foods with low water content, the mutagens appear at 300°C; for those with high water content, the mutagens appear at 400°C.

As noted in the sections on PAHs and NNAs in foods, estimates of daily exposures to these classes of compounds in foods, beverages, and other factors have been made by numerous investigators. Estimates of exposures to mutagenic *N*-heterocyclic amines are limited. Part of the reason is the difference in time span since the particular class of compounds was found to be tumorigenic and/or mutagenic. Exposures to PAHs tumorigenic in laboratory animal bioassays have been studied for more than seven decades since the early 1930s and the identification of B[*a*]P in coal tar by Cook et al. (796a, 797), and exposures to NNAs tumorigenic in laboratory animal bioassays were studied [Magee and Barnes (2441a)] since the mid-1950s. In contrast, exposures to mutagenic *N*-heterocyclic amines reported to be tumorigenic in laboratory animal bioassays have only been studied for about 30 years (since the mid-1970s and the availability of the Ames test).

In his mid-1980s review, Sugimura (3828c) attempted to estimate the exposure of humans to mutagenic *N*-heterocyclic amines with the limited data at his disposal. He wrote:

> Taking various factors into consideration, it is probably impractical and not realistic to make risk estimations from the carcinogenicity data on rodents given a single carcinogen. However, for a simple extrapolation of animal data for risk estimation, TD_{50} values, which are the doses needed to develop cancers in 50% of animals fed on carcinogens [IQ, Trp-P-1, Trp-P-2, Glu-P-1, Glu-P-2, A*a*C, and MeA*a*C] for

TABLE 26.23
Mutagenicity of Common Beverages *vs.* CSC

Agent	Exposure Level	*ST* Strain	S-9 Mix	Revertants
Cigarette	One, inhaled	TA 98	Yes	4,000
Coffee	200 mL	TA 100	No	180,000
Tea[a]	200 mL	TA 100	No	Mutagenic
Brandy	50 mL	TA 100	No	10,500

ST, S. typhimurium.
[a] Japanese green tea.

TABLE 26.24
B[*a*]P Equivalency of Extracts of Charred Fish and Meat

Analyte	Sample wt., g	B[*a*]P Equivalency, ng	Cigarette Equivalency Based on B[*a*]P[a]
Sardine	100 (3.5)[b]	35,800	2983
Mackerel	60 (2.1)	68,200	5683
Beefsteak	190 (6.7)	85,500	7125

[a] Calculation based on assumption of MSS yield of 12 ng/cig of B[*a*]P.
[b] Number in parentheses is weight in ounces.

> their life time, have been calculated based on mouse experiments … If we assume the average TD_{50} value of heterocyclic amines should be about 8mg/kg/day, we can roughly estimate the risk of these carcinogenic heterocyclic amines for human beings. The intake of heterocyclic amines was calculated from available data on their quantities in foods. Apparently the human intake is about 0.0002% times the TD_{50} obtained from animal data. This means that heterocyclic amines may not be so serious for human cancer development.

Sugimura added:

> On the other hand, it is also true that human beings are being exposed to many heterocyclic amines and many other carcinogens with tumor promoters and/or suppressing factors for carcinogenesis. At this moment, it is honest to state that no solid information on the estimation of risk of heterocyclic amines has been obtained in any direction, either positive or negative.

Sugimura (3828d) reported comparisons of the mutagenicities (Ames test) of various beverages (coffee, brandy, tea) and CSC. His data are summarized in Table 26.23.

In another comparison of mutagenicities toward *S. typhimurium* TA 98, Nagao et al. (2667c) calculated the B[*a*]P equivalency of extracts of charred fish and meat. Their data, with additions (charred food weight in ounces, cigarette equivalents based on B[*a*]P), are shown in Table 26.24.

26.3 SUMMARY

It is obvious from the numerous Hoffmann et al. lists (1727, 1740, 1741, 1743, 1744, 1773, 1808, 1870) summarized in Table 26.1 plus many other listings (1217, 2825) and articles that some 70 tobacco smoke components are defined as significant toxicants with most of the 70 being defined as significant tumorigens. Of the 70, 40 or so have recently been defined as "Hoffmann analytes," and their cigarette MSS yield reductions are used to define a "potentially reduced exposure product" (PREP). It should be noted that the various bioassays that generated the data used to define the tumorigenicity of the various cigarette smoke components are similar to and/or identical with the various bioassays that generated the data to define the antitumorigenicity of various compounds to several known potent tumorigens such as B[*a*]P or DB[*a,h*]A. Many of the compounds with demonstrated antitumorigenicity have been identified in CSC and are present in it at much higher levels than such potent tumorigens as B[*a*]P, DB[*a,h*]A, and DMB[*a*]A.

Why do so many of the proponents of the hazards of cigarette MSS seldom discuss in detail the many anticarcinogens, antitumorigens, or antimutagens present in MSS or the many alternate exposures to the various compound classes, the PAHs, aza-arenes, NNAs, and *N*-heterocyclic amines, defined as significant cigarette MSS problems?

At the 1962 American Association for Cancer Research conference (4314), in their 1964 review [see pp. 330–331 in (4319)], and in their 1967 book, Wynder and Hoffmann [see pp. 370–371 in (4332)] also described the results of their experiments on the antitumorigenicity of two tobacco smoke paraffinic hydrocarbons, *n*-hentriacontane ($C_{31}H_{64}$) and *n*-pentatriacontane ($C_{35}H_{72}$), coadministered separately at two different levels with B[*a*]P. Subsequently, they noted [see pp. 628–629 in (4332)]:

> An explanation of the tumorigenic activity of tobacco smoke condensate in terms of single constituents is made more difficult by the presence of substances that may act as anticarcinogens and/or absorption retarders, especially for tumorigenic agents. It is known that noncarcinogenic hydrocarbons can inhibit the effect of carcinogenic* hydrocarbons … The presence of substances such as long-chain paraffinic hydrocarbons may interfere with absorption of tumorigenic* components.

In their book, Wynder and Hoffmann described not only the 1951 results reported by Steiner and Falk (3814) on the antitumorigenicity of B[*a*]A to B[*a*]P when coadministered subcutaneously but also their own 1963 results of the antitumorigenicity of B[*a*]A to B[*a*]P when administered in a skin-painting bioassay [see pp. 246–247 in (4332)]. They noted:

> The existence of anticarcinogens, however, must be considered in evaluating any complex mixture such as tobacco smoke condensate.

Despite such a statement, neither Wynder and Hoffmann nor any of the proponents of the hazards of cigarette smoking

* It is interesting to note the authors' interchange of the two terms carcinogenic and tumorigenic.

discussed in any detail the presence of antitumorigens in cigarette MSS.

The same proponents usually disregard alternate exposures to various tumorigens despite the many pre-mid-1950s articles by Kennaway and Hueper on respiratory effect of air pollutants. Because of the chronology of the discovery of the tumorigenicity of NNAs in the mid-1950s and *N*-heterocyclic amines in the late 1970s, it is obvious that neither Kennaway nor Hueper could discuss alternate exposures to them. Examples of more recent research are the many publications by Grimmer et al. on exposure to PAHs (1397–1402, 1405, 1406a, 1406b, 1407b) and aza-arenes (1407a) as air pollutants.

In the Searle-edited monograph, comprising over 1400 pages on chemical carcinogens (3568), all but one of the major classes (PAHs, aza-arenes, *N*-heterocyclic amines) of tumorigenic components in MSS are not mentioned. The exception, the presence of NNAs in tobacco and smoke, was described briefly by Preussmann and Eisenbrand [see pp. 839–842 in (2990)]. The bulk of the material they cited on NNAs in tobacco and/or smoke included tabulated results by Hoffmann et al. on NNAs and TSNAs in tobacco smoke (514, 1680) and tobacco [including snuff (1675, 1677, 1685)]. However, Preussmann and Eisenbrand cited many pre-1984 publications in which much data were presented on exposure to NNAs from many alternate sources such as food [see pp. 832–834 in (2990)] beverages [see pp. 834–839 in (2990)], cosmetics [see pp. 842–844 in (2990)], prescriptions [see pp. 844–845 in (2990)], pesticides [see pp. 845–846 in (2990)], rubber products [see pp. 846–848 in (2990)], water [see pp. 848–849 in (2990)], and occupations [see pp. 851–857 in (2990)]. In his chapter in Searle (3568), Grasso (1345) described the results of much research on PAHs and NNAs in foods but none on *N*-heterocyclic amines in food. Many references to alternate exposures to NNAs are presented herein, but a great many more may be obtained by a search of the Internet.

27 Free Radicals

27.1 INTRODUCTION

Free radicals and reactive oxygen species (ROS) are common to all living animals and plants, including tobacco. ROS in plants include hydrogen peroxide (H_2O_2) and singlet oxygen ($^1O_2$), as well as several free radicals and radical anions such as nitric oxide (NO), superoxide anion radical ($O_2^{-\bullet}$), hydroxyl radical ($HO^\bullet$), and perhydroxyl radical ($HO_2^\bullet$) [Bartosz (27A06), Dat et al. (27A23), Halliwell (27A40)]. These highly reactive oxidation byproducts are created by normal cell metabolism and environmental factors such as pollution and are continuously produced by living organism.

Free radicals play an important role in the life processes of plants. Free radicals and ROS are produced predominantly in plant cells during photosynthesis and photorespiration and, to a lesser extent, in respiration processes. Free radicals and ROS play crucial roles as signaling molecules in various physiological processes. For example, during periods of environmental stress, intra- and intercellular levels of H_2O_2 and NO tend to increase. Additionally, specific types of free radicals and ROS interact with thiol-containing proteins and activate different signaling pathways as well as transcription factors, which in turn regulate gene expression and cell-cycle processes. Therefore, free radicals and ROS control numerous types of cellular redox reactions (homeostasis), signaling processes (photosynthetic and respiratory metabolism), and processes that regulate plant growth, development, acclimatory and defense responses [Ślesak et al. (27A105)].

The role of free radicals and ROS in plant biochemistry and physiology has been described in many review papers [Kuźniak and Urbanek (27A63), Neill et al. (27A80, 27A81), Apel and Hirt (27A02), Hung et al. (27A47)]. There are no free radicals or ROS that are unique to tobacco. As a result, there will not be an in-depth discussion of free radicals or ROS specifically found in tobacco. In most cases, the free radicals in biological systems are highly reactive and have half-lives of 10^{-6}–10^{-3} s. Nonetheless, free-radical activity has been observed in tobacco. Analytical methodologies rapid and specific enough to monitor and identify these free radicals are just emerging.

It is believed that the presence of oxygen (O_2) in the Earth's atmosphere originated from photosynthetic activity. However, oxygen is involved in two very different roles in biological systems. It is a prerequisite for aerobic metabolism and consequent normal growth and development, but at the same time, a reduction or an increase of molecular oxygen in biological systems very often results in the formation of ROS that can cause deregulation of normal cellular processes and eventually cause cell death. Therefore, in plants and in other aerobic organisms, antioxidant systems have evolved.

The balance of oxidants and antioxidants in plants and animals is critical for survival. The production of ROS is normally carefully controlled by living organisms. A dynamic equilibrium exists between the formation of ROS and the activity of the antioxidant scavenging systems [Hancock et al. (27A45), Irshad and Chaudhuri (27A49), Mittler et al. (27A74), Mittler (27A73), Vranova et al. (27A119)]. To protect themselves from ROS, plants possess a number of free-radical scavenging enzymes, such as ascorbate peroxidase, catalase, and superoxide dismutase (SOD), and low-molecular-weight antioxidants, like ascorbate and tocopherols [Hancock et al. (27A45), Vranova et al. (27A119)]. Antioxidants in tobacco and tobacco smoke are discussed in Chapter 26.

At the senescence stage in tobacco growth, enzyme activities (especially hydrolytic and other degradative enzyme systems) are intensified. These systems are responsible for breakdown of functional and structural components of the cell, such as proteins, nucleic acids, carbohydrates, and lipids. The latter stage of senescence resembles the early stage of leaf curing [Tso (27A114)]. During each of these processes, free-radical reactions are occurring in tobacco leaf. In 1955, Frankenburg et al. reported that free-radical reactions were occurring in cured tobacco leaves to form a nicotine dimer (1224, 1226).

After tobacco is grown, cured, and aged, there are free radicals still found in the lamina. It is believed that free radicals are present on the polyphenols, carbohydrates, and lignin present in tobacco. This is supported by evidence for the generation of free radicals in cellulose by irradiation with ultraviolet light [Kleinert (27A61)]. The existence of stable free radicals in lignin has also been demonstrated [Rex (27A98), Steelink (27A107), Steelink et al. (27A108)]. The formation of free radicals in wood by ionizing radiation has been shown as well as the generation of free radicals in wood resulting from exposure to light [Kalnins et al. (27A57)].

Free radicals are ubiquitous. They are found in living plants and for practical purposes are essential to all life. They also exist in plant material that is dried. These types of free radicals are called persistent free radicals and are normally associated with free radicals present in the structural biomass of the plant (polyphenols, carbohydrates, and lignin). The tobacco precursors of free radicals found in the particulate phase of cigarette mainstream smoke (MSS) are also long-lived, persistent free radicals but arise from the thermolysis of the tobacco biomass to form numerous types of phenolic and quinoidal free radicals [Wooten et al. (27A120)]. Short-lived free radicals are also present in the vapor phase of MSS. Although the types of free radical in tobacco may be similar in form to those in tobacco smoke, in some cases, e.g., NO, they are formed/generated in very different manners.

Free radicals can participate in a wide variety of reactions such as additions, substitutions, eliminations, rearrangements, reductions, electron transfers, and oxidations (27A01). From the beginning of the twentieth century, free-radical chemistry has spread its influence over a wide range of research areas that impinge on our progress and well-being. Apart from polymer chemistry, synthetic organic chemistry, and environmental chemistry, much effort in recent times is expended on research in health and nutrition [Nagendrappa (27A78)].

There are some general features of a free-radical reaction. Free-radical reactions take three distinct, identifiable steps. The first is formation of the free radical that can happen by enzyme catalysis, homolysis, thermolysis, radiation, light induction, combustion, and pyrolysis, or other means. The second step, called propagation, is the heart of a free-radical reaction. In this step, free radicals are repeatedly regenerated and can react with neutral molecules to produce new free radicals. If there is no intervention, two free radicals can react to form a neutral molecule, and the reaction is terminated, which represents the third step in the general reaction scheme. Because of this repetitive nature of the reaction, free-radical reactions are called "chain reactions" and are often represented as a cyclic process [Nagendrappa (27A78)].

27.2 ANALYTICAL METHODS FOR DETERMINATION OF FREE RADICALS

The instrumental method historically used for the detection of free radicals is electron spin resonance (ESR) (sometimes called electron paramagnetic resonance [ERP]). ESR is a spectroscopic technique which detects species that have unpaired electrons. Free radicals can be organic compounds that have a free electron on carbon, oxygen or nitrogen, or inorganic compounds or complexes that have a free electron usually residing on a metal [EPR (27A31)]. ESR spectroscopy is the preferred and major analytical technique for the detection and quantification of free radicals [Demopoulos (27A28)]. ESR has been used in many fields of science to explore the presence and effects of free radicals in chemistry, physics, and biology.

Free radicals can be gases, liquids, or solids and generally exist in very low, and in some cases, steady-state concentrations. ESR can be used to make direct measurements of free radicals that exist in steady-state concentrations [Demopoulos et al. (27A29)]. For short-lived, highly reactive free radicals, regardless of their physical and chemical form, numerous methodologies are now available to convert these free radicals into longer-lived species for analysis. Short-lived free radicals are first treated with another reagent called a spin trap. The resultant product, the spin adduct, is a more stable free-radical species that can then be measured by ESR. Concentrations of free radicals are determined by measuring the spin-trap adducts. A wide variety of spin-trapping reagents have been used. Figure 27.1 shows the chemical structures for a selection of these spin traps.

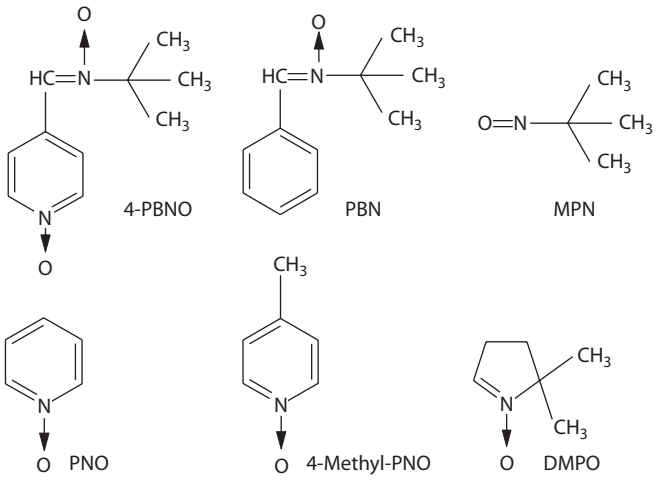


FIGURE 27.1 Chemical structures of 4-POBN, PBN, MNP, PNO, 4-methyl-PNO, and DMPO spin traps [McCormick et al. (27A71)].

Techniques that use ESR alone or ESR with spin-trapping methodologies have advanced tremendously over the last 40 years [Janzen and Gerlock (27A54), Janzen (27A52, 27A53), Janzen et al. (27A55)].

Unlike other typical analytical techniques, e.g., infrared spectroscopy, ESR measurements require a high level of technical skill and expertise. ESR sample measurements are highly dependent on sample collection, sample preparation, types of solvents, temperature, choice of spin trap, and instrument calibration of electrical and magnetic fields, among other things.

ESR, by itself, is considered a very specific, yet semiquantifiable, technique for the measurement of free radicals. It can be used in conjunction with other analytical techniques, such as gas chromatography (GC), mass spectroscopy (MS), and high-performance liquid chromatography (HPLC), for the study of free radicals [Cranton and Frackelton (27A20)]. ESR used in conjunction with other analytical techniques is an emerging field.

Free radicals can also be measured in biological samples. In a recent review by Sanchez-Moreno (27A103), several ESR techniques were described for the collection and determination of free radicals (superoxide, hydroxyl, and peroxyl) that occur in biological systems. These techniques include the total radical-trapping antioxidant parameter method (TRAP), the oxygen radical absorbance capacity method (ORAC), and the Trolox equivalent antioxidant capacity method (TEAC). McAnalley et al. (27A70) have provided descriptions and applications of these (and other) methodologies for the determination of free radicals in biological media. Sanchez-Moreno (27A103) concludes that "in spite of the diversity of biological methods, there is a great need to standardize measurements of antioxidant activity."

Sophisticated ESR instrumentation is now becoming available that allows for the direct study of free radicals and free radical damage in living systems. In 2006, Hirata and Fujii (27A46) reviewed newly developed technologies in ESR spectroscopy and imaging equipment that are useful for

the analysis of free radicals in living (biological) systems. Automatic control techniques used for a continuous-wave ESR spectrometer were discussed. Recent developments in time-domain ESR spectroscopy were also reported. Time-domain ESR spectroscopy is a technically challenging method but can be very useful for the detection of free radicals with very short relaxation times in biological tissues. ESR imaging techniques were also reviewed which are able to visualize free radicals in animal subjects noninvasively. Applications of in vivo ESR spectroscopy and imaging for the detection of free radicals generated in biological specimens is another emerging field especially designed for the noninvasive direct detection of free radicals in biomedical applications. Shulaev and Oliver (27A104) and Tarpey et al. (27A113) have also recently written reviews on ESR methods for the detection of reactive oxygen- and nitrogen-centered free-radical metabolites in in vitro and in vivo systems employing metabolic and proteomic markers for oxidative stress.

Additional articles, reviews, and books on ESR and methodologies to detect and measure reactive free radicals in vitro and in vivo in plants and animals have been written by Khan and Swartz (27A58), Khan et al. (27A59), Bacic and Mojovic (27A03), Muckenschnabel et al. (27A75), Halliwell and Whiteman (27A43), Utsumi and Yamada (27A116), Utsumi et al. (27A117), and Halliwell and Poulsen (27A42).

The newest methodologies for the detection, quantification, and identification of free radicals in cigarette smoke employ HPLC and high-resolution MS analysis of stable radical adducts [Bartalis et al. (27A05)], hyphenated LC-MS/MS techniques with a C18 reverse-phase column fitted to a triple quadrupole instrument for analysis of stable radical adducts [Rolando et al. (27A99, 27A100)], and electrospray ionization (ESI)–HPLC/MS analysis of stable radical adducts [Masselot et al. (27A68, 27A69)].

27.3 FREE RADICALS IN TOBACCO SMOKE

Tobacco smoke contains free radicals. As presented in previous chapters, tobacco smoke is a highly complex aerosol composed of more than 5000 components distributed between the vapor and the particulate phases. The enormous complexity of cigarette smoke is the result of multiple thermolytic processes that occur in heated tobacco within the confines of the burning cigarette rod. These processes involve distillation, pyrolysis, and combustion and are influenced by several factors including the design of the cigarette [Norman (27A82)] and the composition of the tobacco blend [Bokelman and Ryan (385), Leffingwell (2338)]. As indicated in the preceding Chapters 1 through 21, numerous classes of organic compounds are represented in cigarette smoke including saturated, unsaturated, and polycyclic aromatic hydrocarbons (PAHs), alcohols, aldehydes, ketones, carboxylic acids, esters, phenols, nitriles, *N*-nitrosamines, terpenoids, and alkaloids [see also Baker (172), Dube and Green (1067), Hoffmann et al. (1744)]. Invariably, the combustion of tobacco, like that of any organic matter, also produces free radicals via oxidative processes involving homolytic reactions. The high temperatures produced during the smoking process are easily capable of causing bond scissions that lead to free-radical production [Badger et al. (141), Brown (27A14)].

An elaborate description of the fluctuating thermal gradients and vapor environment inside a cigarette during smoking has been given by Baker (172). The chemical complexity of cigarette smoke is strongly dependent on the heating conditions inside the lit cigarette. To summarize briefly, when a smoker lights and draws on a cigarette, the temperature of the ignited tobacco rises rapidly, and a hot coal forms at the lit end of the cigarette (the combustion zone and pyrolysis zone). Peak temperatures inside the coal can exceed 900°C. The high temperature inside the coal during a puff causes an increase in the viscosity of the air flowing through the coal and a concomitant increase in the resistance to the draw of air through the cigarette. This effect forces air to be drawn primarily into the periphery of the coal at the paper burn line rather than through the center of the coal. The depletion of oxygen due to combustion inside the coal and the flux of air around the coal results in the formation of a region immediately behind the coal that is depleted of oxygen, but where the temperatures remain high enough to promote the thermal decomposition of the unburned tobacco. This area behind the coal is known as the pyrolysis/distillation zone. Large amounts of volatile and semivolatile smoke constituents evolve from this zone. These constituents result, in part, from the pyrolysis of tobacco and, in part, from the distillation of volatile constituents native to tobacco because of the heat of the encroaching coal. Numerous types of MSS free radicals are formed in this pyrolysis/distillation zone [Wooten et al. (27A120)].

Cigarette smoke can be divided into two phases, particulate- and vapor-phase smoke, by the use of Cambridge filter [Dube and Green (1067)]. The radicals in these two fractions differ greatly. The MSS particulate phase contains more than 10^{17} stable, long-lived radicals per gram of TPM. The vapor phase of smoke contains more than 10^{15} short-lived radicals per puff [Baker (27A04), Wooten et al. (27A120)]. Free radicals in tobacco smoke were initially detected in whole smoke by Lyons et al. (2429). After some years, scientists became interested in examining the population of free radicals in the particulate and vapor phase of MSS. This trend has continued for nearly 45 years. It has not been until recently that it was proposed that artifacts may be forming during the separation of the whole smoke [Culcasi et al. (27A22), Bartalis et al. (27A05)].

27.4 HISTORICAL REVIEW OF FREE-RADICAL RESEARCH ON CIGARETTE SMOKE

The following paragraphs chronologically summarize research reported on free radicals in MSS [Prier (27A84)] and important discoveries that shaped the mechanisms proposed to explain the generation of free radicals in MSS and their possible biological impact. This historical review of

free radicals in cigarette smoke is not exhaustive but attempts to capture much of the fundamental research that has shaped this field of science and gives the researcher ready sources for further examination.

In 1958, Lyons et al. (2429) first observed free radicals by ESR in whole cigarette smoke that was condensed at liquid oxygen temperature. These workers reported that whole cigarette smoke contains two populations of free radicals, an unstable population that can only be observed at −183°C and that vanishes when the condensate is warmed to 60°C, and a persistent, stable population that exists for "several days" at room temperature. They reported that the unstable population accounts for about one-sixth of the total free-radical population determined at −183°C and consists of about 10^{15} free electrons per gram of tar. This work was repeated by Forbes et al. (1211) in 1967 with very similar results.

In a second set of experiments, Lyons and Spence in 1958, studied the effect of extracting benzene solutions of the stable free radicals with water, 2*N* sodium hydroxide, and 2*N* sulfuric acid. They reported that the ESR signal of the stable free radicals was reduced in intensity following each extraction by 20%, 50%, and 57%, respectively. They concluded that whole cigarette smoke contains several different types of free radicals, some of which are very stable while others exist only fleetingly. They also suggested for the first time that free radicals might be involved in the carcinogenicity of cigarette smoke (2432).

In a follow-up study, Lyons and Spence in 1960 reported the detection of free radicals in sidestream smoke (SSS) as well as in MSS. They reported that dried SSS condensate contains 5×10^{14} spins per gram of tar, while MSS condensate contains 6×10^{15} spins per gram of tar. These results were compared to chimney soot and to the condensed exhaust material from diesel-powered automobiles that contain 5×10^{18} and 2×10^{19} spins per gram of material, respectively (2435).

Ingram and Allen in 1959 (1862) and Ingram in 1961 (1861) published two further extensions of earlier work in which the pyrolysis of organic material was related to the production of free radicals detected by ESR. They demonstrated that free-radical production by pyrolysis is a general phenomenon that occurs with various types of hydrocarbons and that the concentration of free radicals produced is proportional to the percent of carbon in the pyrolyzed material. A maximum free-radical concentration was detected at about 90% carbon. They concluded that such a high percentage of carbon is consistent with a PAH and that free electrons must reside within such a structure. Ingram (1861) postulated that the stable free radicals generated from the pyrolysis of tobacco could be benzosemiquinone radicals. He also postulated that PAH free radicals would be present in tobacco smoke condensate.

In 1963, Marsden and Collins (2466) reported on their results from measurements of α-activity in leaf tobacco used for cigarettes marketed in the United Kingdom and in specially made standard size unblended cigarettes made from tobaccos originating from widely separated geographical locations. The origin of free radicals in tobacco smoke was discussed. They speculated on contributions of α-radiation and free radicals in cigarette smoke in the induction of lung cancer.

In that same year, Westermark (4220a) suggested that free radicals generated during smoking could lead to a free-radical chain reaction, which could possibly generate enough free radicals to be carcinogenic.

Wynder and Hoffmann in their lengthy 1964 review of tobacco carcinogenesis (4319) discussed tobacco smoke as a "complete carcinogen" and in their evaluation of the role of tobacco smoke components in experimental carcinogenesis listed radicals with the comment that radicals are "suggested as possible carcinogens in disagreement with the experiments" [see p. 391, Table XXII in (4319)].

Takeshita and Ohe in 1964 published a paper on the effects of aging of cigarette smoke and its relation to radical concentration (3864). In their study, they used the radical scavenger α,α′-diphenyl-β-picrylhydrazyl (DPPH) and were able to detect free radicals in condensed whole smoke from flue-cured tobacco after 300 h, employing a colorimetric method. DPPH is a fluorescent stable free radical and will react with other radicals to form a neutral non-fluorescent hydrazine species. DPPH is not considered a spin trap which generally involves free radical addition to a nitroso function. The reaction produces stable nitroxides which build up to readily detectable concentrations in the presence of a free-radical source. The usefulness of radical addition reactions with nitrones has been found to exceed that of the nitroso compound because of their greater stability in a variety of reaction conditions. Much work has been done with phenyl α-*N*-*tert*-butylnitrone (PBN) in solution, although many new spin adducts are now available. The free-radical addition reaction is called a spin-trapping reaction. The nitrone or nitroso compound is called a spin trap, and the radical addition product is called a spin adduct [Janzen and Gerlock (27A54)].

In 1965, Boenig (369) reported on the pyrolytic products of cigarettes irradiated with ^{60}Co γ-radiation. ESR experiments were not conducted on the tobacco to determine the presence or extent of free radicals, although a reduction in concentration of free radicals in smoke condensate (as measured by ESR) was noted along with reductions in MSS tars and tar-like components. Later in 1975, Severson et al. (3610) conducted studies on γ irradiation of cigarettes and concluded that γ irradiation had no major effects on smoke composition. Their study negated the possibility of decreased formation of PAHs as a result of fewer free radicals and other suggested changes in smoke chemistry.

Boenig reviewed the literature on free radicals and health in 1966 (370, 371). In his reports, he considered the fundamental processes involved in the pyrolysis of tobacco during smoking, i.e., distillation, steam distillation, thermal oxidation, decomposition, and thermal cracking (thermal cracking apparently playing a major role in this combustion). He emphasized that thermal cracking probably is the most important step, during which free radicals are formed.

Interaction of a considerable proportion of these free radicals then leads to the formation of various types of molecules including the PAHs. He proposed a mechanism that would explain the formation of PAHs from various tobacco constituents and a variety of small reactive free radicals, e.g., NO, hydroxyl, alkyl. Later that year, he authored a paper in which he proposed a unifying concept that free-radical exposure and health are intimately linked (372).

Browning and Patton presented a paper at the *20th Tobacco Chemists' Research Conference (TCRC)* in 1966 on a quantitative analytical procedure to determine stable free radicals in tobacco smoke condensate by ESR (448). Their analytical method for the determination of stable free radicals in tobacco smoke condensate was generally applicable to all types of tobacco tars. Accuracy for the method was based upon standard coal reference samples that yielded 7.52×10^{16} spins/g of tar. The experimental precision was 10%. They discussed the limitations (heating effects, sample isolation and concentration, solvent effects) and utility of the method.

In 1966, Forbes reported on the role of free radicals in tobacco smoke carcinogenesis (1210). In that publication, he concluded that tobacco smoke condensates contained a variety of free-radical species that had a broad range of stability. Some of the free radicals had lifetimes of only a few seconds, while others are stable over long periods of time. The chemical nature of the radicals formed in tobacco smoke was not fully identified. Forbes postulated that some of the free radicals formed resembled radicals obtained from benzo[*a*]pyrene.

In 1967, Forbes et al. further examined free radicals present in tobacco smoke condensates by ESR (1211). They prepared and examined sulfuric acid solutions of smoke condensates. They reported that the free-radical species present in sulfuric acid solutions of smoke condensates corresponded to a modified benzopyrene-type cation radical and to the spectrum of a modified anthracene cation radical, with the latter decaying fairly rapidly. No definitive proof was given for these two cation radicals.

Rowlands et al. (27A101) studied the effect of MSS free radicals on the tissue of perfused rabbit lungs in 1967. The lungs were removed from the animals and attached to bell jars that were used to simulate the breathing operation. The animal blood was circulated through the veins and arteries attached to the lung while smoke were periodically drawn into the lung. The blood was then sampled and studied by ESR. They found a three-line ESR spectrum superimposed on a second broad singlet. They theorized that a covalent, hexa-coordinated ferric hemoglobin complex explained the ESR spectra.

In 1968, Rowlands et al. (27A102) published an extension of their previous work in which the reaction of cigarette smoke condensate (CSC) with hemoglobin was studied in more detail. In addition, the electron transfer properties of the smoke condensate were studied. The involvement of the oxides of nitrogen in the free-radical properties of the smoke was suggested by a selective condensation experiment in which the smoke was fractionated at various temperatures and the various condensates reacted with hemoglobin.

Cooper et al. published a paper (814) in the 1968 National Cancer Institute monograph "Toward a less harmful cigarette" (4343) in which they suggested that free radicals in MSS were possible contributors to tobacco smoke carcinogenesis. They summarized research from the previous decade on free radicals in tobacco smoke and discussed the possible role of free radicals as a cause of cancer (814). It should be noted that as early as 1954, Dorn reviewed the published experimental evidence that indicated that the products formed by the combustion of tobacco may cause skin cancer in mice. He stated that compared to other known carcinogens, the combustion products of tobacco smoke are relatively weak (27A30).

In their 1967 book, Wynder and Hoffmann [see pp. 461–463 in (4332)] briefly described the studies on cigarette smoke free radicals conducted up to that time. Summing up the available evidence, they wrote:

> Several facts seem to exclude an importance of radicals in tobacco smoke condensate carcinogenesis. Even though sidestream smoke condensate contains only about one tenth the amount of free radicals found in the mainstream smoke condensate, the tumor response of both sidestream and mainstream "tar" on mouse skin is not different statistically … Since both types of radicals are present mainly in the particulate matter, it remains questionable whether in freshly generated tobacco smoke organic radicals participate in the carcinogenic effect.

During 1968, Stedman wrote his review on the chemical composition of tobacco and smoke (3797). In his review, he summarized much of the prior work on free radicals in MSS. At that time, no free radicals in tobacco or tobacco smoke had been identified. As free radicals were considered to be playing some role in the induction of cancer, efforts were concentrated on determining the quantity of free radicals in smoke and their stability.

In 1961, Larson et al. (2264) published their book on experimental and clinical studies on tobacco. Free radicals in smoke were not mentioned. However, in Supplements I, II, and III, issued successively in 1968, 1971, and 1975, respectively, Larson and Silvette (2266) summarized reported research on free radicals in tobacco smoke. In the nearly 800-page 1968 Supplement I, they reviewed the free-radical findings of Lyons and Spence (2432), Ingram (1861), Ingram and Allen (1862), and Westermark (4220a) in a few paragraphs. In the over 500-page 1971 Supplement II, Larson and Silvette summarized the findings on free radicals in tobacco smoke by Boenig (370, 371), Peacock and Spence (27A82b), and Cooper et al. (814) in less than a page. In the nearly 800-page 1975 Supplement III, their only reference to radicals in tobacco smoke was in two separate paragraphs on a study by Dontenwill et al. (1046a) in which the specific tumorigenicities of the CSCs from control and tobacco treated with *n*-propyl gallate were compared. The *n*-propyl gallate was a known scavenger of free radicals. No tumorigenic difference was observed.

During 1969, Rathkamp and Hoffmann (3086) reported on the inhibition of the pyrosynthesis of several selective

smoke components. They suggested from the results of their pyrolysis studies on tobacco containing KNO_3 or I_2 that PAHs are at least partially formed via C and H free radicals.

In 1969, Tully et al. (27A115) were the first authors to publish a study of the free radicals in the vapor phase of MSS cigarette smoke that was condensed at liquid oxygen temperature. The condensed vapor phase of MSS produced no ESR signal until the temperature of the ESR cavity holding the sample was raised to −100°C. At this temperature, a three-line ESR spectrum was obtained that had nitrogen splitting [a(N)] of 1.26 mT. For cigarettes made with tobacco that contained 3.4% copper nitrate by weight, a complex ESR spectrum consisting of at least 17 lines was observed. The three-line spectrum from the untreated tobacco increased to a maximum intensity after 1.5 h at −100°C. When warmed to room temperature, the ESR signals observed at −100°C vanished irreversibly. These authors concluded that the observed free radicals may have formed as a result of some unspecified participation by nitrogen oxides (NO_x) in free-radical reactions within the smoke. Interestingly, nitrogen dioxide (NO_2), itself a free radical, adds to olefinic double bonds to produce carbon-centered free radicals [Estefan et al. (27A35)]. ESR spectra taken on solutions of NO_2 mixed with different olefins show three-line spectra that are very much like those observed by Tully et al. (27A115). In each case, a three-line spectrum with a(N) = 1.22–1.33 mT is obtained [Estefan et al. (27A35), Bielski and Gebicki (27A09), Pryor et al. (27A91)].

Short-lived particulate- and vapor-phase free radicals that cannot be measured directly by ESR can be measured with the aid of spin traps. The first application of spin trapping to the study of free radicals in tobacco smoke was reported in 1971 by Bluhm et a1. (349). MSS from commercial cigarettes, pipes, and cigars was bubbled through solutions of PBN in benzene (a spin trap). In each case, a doublet of triplets with a(N) = 1.376 and a(H) = 0.199 mT was obtained along with a triplet with a(N) = 0.801 mT. The former splittings were assigned to an alkoxyl free-radical adduct of PBN, while the latter signal was assigned to benzoyl *tert*-butyl nitroxide ($PBNO_x$). The intensity of the spin-adduct signal from cigarette smoke was the weakest, while that from cigars was the strongest. The identity of the specific alkoxyl radical was not determined.

Bilimoria et al. investigated the inhibition of radical-initiated polymerization of vinyl acetate by tobacco smoke and some PAHs in 1973 (329). Their results indicated that vapor phase of smoke is an efficient inhibitor of vinyl acetate polymerization and that conjugated dienes like isoprene are responsible for the inhibition. There were no free radicals from tobacco smoke specifically identified in this research. Nisbet and Schmeller presented the results of this research at the *27th TCRC* in 1973 (2789a).

At that same TCRC in 1973, Johnson (1956) presented a paper on the antioxidant activity of tobacco smoke. The investigation was undertaken to determine whether or not smoke initiates or promotes the formation of radical peroxides which would in turn lead to lipid peroxidation. He found that both the vapor phase and particulate phase of smoke behaved as an antioxidant. Fractionation of the total smoke condensate showed antioxidant activity in the neutral and water-insoluble acidic fractions, with virtually no activity in the basic fractions. The mode of antioxidant action of tobacco smoke was discussed in terms of free-radical mechanisms involving atom transfer, addition, substitution, and coupling.

De Hys et al. in 1973 (27A25) studied the spin trapping of free radicals in the filtered MSS of 1R1 research cigarettes. They obtained spin-adduct spectra that did not exhibit hydrogen splitting, although the three-line spectra were very broad (the hydrogen splitting was not resolved). They reported that smoke held in the syringe for 15 s before being bubbled through the PBN solution showed no change in spectral features, while smoke held in the syringe for 30 s resulted in a 50% decrease in the spin-adduct spectral intensity. These authors also found that spin-trapping unfiltered smoke resulted in no spin-adduct spectrum. Experiments were also performed using 2-nitrosotoluene and 5-nitroso-8-quinolinol as spin traps. In the first case, a three-line spectrum was obtained with a(N) = 1.56 mT, while the second spin trap gave no spin adduct. No attempt was made to identify the free radical trapped with 2-nitrosotoluene. These results indicate that time and smoke filtration impact free-radical collection and measurement.

NO_2 was bubbled through a solution of PBN in benzene and the resulting solution studied by ESR. A strong three-line ESR spectrum with a(N) = 1.0 mT was observed. Smoke bubbled through cyclohexene produced no ESR signal, although NO_2 can react with olefins to give the three-line spectrum described previously (27A35, 27A09, 27A91). These authors concluded that the free radicals in the vapor phase of cigarette MSS have half-lives of about 30 s and that NO_2 is not the dominant free-radical species responsible for production of spin adducts from cigarette smoke.

In 1974, Morie evaluated the effectiveness of free-radical traps in cellulose acetate filters for the removal of nitrogen oxides from cigarette smoke (2625). Four free-radical spin traps were tested as cigarette filter additives for the removal of nitrogen oxides from tobacco smoke. A filter consisting of cellulose acetate fibers containing 20 mg of 4-(3,5-di-*tert*-butyl-4-hydroxybenzylidene)-*tert*-butylamine *N*-oxide removed 42% of the nitrogen oxides from cigarette smoke. Three other free-radical traps when placed on cellulose acetate fibers or activated carbon within cigarette filters reduced the concentration of nitrogen oxides in the smoke to a lesser extent. The mechanism proposed by Morie for the removal of nitrogen oxides was that the free-radical spin trap reacted with a free radical in the tobacco smoke to yield a long-lived nitroxide radical, which in turn reacts with nitrogen oxides in the smoke.

A spin-trapping study of the free radicals in the MSS from 1R1 research cigarettes was performed by Menzel et al. in 1976 (27A72). These authors used spin-adduct spectral line broadening to determine that the MSS vapor-phase results in 1×10^{18} spin-trapped free radicals per cigarette puff (about 10^{19} spins/g of tar produced). Using spin-trap solutions in series, they estimated the efficiency of spin trapping of the

tobacco smoke free radicals with PBN to be about 47%. They obtained extremely broad spectral lines (by ESR) showing no hydrogen splitting. Their results were somewhat suspect as the spin-adduct concentration that they obtained (2×10^{19} spins/g) was much larger than any other free-radical concentration reported before or since (2429, 2435, 27A95).

During 1976, Pryor edited and contributed to a book on free radicals in biology (2998a). In that book, he authored a paper on the role of free radicals in biological systems where he discussed free radicals in cigarette smoke and the possible action of free radicals in smokers.

A comprehensive study of free radicals in the vapor phase of MSS produced by 1R1 research cigarettes was reported in 1976 by Pryor et al. (27A95). Using three different spin traps, PBN, 5,5-dimethyl-1-pyrroline-*N*-oxide (DMPO), and 3,5-(di-*tert*-butyl-4-hydroxyphenyl)-*N*-*tert*-butylnitrone (OHPBN), they found that MSS produces three types of spin adducts: an alkoxyl or aroyloxyl spin adduct, $PBNO_x$, and an unknown adduct with $a(N) = 1.00$ mT. They reported that the intensity of the alkoxyl adduct increases with the distance that the smoke must travel from the cigarette to the spin-trap solution and then decreased thereafter. They called this phenomenon the path length effect. The concentration of spin-trapped free radicals was found to be about 1×10^{15} spins/g of tar. In addition, the effect of aging on the absolute and relative concentrations of the spin adducts was studied. The conditions of collection also had an impact on free-radical measurement. Their data did not allow them to specify the identity of either the aromatic group in the aroyloxy ($ArCO2^{\bullet}$) radical or the alkyl group in the alkoxy ($RO^{\bullet}$) radicals.

Ishiguro and Sugawara published their review on chemistry of tobacco smoke in 1980 (1884). This was the last major review of compounds identified in tobacco smoke. In their massive report, they reviewed the literature on free radicals in tobacco smoke. There were no identified free radicals specifically mentioned in their review. They stated that:

> The study of radicals in smoke has not advanced very far because of the difficulty of identifying the radicals. It is hoped that further progress will be made in this field so that the formation routes of many components can be understood and the composition of smoke components can be better controlled.

In a paper written in 1982 entitled "Free radical biology: Xenobiotics, cancer, and aging," Pryor suggested that free radicals in cigarette MSS could pose a significant health risk to smokers (2998b). In that paper, he proposed several complicated interactions between MSS components, e.g., NO, dienes, phenols, and free radicals that he believed were operative means leading to carcinogenesis.

In 1983, Slaga et al. suggested that free radicals may be involved not only in initiation but also in the promotion of carcinogenesis (3687).

In 1983, using ESR spin-trapping techniques with PBN as the spin trap, Pryor et al. (2999a) observed free radicals in the vapor phase of both cigarette MSS and SSS. The principal vapor-phase free radicals appeared to be alkoxyl radicals ($RO^{\bullet}$). Pryor et al. determined that each of the vapor phases of cigarette MSS and SSS has about the same concentration of radicals, about 1×10^{16} radicals/cig (or 5×10^{14} per puff) (2999a).

In that same year, Pryor et al. (2999) examined and found that the particulate matter from both MSS and SSS contained persistent free radicals. The ESR signal was obtained when the particulate matter collected on Cambridge pads was measured directly and when the particulate matter was extracted from the Cambridge pad with various solvents. Pryor et al. listed the occurrence of four paramagnetic radical species in CSC. Three of these radicals, an inorganic phosphorus radical, a graphitic carbon associated radical, and a radical that appeared associated with an odd electron delocalized over an aromatic ring system, appeared to have relatively short half-lives. However, the fourth type of free radical had an unusually long half-life of several days. It was speculated that the dominant ESR signal from this fourth type was from free radicals generated from catechol and hydroquinone (HQ). Neither of these free radicals was unequivocally identified (2999). Treatment of alcoholic solutions of particulate matter with base generated a new group of radicals that appeared to be semiquinone radicals derived from the oxidation of phenolic and polyphenolic species in the particulate matter. Pryor et al. suggested this latter radical was associated with a quinone (QH)/HQ acceptor/donor chain (2999). Again, the identification of the specific free radicals was not obtained.

In these two papers and again in 1984 (3001), Pryor et al. suggested the possible involvement of particulate-phase MSS free radicals in smoking-related diseases (2999, 2999a). In vitro assays were performed that suggested that cigarette smoke may cause oxidative stress or oxidative damage to essential biological molecules (3000, 27A120). Specifically in 1984, ESR evidence of the binding of the particulate-phase MSS free radicals to DNA and polynucleotides was shown (3001).

In the 1984 American Chemical Society monograph on chemical carcinogenesis, edited by Searle (3568) and with contributions from experts in carcinogenesis, there was no mention on the carcinogenicity of free radicals, nor any tumorigenic PAH or aza-arene in tobacco smoke despite the reports by Snook et al. (3756–3759, 3750, 3752, 1544, 3664, 3665, 3908).

In 1985, Nakayama et al. published a report that described the generation and identification of H_2O_2 and superoxide anion radical from cigarette smoke (2677). H_2O_2 and superoxide anion radical were generated in a neutral buffer solution through which cigarette smoke was bubbled. They speculated that the H_2O_2 may have been formed by the autoxidation of polyphenols such as catechol and HQ in the cigarette smoke.

During 1985, Halpern and Knieper isolated and tentatively identified the *tert*-butoxy radical by the spin trapping of radicals in the vapor phase of cigarette smoke (27A44).

Cosgrove et al. in 1985 (828a) showed that it was possible to detect hydroxyl radicals in an aqueous extract of the particulate phase of cigarette MSS under metal-mediated conditions. An unidentified alkyl radical and the carbon dioxide

anion radical were also observed under their experimental conditions. They concluded that the results of their experiment indicated that the major particulate-phase free radical was a QH/HQ redox system in a polymeric matrix and that the radical signal could become associated with DNA. Unequivocal proof was not provided for these claims.

Church and Pryor in a 1985 publication (746) summarized their work (to that point) on the free-radical chemistry of cigarette smoke and its toxicological implications. They stated that cigarette smoke contains two very different populations of free radicals, one in the particulate phase and one in the vapor phase. The particulate phase contains several relatively stable free radicals. Church and Pryor stated that they had "identified" the principal radical as a Q/QH_2 complex held in the tarry matrix. However, no unequivocal identification was ever made. They suggested that this Q/QH_2 complex was an active redox system that is capable of reducing molecular oxygen to produce superoxide, eventually leading to H_2O_2 and hydroxyl radicals.

In that same publication, Church and Pryor (746) stated that the vapor phase of cigarette smoke contains small oxygen- and carbon-centered radicals that are much more reactive than the particulate-phase radicals. Although no vapor-phase radicals were specifically identified. They stated that the vapor-phase radicals do not arise from the initial combustion of the tobacco but are rather produced in a steady state by the oxidation of NO to NO_2, which then reacts with reactive species already present in smoke, such as isoprene. They suggested that these reactive vapor-phase free radicals and the metastable products derived from these radical reactions may be responsible for the inactivation of α1-proteinase inhibitor by fresh smoke.

Church and Pryor (746) proposed that the excess superoxide that is expected to form in lung tissue exposed to cigarette smoke is one possible means of inactivating α1-protease inhibitor, a protein associated with the onset of emphysema in deficient individuals. In the same report, the authors noted that after particulate-phase MSS was incubated with deoxyribonucleic acid (DNA), an ESR signal was observed in the recovered DNA. Later, it was suggested that hydroxyl free radicals generated from the particulate-phase MSS free radicals may cause DNA damage [Kiyosawa et al. (27A60), Pryor (27A85), Pryor et al. (27A93)]. Later in 1992, Pryor (27A85) noted that such molecular damage is not unique to tobacco smoke but also occurs with smoke from other sources such as diesel fuel and wood.

In 1986, Pryor wrote a paper on the formation, lifetimes, and reactions of oxy-radicals and related species (2998c). In his overview, he discussed some of the ways in which free radicals and other highly reactive species are produced in biological systems. He discussed the reactivity and lifetimes of these species and listed some pathological conditions and chronic diseases in which these species may be involved. He discussed that cigarette smoking is a rich source of free radicals and that much of the toxicity associated with cigarette smoking may be due to the presence of free radicals in MSS.

In 1986, the International Agency for Research on Cancer (IARC) issued its monograph on tobacco smoking (1870). Free radicals in tobacco smoke were discussed as follow:

> Smoke can be a major indirect or direct source of chemical oxidants and radicals, and also causes a rapid influx of pulmonary alveolar macrophages and polymorphonuclear neutraphils in the lung. These actively phagocytic cells release a variety of oxidative intermediates when exposed to particulates such as those in cigarette smoke. The intermediates found in cigarette smoke and/or released by activated macrophages include superoxide anion, hydrogen peroxide and hydroxyl radical …

Other than referring to the article on free radicals in cigarette smoke by Church and Pryor (746), IARC cited none of the many other pre-1986 references to free radicals in tobacco, e.g., Bilimoria et al. (329), Bluhm et al. (349), Boenig (370–372), Browning and Patton (448), Cooper et al. (814), Cosgrove et al. (828a), Forbes (1210), Forbes et al. (1211), Ingram (1861), Ingram and Allen (1862), Lyons et al. (2429), Lyons and Spence (2432, 2435), Marsden and Collins (2466), Morie (2625), Nakayama et al. (2677), Nisbet and Schmeller (2789a), Pryor (2998a, 2998b), Pryor et al. (2999, 2999a, 3001), Slaga et al. (3687), and Takeshita and Ohe (3864).

During the 1980s, R.J. Reynolds Tobacco (RJRT) Company developed a new cigarette product called Premier that heated rather than burned tobacco. A tremendous amount of research was conducted on that product prior to introduction. The research on Premier was summarized in a monograph by RJRT (3190). Free-radical analyses comparing the Premier product and University of Kentucky 1R4F reference cigarette were conducted by Rice and Hayes in 1989 (1555c, 3129). In two studies, Rice and Hayes reported that Premier had a 99% reduction in vapor- and particulate-phase free radicals compared to the 1R4F reference cigarette. Similar ESR spectra were obtained, but the yields of radicals in both phases were decreased. In the 1R4F cigarette, the particulate-matter free radicals appeared to be from species with an odd electron delocalized over an aromatic ring system, e.g., a PAH. The second source of particulate-matter free radicals appeared to come from what Church and Pryor (746) suggested was a donor/acceptor chain involving HQ as the donor and QH as the acceptor. ESR analysis of 1R4F vapor phase indicated the presence of radical species similar to those previously reported for tobacco-burning cigarettes. No identification of specific free radicals was conducted in these studies.

In 1988, O'Brien (27A82a) discussed the fate of free radicals and their effect on chemical carcinogenesis. Only one comment was included on cigarette smoke, and it involved the PAH B[*a*]P in MSS and the assertion of its involvement in lung cancer induction. O'Brien stated that PAHs like B[*a*]P donate a single electron to an enzyme which may be involved in the generation of tumorigenic diol epoxides of the PAH.

In 1989, Nakayama et al. (27A79) reported on a reliable method for the detection and quantitation of H_2O_2 generated

in aqueous extracts of cigarette smoke tar. Aqueous tar extracts (ACT) were passed through a short reverse-phase column, and the H_2O_2 concentration was determined by differential pulse polarography using an automatic reference subtraction system. The H_2O_2 concentration in the ACT increased with aging, pH, and temperature; the presence of SOD led to lower H_2O_2 concentrations. Their method was applied to several types of research and commercial cigarettes. They reported that, with few exceptions, the amount of H_2O_2 formed after a fixed time from each cigarette smoke was proportional to its tar yield.

Brunmark and Cadenas (27A15) reviewed the major mechanisms that are involved in QH-induced cytotoxicity in 1989. The redox chemistry of quinoid compounds was surveyed in terms of (1) reactions involving only electron transfers, as those accomplished during the enzymatic reduction of QHs and nonenzymatic interaction with redox couples generating semiquinones, and (2) nucleophilic addition reactions. In their explanation of the mechanisms involved, QH is reduced to the HQ or semiquinone radical by cellular reductase. The semiquinone radical then undergoes rapid autoxidation with the generation of the parent QH and concomitant formation of superoxide. The HQ reacts rapidly with superoxide to form H_2O_2 and the semiquinone.

In 1992, Pryor (27A85) reviewed, compared, and contrasted the chemistry of cigarette smoke, wood smoke, and the smoke from plastics and building materials that was inhaled by persons trapped in fires. He contended that cigarette smoke produced cancer, emphysema, and other diseases after a delay of years. He discussed that acute exposure to smoke from a fire could produce a loss of lung function and lead to death after a delay of days or weeks. Tobacco smoke and the smoke inhaled in a burning building have some similarities from a chemical viewpoint, e.g., both contain high concentrations of CO and other combustion products. In addition, both contain varied concentrations of free radicals, which if inhaled could lead to biological harm (27A65). At this time, personnel in Pryor's laboratory had studied these free radicals, largely by ESR methods, for about 15 years. The article reviewed what was known about the radicals present in these different types of smokes, soots, and tars. His article summarized the evidence that suggested that free radicals could be involved in cigarette-induced pathology and smoke-inhalation deaths.

In 1993, Diana and Pryor edited a book entitled *Tobacco Smoking and Nutrition: Influence of Nutrition on Tobacco-Associated Health Risks* (960c). In that book, Pryor and Stone wrote a chapter on oxidants (free radicals, H_2O_2, peroxynitrate, and peroxynitrite) in cigarette smoke (3000). They reported that methyl nitrite (CH_3ONO), NO, and NO_2 were primary oxidants in the vapor phase of MSS and that the proposed QH/semiquinone/HQ equilibrium complex was the primary oxidant in particulate-phase MSS. They postulated that peroxynitrite (HOO-N=O) and/or peroxynitrate (HOO-NO_2) or their esters (RO-ONO and RO-ONO_2) were present in the vapor phase of MSS. They argued that hydroxyl radicals were generated from H_2O_2 via the Fenton reaction (27A36), that carbon-centered radicals were generated from dienes in MSS and that peroxyl radicals ($ROO^{\bullet}$), alkoxyl radicals ($RO^{\bullet}$), and superoxide radicals ($O^{\bullet -}$) were present in the vapor phase of MSS. In that same book, Niki et al. in 1993 reviewed information on membrane damage from lipid oxidation by free radicals in cigarette smoke (2786a).

Cigarette smoke contains metals and metal ions (see Chapter 20). Certain metal ions are important in free-radical reactions, e.g., Fenton-type metal-catalyzed free-radical reactions. In 1993, Li and Trush (27A67) reported on the oxidation of HQ by copper and provided chemical mechanisms for the generation of QH species and their biological effects. Since the interaction of several xenobiotics with copper had been shown to result in their metabolism, Li and Trush investigated the role of copper in the oxidation of HQ and HQ-induced toxicity to mice bone marrow stromal cells, target cells of HQ in the bone marrow. In phosphate-buffered saline, HQ underwent autoxidation slowly to benzoquinone (BQ), while the presence of Cu^{+2} ions (1–50 μM) strongly accelerated the oxidation of HQ to BQ in a concentration-dependent manner. Reaction of HQ with Cu^{+2} was also accompanied by the reduction of Cu^{+2} to Cu^{+1}, the utilization of O_2, and the concomitant generation of H_2O_2. Their results indicate that Cu^{+2} strongly induced the oxidation of HQ and as such may be a factor involved in the oxidative activation and toxicity of HQ in target cells. As copper, HQ and BQ are known components of MSS, the relevance of the work of Li and Trush became important in light of the postulated mechanism of Pryor and Stone (3000).

Cueto and Pryor in 1994 (27A21), following up on the report by Pryor and Stone in 1993 (3000), reported their work on the conversion of NO to NO_2 by Fourier Transform IR. They also reported their results on the reactions of olefins with nitrogen oxides. In order to explain the apparent longevity of the presumably short-lived free radicals in aging filtered smoke, a steady-state production mechanism was proposed involving oxygen, nitrogen oxides, and vapor-phase olefins. No specific reaction products were discussed.

Tanigawa et al. (27A112) published a paper on the spin trapping of superoxide in aqueous solutions of fresh and aged cigarette smoke in 1994. Superoxide generation was determined as a function of the age of the smoke using spin trapping. DMPO was used as the spin trap. The superoxide adduct of DMPO was detected in a solution of fresh MSS for over 1 h. The superoxide-generating potential of smoke was rapidly lost as the smoke was kept in a plastic syringe. Smoke aged for 3 min did not generate superoxide. Additional evidence of superoxide generation in aqueous solutions of cigarette smoke was obtained by the chemiluminescence method.

Church in 1994 (27A19) published an article on the spin trapping of organic radicals. In that article, he postulated a steady-state mechanism that he believed explained the formation of longer-lived vapor-phase free radicals in cigarette MSS.

The proposed mechanism was based on the observation that NO_2 concentration in MSS followed the concentration of the free radicals in the vapor phase of MSS.

In 1995, Stone et al. (27A111) reviewed the previous work conducted in the laboratories of Pryor which showed that extracts from MSS or SSS nicked DNA. These solutions were believed to contain the semiquinone free radical. Aged solutions of catechol containing a semiquinone species that had ESR properties similar to those of the radical in cigarette tar extracts were used as a model for the MSS particulate-phase radical. Both the radical in aged catechol solutions and the cigarette tar radical become associated with the DNA in mammalian cells and nicked DNA. The nicking of DNA caused by both the MSS particulate-phase radical and aged catechol solutions followed saturation kinetics. The authors believed that aged catechol solutions could be used as a model for the MSS particulate-phase radical. Unfortunately, their model did not take into account the fact that MSS is a complex mixture and that other constituents in MSS could have altered their finding.

Stohs and Bagchi (27A109) reviewed the role of ROS, with the subsequent oxidative deterioration of biological macromolecules in the toxicities associated with transition metal ions in 1995. Studies have shown that metals, including iron, copper, chromium, and vanadium, undergo redox cycling and that this cycling can result in the production of ROS such as superoxide ion, H_2O_2, and hydroxyl radical. As a consequence, lipid peroxidation can be enhanced, DNA can be damaged, and calcium and sulfhydryl homeostasis can be altered. Various studies have suggested that the ability to generate ROS by redox cycling QHs and related compounds may require metal ions. Cigarette MSS contains metal ions. Some mechanisms associated with the toxicities of metal ions are very similar to the effects produced by many organic xenobiotics. Specific differences in the toxicities of metal ions may be related to differences in solubility, the complex mixture containing the metal, absorbability, transport, chemical reactivity, and the complexes that are formed within the body. Their review summarized studies (through 1995) that had been conducted with transition metal ions, regarding the production of ROS and oxidative tissue damage.

In 1995, Li et al. (27A66) reported on ESR evidence for the generation of ROS from the copper-mediated oxidation of the benzene metabolite, HQ, and its possible role in DNA damage. Prior to this study, Li and Trush (27A67) had observed that Cu^{+2} strongly induces the oxidation of HQ, producing BQ and H_2O_2 through a Cu^{+2}/Cu^{+1} redox cycle mechanism. The oxidation of HQ by Cu^{+2} also resulted in plasmid DNA cleavage. In this study, using ESR spectroscopy, they investigated whether this chemical-metal redox system could generate ROS which induce DNA damage. Studies were not performed with cigarette MSS but were conducted on solutions of HQ. Results indicated that both H_2O_2 and Cu^{+1} are critical for the formation of reactive oxygen from the HQ/Cu^{+2} systems. Aerobic conditions were necessary for the redox system to function. Reactive oxygen scavengers significantly inhibited the redox mechanism. Overall, the results indicated that it is possible, through a copper-redox cycling mechanism, to generate a ROS of HQ that may participate in DNA damage. The conditions of the experiments were not those that a smoker would experience.

Zang et al. investigated the presence of free radicals in ACT by ESR (27A122) in 1995. They demonstrated that ACT autoxidized to produce semiquinone, hydroxyl, and superoxide radicals in air-saturated, buffered aqueous solutions. Semiquinone species were detected by direct ESR measurements and were tentatively identified as *o*- and *p*-benzosemiquinone radicals by comparison with the ESR signals of catechol and HQ radicals under similar conditions. The rate of formation of these radicals was dependent on pH. Hydroxyl and superoxide radicals were detected as DMPO spin adducts by ESR spin trapping. SOD (20 units/mL) inhibited the formation of the superoxide spin adduct of DMPO completely. Addition of Fe^{2+} to this system increased the ESR signal intensity of hydroxyl radical spin adduct of DMPO. Their results indicated that superoxide and hydroxyl radicals are produced during the autoxidation of HQ- and catechol-related species in ACT under the specific conditions of their experiments.

Borgerding et al. (27A13) presented a paper at the 1995 TCRC on a method for the quantitative determination of free radicals in the vapor phase of cigarette MSS. The method was based on trapping free radicals in a PBN/benzene solution to form a stable radical species, i.e., spin trapping, followed by detection with an ESR spectrometer. Two smoke collection techniques were discussed which differed in the extent of smoke aging prior to spin trapping. Both techniques were found to be acceptable for the comparison of cigarette smoke yields. Free-radical analysis of the vapor phase of MSS from cigarettes which contained a novel carbon filter and experimental low *N*-containing tobacco blend demonstrated that vapor-phase free-radical reductions on the order of 80% were possible when compared to other equivalent "tar" cigarettes.

At the same conference in 1995, Blakley et al. (27A10) reported the results of their studies on MSS vapor-phase radical formation and possible formation mechanisms. Church and Pryor (746) had previously suggested a mechanism for formation of mainstream vapor-phase radicals that involved a reaction between NO_2 and reactive dienes, such as isoprene. Experiments were conducted to systematically explore the Church–Pryor proposed mechanism. Included in the experiments were cigarettes from different "tar" categories, cigarettes comprising a new type of carbon filter [Blakley et al. (27A12)] and blends, and cigarettes that primarily heated, rather than burn tobacco. Some results indicated that the suggested NO_2/diene mechanism was viable, while other results did not support the Church–Pryor mechanism. For many of the cigarettes studied, vapor-phase radical yields increased as either isoprene or NO_x smoke yields increased. (It should be noted that in 1978, Cooper and Hege (816) reported that there is very little NO_2 in cigarette smoke, most of the NO_x is NO.) However, in a series of experimental cigarettes where isoprene yield was held constant and NO_x levels substantially increased, vapor-phase free radicals were dramatically reduced.

In addition, preliminary research suggested that some processed tobaccos yielded diminished radicals as compared to unprocessed tobaccos, while NO_x smoke concentrations remained constant. Data were also presented on a cigarette constructed from wood shavings that produced a substantial free-radical response with virtually no isoprene or NO_x present in the smoke.

Rahman and MacNee (27A96, 27A97) reviewed the literature in 1996 on the imbalance between oxidants and antioxidants concerning the pathogenesis of smoking-induced lung diseases, such as chronic obstructive pulmonary disease (COPD), particularly emphysema. There was evidence that indicated that increased neutrophil sequestration and activation occurred in the pulmonary microvasculature in smokers and in patients with COPD, with the potential to release ROS. ROS generated by airspace phagocytes or inhaled directly from the environment can increase the oxidant burden and may contribute to the epithelial damage. Although much research has focused on the protease/antiprotease theory of the pathogenesis of emphysema, less attention had been paid to the role of ROS in this condition. The possible effects of the increased oxidant burden in smokers and in patients with COPD are opposed by the lung antioxidant defenses. In their article, they reviewed the evidence for the presence of an oxidant/antioxidant imbalance in smoking-induced lung disease and its relevance to therapy in these conditions. They noted that the involvement of MSS vapor-phase free radicals in oxidative damage was unclear because generally, the reactive vapor-phase free radicals in MSS are quenched immediately on contact with moist surfaces of the respiratory tract.

In 1997, Kodama et al. (27A62) analyzed multiple components in cigarette smoke for their ability to form active oxygen species using a spin-trapping agent, DMPO. The main source of O_2 and H_2O_2 was ascribed to polyphenols in a particulate phase of MSS. $OH^{\bullet}$ were identified in the vapor-phase of MSS. Carbonyl sulfide in the vapor phase was shown to be a source of DMPO-OH adduct. NO in the vapor phase of MSS did not show appreciable reactivity. They added that the quantification and identification of active oxygen species in cigarette smoke could provide important information for elucidating the mechanism of tobacco carcinogenesis, as certain types and concentrations of free radicals have shown genotoxic effects to induce DNA strand breaks, as well as epigenetic effects, to act as cell proliferation signals.

In 1997, Pryor summarized the free-radical mechanisms developed in his laboratory over the previous 21 years (27A86). He stated

> Cigarette smoke is a rich source of free radicals, as well as other oxidants and puts an oxidative burden on the entire organism. Smoke contains two phases, operationally defined as gas-phase smoke, which passes through a glass-fiber Cambridge filter and particulate matter, or tar, which is retained on the filter. Gas-phase smoke contains reactive, short-lived radicals that can be detected and quantified using electron spin resonance (ESR) spin trap methods. The radicals in gas-phase smoke do not result from the flame directly, but rather are continuously generated by the oxidation of NO to NO_x, which then adds to reactive species in the smoke (primarily isoprene) to give $R^{\bullet}$ radicals, which react with O_2, to give RO^- and $ROO^{\bullet}$ radicals. Gas-phase smoke, with up to 500 ppm NO as well as oxyradicals, also produces a variety of reactive nitrogen species (RNS), including HOONO, $NOONO^{\bullet}$, $ROONO^{\bullet}$, and $ROONO^{\bullet}$. Gas-phase smoke oxidizes α-I-antiproteinase by a process involving H_2O_2 and RNS. Cigarette tar contains a stable semiquinone radical $Q^{-\bullet}$, that can be observed by direct ESR; the tar radical reduces O, and thus aqueous cigarette tar (ACT) extracts contain $O_2^{-\bullet}$, H_2O_2 and $^{\bullet}OH$. The tar radical binds to and associates with DNA (both by ESR and by ^{14}C). ACT extracts nick DNA, and $^{\bullet}OH$ or a species like it are responsible for the damage. Fractionation of ACT shows that the fractions that contain the tar radical $O_2^{-\bullet}$ are responsible for >85% of the nicks.

In 1997, Stohs et al. (27A110) reviewed the potential of metal ions reacting in conjunction with other constituents of tobacco smoke to cause cellular damage by free-radical reactions. Various studies had demonstrated the role of ROS in the toxicity of transition metals. They concluded that the presence of several reactive metal ions in tobacco smoke indicates that there may be a role for metal ions in the subsequent toxicity and carcinogenicity of tobacco smoke. They described the metal-catalyzed mechanisms that might be involved.

By the early 1990s, free radicals generated from MSS were considered a significant health risk because of their potential involvement in oxidative stress. Müller et al. (27A77) reported that NO in cigarette smoke could react with superoxide derived from the reducing constituents in the particulate phase of cigarette smoke to form peroxynitrite ($ONOO^-$). NO may also be converted to a number of more reactive nitrogen derivatives, such as NO_2, dinitrogen trioxide (N_2O_3), and dinitrogen tetraoxide (N_2O_4). Their results were consistent with a rapid NO-consuming reaction coupled with superoxide-generating properties of the particulate phase of MSS.

The roles of superoxide ($O_2^{\bullet-}$), peroxynitrite, and carbon dioxide (CO_2) in the oxidative chemistry of NO was reviewed by Squadrito and Pryor (27A106) in 1998. Each of these ROS can cause biological damage at high concentrations. They contended that NO and superoxide are produced by several cell types and can rapidly combine to form peroxynitrite. Peroxynitrite is a potent and versatile oxidant that can attack a wide range of biological targets, if not held in check. In previous publications, Pryor implied that NO and superoxide (both known MSS components) could be linked to numerous diseases associated with smoking. Of course, CO_2 is also present in MSS. Peroxynitrite is normally scavenged by antioxidants, but CO_2 can also compete with certain antioxidants. Squadrito and Pryor proposed a mechanism for the reaction of CO_2 with $OONO^{\bullet}$ that produced metastable nitrating, nitrosating, and oxidizing species as intermediates. An analysis of the lifetimes of the possible intermediates and of the catalysis of peroxynitrite decomposition suggested that the reactive intermediates responsible for reactions with a

variety of substrates may be the free radicals NO_2 and $CO_3^{\bullet-}$. In closing, Squadrito and Pryor noted that increased formation of peroxynitrite has been linked to Alzheimer's disease, rheumatoid arthritis, atherosclerosis, lung injury, amyotrophic lateral sclerosis, and other diseases.

Flicker and Green (27A38) developed a new HPLC method for the detection of free radicals in cigarette smoke and diesel exhaust in 1998. Carbon-centered radicals were trapped from the vapor phase of cigarette smoke and diesel engine exhaust by reaction with a nitroxide, 3-amino-2,2,5,5-tetramethyl-1-pyrrolidinyloxy (3AP). The resulting mixture of stable, diamagnetic adducts was derivatized with naphthalenedicarboxaldehyde (NDA) to produce highly fluorescent products. Derivatives were separated by HPLC, which revealed distinctly different sets of radicals present in the two systems. Integration of HPLC peaks gave approximately 22 ± 7 nmol of radicals per cigarette and 3 ± 1 nmol of radicals per liter of diesel engine exhaust. An estimated 8–10 different carbon-centered radical species are present in each system. No identification of the free radicals was made.

In 1999, Halliwell and Gutteridge (27A41) published a second edition of their book *Free Radicals in Biology and Medicine*. It has become a classic text in the field of free-radical and antioxidant research. In their book, they reviewed the role of free radicals in the life and biomedical sciences and provided methods available to measure reactive species and oxidative damage (and their potential pitfalls), as well as the importance of antioxidants in the human diet. It is important to note that free radicals in cigarettes were not discussed. Although, their text has often been cited concerning oxidizing species/free radicals found in MSS that are known to cause oxidative damage in essential biomolecules.

In 1999, a World Patent was granted to Emami on a cigarette filter additive to capture and remove free radicals from cigarette MSS (27A34). The filter additives described in the patent were based on natural polyphenols which efficiently scavenge free radicals in cigarette smoke. Among the various polyphenols tested, oils of rosemary extracts from *Rosemarinus officinalis* L. proved to be the most active in reducing the yields of both vapor- and particulate-phase free radicals. The additive-containing filters were stable at high temperature, had a 12-month shelf life, were not air sensitive, and had normal pressure drop characteristics.

Emami et al. reported on the free-radical scavenging efficiency of the cigarette filters containing rosemary extract in 2000 (1143). Employing ESR, Emami et al. were only able to tentatively identify the presence of hydroxyl, methoxyl, and cyano free radicals in MSS. Unfortunately, ESR techniques alone give poor structural information on the nature of free radicals.

In 2000, Liu et al. (2380a) presented their research on the design of a unique low-"tar" cigarette designed to yield approximately 40% less particulate-phase free radicals. The cigarette employed a special filter, casing additives to reduce free radicals (vitamin E, vitamin A, cysteine, and selenic compounds of mannitol), a specially formulated casing with burn control agents, expanded tobacco, and tobacco filler rich in selenium. Although it was not possible to determine the interactive effects of all the changes in the uniquely designed cigarette, ESR results confirmed a reduction in particulate-phase free radicals.

Blakley et al. (27A11) published a paper in 2001 that questioned published reports postulating that the particulate-phase free radicals of cigarette MSS consisted of a HQ/semiquinone/QH shuttle. Their results showed that there was no positive correlation between the smoke yield of HQ and the presence of particulate-phase free radicals. When a 10-fold reduction in MSS HQ yield was obtained when KNO_3 was applied to the surface of tobacco of an American blended cigarette, there was no significant corresponding change in the yield of particulate-phase free radicals. In experiments testing MSS from low and high HQ-yielding tobaccos, there was no consistent corresponding relationship between HQ and particulate-phase radical yields. In one series of blends, there was at best an inverse relationship between HQ and particulate-phase radical yields. In contrast with the published literature, Blakley et al. concluded that the particular compound or compounds driving particulate-phase free-radical formation are currently unknown.

Flicker and Green (27A37) published an improved method for trapping carbon-centered free radicals ($R^{\bullet}$) from the vapor phase of the MSSs from cigarettes and cigars in 2001. They compared free-radical concentrations trapped from various cigarettes and model smoke systems. Using a nitroxide trap, 3-amino-2,2,5,5-tetramethyl-1-pyrrolidinyloxy (3AP), on solid support, they trapped radicals directly from the vapor phase, washed them off the support, and analyzed them with HPLC. Separation of the trapped radicals showed that the vapor phase of smoke from each cigarette type produced a unique set of free radicals (4–10 distinct peaks). Vapor mixtures used to model tobacco smoke consisted of NO, air, isoprene, and methanol. The model systems produced a set of free radicals that consisted of four major and several minor peaks, two of which matched peaks in tobacco smoke chromatograms. Quantities of free radicals trapped from cigarettes tested varied from 54 ± 2 to 66 ± 9 nmol. The cigar tested produced 185 ± 9 nmol of free radicals. In their experiments, oxygen competed with the nitroxide trap for MSS vapor-phase radicals. A kinetic analysis of the O_2 competition shows that actual radical concentrations in the smoke were approximately 100-fold higher than measured.

Valavanidis and Haralambous reported in 2001 (27A118) on the free-radical populations in the MSS and SSS of cigarettes with conventional acetate filters compared to biofilters (BF) that claimed reductions in yields of certain toxic substances and oxidants in the vapor phase of the MSS [Deliconstantinos et al. (27A26)]. They found that BF cigarette smoke had similar tar radical species with the same intensity ESR signals to those of the other cigarettes containing cellulose acetate filters. The ability of the ACT to produce hydroxyl radicals in the cigarettes with the BF filter was very similar to, or even higher than, the other three brands tested. The vapor phase of the MSS of the BF cigarette showed a 30%–35% reduction in the production of oxygen-centered radicals.

In the case of the SSS, BF cigarettes produced substantially higher concentrations of vapor-phase free radicals, compared to the other brands. Their results suggested that cigarettes with the BF were partially effective at removing some of the vapor-phase oxidants but not effective in the reduction of tar and its radical species in the MSS and SSS.

In their paper at the *55th TSRC* in 2001, Wooten et al. reviewed free radicals and proposed mechanisms for their generation in tobacco smoke (4277). Their review was mainly a synopsis of work published by Pryor et al. over the previous 20+ years. No specifically identified free radicals were presented.

The free-radical NO is both found in all living organisms and is required for many physiological functions. NO is also an important regulatory molecule for immune response and cytotoxicity. It is naturally produced from *l*-arginine by NO synthases (NOS). As a free radical, it produces many reactive intermediates that account for its bioactivity. NO is also a component of MSS. One mechanism for NO-induced cytotoxicity was through its interaction with superoxide to produce peroxynitrite, which can cause DNA damage. Müller et al. (27A76) and Squadrito and Pryor (27A106) previously suggested that this same mechanism may be operative for free radicals in MSS. In 2001, Lala and Chakraborty published a paper on the role of NO in carcinogenesis and tumor progression (27A64). However, they also suggested that selective inhibitors of NOS may have a therapeutic role in certain cancers associated with free radicals.

In 2002, Takanami et al. reviewed their research on the detection of free radicals in vapor phase of cigarette smoke by ESR at the *56th TSRC* (3862).

Usually, highly reactive free radicals are detected by ESR techniques once stable spin adducts are formed, but this may lead to many pitfalls. In 2002, Masselot et al. (27A68) reported a new methodology to study free radicals based on ESI and MS. The concentration of free radicals in MSS smoke is too low, compared to the total concentration of MSS, to allow for their identification by molecular ion identification alone. Stable spin adducts of free radicals from samples of MSS were analyzed by ESI–MS/MS, and the resulting fragmentation spectra were used to determine the nature of the free radicals trapped in MSS. With this methodology, Masselot et al. successfully identified two free radicals in the cigarette smoke, the $OH^{\bullet}$ and the $CH_3^{\bullet}$ radicals, and were able to tentatively identify the $O_2^{\bullet -}$ radical. When coupled to LC techniques, the ESI–MS/MS analyses allowed not only for radical identification but also for their quantification. Masselot et al. applied their new method to characterize and optimize a new filter, based on rosemary extracts which efficiently scavenged free radicals in cigarette smoke and had been patented by Emami in 1999. The relative efficiency in the removal of the various free radicals present in cigarette smoke (C centered, O centered) was discussed.

In 2002, Anderson et al. presented a review on the importance of previous work conducted on free radicals in cigarette smoke at the *56th TSRC* (74).

Ingebrethsen and Lyman (27A48) examined the mechanism proposed by Cueto and Pryor (27A21) and Pryor and Stone (27A93a) for the formation of reactive free-radical species from NO and NO_2 in the vapor phase of cigarette MSS in 2002. Inspection of the generic reaction scheme proposed by Cueto and Pryor (27A21) and Pryor and Stone (27A93a) suggested that some condensable materials were likely to result. The possibility of particle formation and growth due to this condensable material suggested only one route for phase transformation in filtered smoke. From a practical perspective, those working with cigarette smoke have long been aware that totally filtered smoke can yield condensable deposits in smoking machine plumbing even in the absence of temperature gradients. Ingebrethsen and Lyman reported that aerosol particle formation and growth were observed in aging, initially particle-free vapors obtained from filtered cigarette MSS. The timescale of particle formation and growth was on the order of minutes and was highly dependent on cigarette tobacco type. Measurements by both ensemble and single particle light-scattering methods were consistent with scattering from an aerosol with a fixed number of particles that grew into the 10th micron range. The rate of particle size increase agreed best with that predicted for growth controlled by condensable species formation by vapor-phase reaction slower than the diffusion rate of the reaction products. A simple reaction scheme involving NO oxidation and reaction with isoprene reproduced the observed form of the particle growth curves but did not yield a consistent reaction rate constant for the various cigarette tobacco types. Their results were inconsistent with the proposed mechanisms of Cueto and Pryor (27A21) and Pryor and Stone (3000) and suggested that additional reactants are involved in the particle formation.

Müeller and Intorp reported on the longer-lived particulate-phase free radicals (QH, HQ, and semiquinone species) they detected in MSS by ESR directly after extraction of Cambridge filter pads in 2003 (27A76). They also reported on their study of short-lived vapor-phase free radicals (alkoxy and alkyl species) in MSS. These radicals were spin trapped with PBN and detected by ESR. No specific identification of the free radicals was reported.

In 2003, Baum et al. (27A08) reported on a rigorous set of experimental protocols they believed were necessary to conduct ESR experiments on particulate- and vapor-phase free radicals in MSS. In their paper, they discuss experiments that were conducted in order to determine the optimal conditions for maximum signal intensities and reproducibility of results. Their results showed that radical concentrations in smoke vary among cigarettes in both the vapor phase and particulate phase of MSS. By use of a series of commercial cigarettes, where many parameters change from cigarette to cigarette, no statistically significant correlations were found between radical levels and total particulate matter in smoke. However, a weak correlation was found between the vapor-phase free-radical levels and total particulate-matter levels in smoke. They also reported that there may also be a complex effect of tobacco type on radical levels in smoke.

Emami et al. presented a paper at the 2003 CORESTA meeting in Freiburg, Germany, on an improved method for the detection, quantification, and identification of vapor-phase free radicals in MSS (27A32). They commented that the detection and quantification of vapor-phase free radicals by ESR have two main limitations: (1) Free-radical/spin-trap adducts are readily oxidized to give nonradical species, which cannot be detected by ESR; and (2) ESR techniques have a low capability to give structural information in the case of mixtures. Consequently, the unequivocal identification of many free radicals in cigarette smoke is still to be determined, and in addition, quantitative results for comparison studies are difficult to obtain (27A08). Masselot et al. (27A68, 27A69) had previously reported on use of 4,5,5-trimethylpyrroline-*N*-oxide for characterizing *O*-centered radicals and of 3-amino-2,2,5,5 tetramethyl-1-pyrrolidinyloxy for C-centered radicals. These two free-radical-trapping agents were used to identify the hydroxyl ($OH^{\bullet}$) and methoxyl ($CH_3O^{\bullet}$) radicals and cyano ($CN^{\bullet}$) radical, respectively. In this report, they described the quantitation of these radicals employing a hyphenated LC-MS/MS technique with a C18 reverse-phase column fitted to a triple quadrupole MS instrument. The addition of a stable free radical as internal standard (TEMPO, 2,2,6,6-tetramethyl-1-piperinodyloxy) allowed them to cleanly quantify the detected free radicals by the so-called multireaction monitoring (MRM) mode. The absolute quantification they obtained (ca. 10^{16} radicals/cig) was in good agreement with previous experiments based on ESR techniques. They applied their improved free-radical method to characterize a new filter containing rosemary extracts which scavenge free radicals in cigarette smoke patented by EMAMI in 1999 (27A34). The relative efficiency in the removal of the various free radicals present in cigarette smoke (C centered, O centered) was 50% for filters containing 50 mg of formulated rosemary extract.

Numerous presentations on free radicals were made in 2004 at the *58th TSRC* and at the *CORESTA Congress* in Kyoto, Japan.

In 2004, Zhou et al. (27A123) presented a systematic approach to the study of these free radicals in particulate-phase MSS at both the *CORESTA Congress* and at the *58th TSRC* (4415). They reviewed much of the prior research on detection methods for free radicals and discussed means to reduce free radical in MSS and the need for more biomedical evaluation.

In 2004, Rolando et al. (27A100) reported on the identification and quantitation of the hydroxyl ($OH^{\bullet}$), methoxyl ($CH_3O^{\bullet}$), cyano ($CN^{\bullet}$), formyl ($HC(O)O^{\bullet}$), peroxyl ($^{\bullet}OOH$), and nitrite ($NO2^{\bullet}$) free radicals employing their previously reported hyphenated LC–MS/MS technique that used a C18 reverse-phase column fitted to a triple quadrupole instrument at the *CORESTA Congress* in Kyoto.

Little et al. presented results of their investigation of phenolic particulate-phase free radicals (e.g., BQ–HQ radicals) in MSS measured by direct ESR measurements at low temperatures (2379) at the *58th TSRC*. Variable temperature ESR studies were performed on the particulate-phase free radicals in MSS. Different particulate-phase free radicals showed temperature dependence. Isolated particulate-phase free radicals began to form at about 450°C. It should be noted that stable BQ–HQ complexes (CAS No. 106-34-3) had been identified in tobacco smoke and Cytrel® smoke in 1969 by Green et al. (1378) and by Newell et al. (2767) in 1974. In neither study was any special procedure used to deal with free radicals.

At the *58th TSRC*, Rickert et al. reported on an ESR method used at LabStat for the determination of the yields of vapor-phase and particulate-phase free radicals generated in MSS (3134). No specific identified free radicals were discussed.

In 2004 at the *58th TSRC*, Johnson and Chapman presented a general review on the identification of free radicals in whole smoke (1957). Again, no specifically identified free radicals were discussed.

Johnson reported at the *59th TSRC*, in 2005, on the results of the identification of spin-trapped vapor-phase free radicals in MSS via an ESI triple quadrupole tandem MS analysis method. Four alkoxyl free radicals were unequivocally identified ($^{\bullet}OC_2H_5$, $^{\bullet}OC_3H_7$, $^{\bullet}OC_4H_9$, and $^{\bullet}OC_5H_{11}$). The superoxide free radical was also tentatively identified (27A56).

Employing an Amplex Red assay, Yan et al. (27A121) were able to detect, quantify, and positively identify H_2O_2 in whole cigarette smoke. Although not a free radical, H_2O_2 has been proposed as an intermediate in certain free-radical reactions. Church and Pryor (746) proposed that HQs present in the particulate phase of MSS can reduce dioxygen (O_2) to produce $O_2^{-\bullet}$ and semiquinone ($Q^{-\bullet}$) radical anions. The superoxide radical anion was thought to be the immediate precursor to H_2O_2, which could then be reduced to the hydroxyl radical by metals such as iron. Church and Pryor (746) suggested that the resulting $HO^{\bullet}$ radical can then damage DNA. Yan et al. found that there was a time dependency of H_2O_2 production in whole cigarette smoke in their experiments. The Amplex Red assay showed an increase in the production of H_2O_2 of up to 120 min and then reached a plateau thereafter, suggesting H_2O_2 was formed over this time period by some reaction(s) involving the highly complex mixture of chemical constituents present in whole cigarette smoke. In the work of Yan et al., concentrations of 3–8 μM H_2O_2 were found in aqueous solutions of whole smoke bubbled samples, while there was negligible H_2O_2 formation from vapor-phase bubbled samples. The data in this work suggest that the major constituents responsible for H_2O_2 formation are in the particulate phase. Aqueous solutions of HQ and catechol, both of which are particulate-phase constituents of cigarette smoke, generated no H_2O_2 even though they are free-radical precursors involved in the production of ROS in the smoke matrix.

In 2005, Chouchane et al. (27A18) studied cigarettes that had varied levels of polyphenols in the tobacco filler (flue-cured, burley, Oriental tobacco, and blends of these tobaccos).

Chouchane et al. found that the yield of particulate-phase free radicals generated in the MSS from these cigarettes was not directly related to the total amount of polyphenolic compounds in the tobacco leaf filler. For example, cigarettes prepared from flue-cured tobacco, which contains a significantly higher amount of polyphenols in comparison to burley tobacco, did not generate a higher yield of particulate-phase free radicals in MSS compared to cigarettes prepared with burley tobacco.

Halliwell and Poulson recently published a book on cigarette smoke and oxidative stress (27A42). The currently proposed mechanisms for free-radical production in cigarette smoke were discussed. They concluded that the proposed mechanisms by which cigarette smoke causes or contributes to inflammatory diseases like chronic obstructive pulmonary disease, cardiovascular disease, and cancer remain unclear. In several chapters in their book, they discussed recent developments in cellular signaling and suggested that cigarette smoke may cause oxidative stress in cellular systems. The assessment, consequences, and possible modulation of biological effects from oxidative stress were discussed. Analytical methods for the determination of isolated free radicals and biological assays for free radicals were also discussed.

In 2006, Rolando et al. (27A99) developed a new methodology based on LC, MS (LC-MS and LC-MS/MS) for the identification and quantification of free-radical spin-trap adducts. The improved method involved the use of a nano-LC fitted with a 75 µm column for separation that allowed for shorter analysis time and higher sensitivity. The main advantage of their improved method was its ability to detect and identify certain free-radical adducts (so-called ESR silent adducts) which had been oxidized or reduced after the trapping. By using spin traps which were specific for the trapping of C- or O-centered free radicals, they unambiguously identified the $OH^{\bullet}$ and $CH_3^{\bullet}$ radicals. Using this new methodology, they were able to ascertain the presence and identification of the cyanide radical ($CN^{\bullet}$) and nitrite ($ONO^{\bullet}$) radical. They stated that they were continuing their work on the structure of more complex free radicals at higher molecular mass by comparing spectra from chemically generated free radicals to those present in MSS.

Free radicals in cigarette smoke have attracted a great deal of attention because they are hypothesized to be responsible in part for several of the pathologies related to smoking. HQ, catechol, and their methyl-substituted derivatives are abundant in the particulate phase of cigarette smoke, and they are known precursors of semiquinone radicals. In the study by Chouchane et al. (27A17) in 2006, the in vitro cytotoxicity of these dihydroxybenzenes was determined with the neutral red uptake (NRU) assay, and their radical-forming capacity was determined by ESR. All of the dihydroxybenzenes studied were found to generate appreciable amounts of semiquinone radicals when dissolved in the cell culture medium employed in the NRU assay. HQ exhibited by far the highest capacity to form semiquinone radicals at physiological pH, even though it was not the most cytotoxic dihydroxybenzene. Methyl-substituted dihydroxybenzenes were found to be more cytotoxic than either HQ or catechol. The formation of semiquinone radicals via autoxidation of the dihydroxybenzenes was found to be dependent on the reduction potential of the corresponding QH/semiquinone radical redox couple. The capacity to generate semiquinone radicals was found to be insufficient to explain the variance in the cytotoxicity among the dihydroxybenzenes in their study; consequently, other possible mechanisms of toxicity must also be involved. The observed interactions between 2,6-dimethylhydroquinone and HQ in the cytotoxicity assay and ESR analysis suggested that care needs to be taken when studying the bioactivity of cigarette smoke constituents, i.e., the effect of the whole cigarette smoke complex matrix on the activity of the single constituent studied must be taken into consideration. Biological studies of the separated particulate and vapor phases of MSS may provide results that are different from those of studies of whole MSS.

In 2006, Culcasi et al. (27A22) also reported on the free-radical-related cytotoxicity of the vapor phase of MSS and the paradoxical temporary inhibition of cytotoxicity of vapor-phase free radicals by the MSS particulate phase. In their ESR studies, the spin-trap 5-(diethoxyphosphoryl)-5-methyl-1-pyrroline-*N*-oxide (DEPMPO) was employed. They experimented with cigarettes made with cellulose acetate filters, empty cavity filters, and cavity filters containing carbon (charcoal). In their study, filters containing carbon were effective in reducing vapor-phase free-radical formation, cytotoxicity, and lipid peroxidation in three cell lines. The results of their experiments also showed that NO and NO_2 are more important than hydroxide free radicals in generating the cytotoxicity of vapor-phase MSS free radicals generated from MSS constituents. Culcasi et al. also suggested that *something* in the MSS TPM reduced the cytotoxicity of vapor-phase free radicals in MSS as there was an unexpected protective effect of TPM on the cytotoxicity of whole smoke compared to that of vapor phase of MSS alone. They concluded that the conventional smoke collection method (separation of the smoke into vapor and particulate phases) distorts the true picture of free-radical activity. In other words, free-radical activity in cigarette smoke should only be evaluated on a "whole smoke" basis.

In 2007, Dellinger et al. (27A27) conducted and reported on the formation and stability of resonance stabilized free radicals of the type hypothesized by Pryor and his associates in the particulate phase of MSS. They concluded that the commonly observed free radicals in the particulate phase of MSS were not a surface associated semiquinone and were more likely an intrinsic, polymeric radical with a delocalized electron. The EPR signal observed by Pryor in the alcohol extract of the particulate phase of MSS may be from an extracted and autoxidized HQ, not a particulate-phase-associated semiquinone radical. The semiquinone radical was observed in the particulate phase of MSS collected below 400°C and has a five-line spectrum with $g \sim 2.006$.

Semiquinone radicals were formed in the particulate phase of MSS only after aging.

Ghosh et al. in 2007 (27A39) presented their research results on the ESR study of free radicals in the vapor phase of the MSS from 2R4F reference cigarettes. The vapor phase of MSS trapped with DMPO contained a mixture of three free-radical species correspond to two oxygen-centered radicals (90%) and an unidentified radical (10%) resulting from the decomposition of the spin adducts. They were able to identify the methoxy free radical in the vapor phase of MSS via computer simulation. The oxygen-centered free-radical concentration in the vapor phase of MSS was in the range of 10^{14}–10^{15} spins/cig smoked under ISO standard smoking conditions.

In 2007, Bartalis et al. (27A05) identified 7 acyl and 11 alkylaminocarbonyl radicals in whole MSS employing HPLC and high-resolution MS analysis of stable radical adducts. Their combined abundance of these free radicals measured in fresh whole smoke from a single 2R4F cigarette was approximately 225 nmol (1.4×10^{17} radicals). The fiberglass Cambridge filter pad conventionally employed to separate the vapor phase from the particulate phase of MSS was found to reduce the apparent yield of these radicals, introducing artifacts of measurement. They stated that the long-accepted steady-state mechanism for the formation of C-centered radicals in cigarette smoke involving NO_2 chemistry cannot account for these newly identified radicals and does not in general appear to be a major source of C-centered radicals in fresh cigarette MSS. Consequently, they suggested that the precise nature of radicals in cigarette smoke warrants reexamination.

27.5 PROPOSED MECHANISM FOR THE GENERATION OF FREE RADICALS IN MSS

Smoking has been implicated in numerous diseases (4012, 27A50, 27A51, 27A83, 27A87). Over the last 50–60 years, extensive research has been conducted to understand relationships between individual smoke constituents and smoking-related diseases. Because cigarette smoke is a complex mixture and a great number of complex biological processes are involved in each disease, no simple correlations have been found between smoking and disease. This is not to say that we have not progressed in our understanding of the biological effects of smoking and disease, but causal relationships are still largely unknown (27A17).

Numerous constituents of cigarette smoke have been identified as potential agents of biological damage, including tobacco-specific *N*-nitrosamines, PAHs, phenolic compounds, and free radicals (746, 1727, 2999, 3712).

Free radicals in tobacco smoke have attracted much attention during the last 30 years. Free radicals in biological systems can cause DNA damage, lipid peroxidation, and protein oxidation [Baskin and Salem (27A07), Halliwell and Gutteridge (27A41)] if not moderated by the body's oxidative stress defenses. Cigarette smoke and other environmental pollutants contain free radicals (2999, 2999a). Although free radicals in tobacco smoke have been implicated in human disease, no unequivocal proof of their harm has been established. Tobacco smoke is a complex mixture containing thousands of chemical constituents that can readily produce free radicals in aqueous media (828a, 2999). Tobacco smoke also contains an even greater concentration of antioxidants, antimutagens, and anticancer agents that have been shown to effectively inhibit several biological processes that could lead to disease. In Chapter 26 on carcinogens, cocarcinogens, anticarcinogens, and antimutagens, this subject is reviewed. Nevertheless, there are still many unanswered questions concerning the involvement of free radicals in the toxicology of tobacco smoke. In-depth studies are needed to delineate their precise effects (27A17).

In 1958, Lyons et al. (2429) first observed free radicals by ESR in whole cigarette smoke that was condensed at liquid oxygen temperature. These workers reported that whole cigarette smoke contains two populations of free radicals, an unstable population that can only be observed at −183°C and that vanishes when the condensate is warmed to 60°C and a persistent, stable population that exists for "several days" at room temperature. The unstable population of free radicals included those in the vapor phase of whole cigarette smoke, and the more stable population of free radicals included those found in the particulate phase of whole smoke. As a result, the early examination of the chemical and physical characteristics of free radicals in tobacco smoke was mainly conducted on free radicals in the particulate phase. In 1969, Tully et al. (27A115) were the first to publish a study of the free radicals in the vapor phase of cigarette MSS that was condensed at liquid oxygen temperature. By passing whole cigarette smoke through a fiberglass filter, called a Cambridge pad, the particulate phase of cigarette smoke can be efficiently separated from the vapor-phase constituents (172, 1067). The use of Cambridge pads allowed investigators to separate and independently investigate the free radicals in both phases of whole smoke. The chemical behaviors of the vapor- and particulate-phase free radicals of MSS smoke were found to be quite distinct. The vapor-phase radicals have been shown to be unstable and very reactive, whereas the radicals in the particulate phase are much longer lived (2999, 2999a, 27A95). Derivative methods or spin-trapping techniques were developed to stabilize the vapor-phase free radicals for quantitation. From about the mid-1960s, chemical and biological research on free radicals in tobacco smoke involved separation of the smoke stream into vapor and particulate phases.

From 1976 through 2006, Pryor and his associates studied both vapor- and particulate-phase free radicals in tobacco smoke (746, 828a, 2999, 2999a, 3000, 3001, 27A19, 27A21, 27A24, 27A84–27A95, 27A106, 27A111, 27A122). They generated experimental evidence that suggested possible mechanisms for the initiation, propagation, and termination of free radicals in tobacco smoke. They also alleged that free radicals in MSS were important to numerous smoking-related diseases. They hypothesized that vapor-phase free radicals in tobacco smoke were formed by a continuous mechanism, whereby NO reacted with molecular oxygen in air to form

NO_2, and subsequent reactions between NO_2 and unsaturated molecules in cigarette smoke, e.g., isoprene and butadiene, yielded alkyl, peroxyl, and alkoxy radicals. They contended that the reaction of peroxyl radicals with NO generated additional NO_2, creating a steady-state cycle (2999a, 27A94).

Pryor and his associates also postulated a mechanism for the generation and reaction of free radicals in the particulate phase of tobacco smoke. In that mechanism, particulate-phase free radicals in MSS were postulated to be semiquinone radicals in a polymeric matrix (2999). They stated that the particulate phase of MSS contained numerous dihydroxybenzenes, which could generate semiquinone radicals (27A122). They supported their hypothesis by showing that HQ and catechol can undergo oxidation in air to form semiquinone radicals and ultimately QHs. They further showed under laboratory conditions that reactions between the semiquinone free radicals and molecular oxygen, either in ACT or in living cells, could lead to the creation of ROS such as superoxide radical, H_2O_2, and hydroxyl radical (27A122). It is important to note that the measurements of Pryor et al. (27A93) and others performing research on free radicals in tobacco smoke are not representative of free-radical formation under physiological conditions or in biological systems (27A17). The free-radical mechanisms proposed by Pryor and his associates were very convincing, but like all mechanisms as scientific curiosity is peaked, they were vigorously tested by others.

In 2001, Blakley et al. (27A11) showed that the yield of particulate-phase free radicals was not correlated with the yield of HQ in MSS. For a series of cigarettes containing different tobacco blends with variable yields of MSS HQ, the amount of free radicals in the particulate phase of MSS remained unchanged. In their experiments, methylene chloride was used to extract the particulate matter from Cambridge pads, the solvent evaporated, and the residue redissolved in benzene for EPR measurements. Under these experimental conditions, HQ would be less likely to undergo autoxidation, which is less favorable in organic solvents. Nevertheless, significant levels of particulate-phase free radicals were observed, which calls into question the exact nature of the radicals that could be involved in biological damage.

Ingebrethsen and Lyman in 2002 conducted experiments on particle formation and growth in vapors from totally filtered cigarette MSS (27A48). In their experiments, they tested a simple reaction scheme involving nitrogen oxide oxidation and its reaction with isoprene. Their experiments reproduced the expected and observed form of the particle growth curves and did not yield a consistent reaction rate constant for the various cigarette tobacco types. Their results were inconsistent with the proposed vapor-phase free-radical mechanisms of Cueto and Pryor (27A21) and Pryor and Stone (3000) and suggested that additional reactants are involved in the particle formation.

Cytotoxicity is regarded as a potential step in several chronic disease processes, including carcinogenesis and emphysema [Butterworth et al. (27A16)]. The cytotoxic constituents of cigarette smoke and their mechanisms of action are poorly understood [Chouchane et al. (27A17)]. Thus far, most research has focused either on the chemistry of cigarette smoke or on the in vitro and in vivo effects of cigarette smoke on biological systems. The lack of a bridge between these two approaches has made it difficult to assess the relationship between cigarette smoke constituents and their effects in biological systems. It is known, e.g., that cigarette smoke contains a substantial amount of dihydroxybenzenes in the particulate phase of MSS (2681, 3175, 3743). In vitro assays have demonstrated that ACT, which contains significant amounts of HQ, catechol, and other mono- and dihydroxybenzenes, can damage DNA [Pryor et al. (27A93)]. However, there is no direct evidence to suggest that pure HQ or catechol can induce the same level of free-radical formation and DNA damage as any isolated fraction of ACT [Chouchane et al. (27A17)]. Again, it must be repeated that the experimental conditions employed by Pryor and others for measurement of free-radical activity in tobacco smoke are not representative of free-radical formation under physiological conditions or in biological systems (27A17).

In 2006, Culcasi et al. (27A22) suggested that *something* in the MSS particulate phase reduced the cytotoxicity of MSS vapor-phase free radicals as there was an unexpected protective effect of particulate phase on the cytotoxicity of whole smoke compared to that of vapor phase of MSS alone. They concluded that the conventional smoke collection method, i.e., separation of the smoke into vapor and particulate phases, distorted the true picture of free-radical activity. In other words, free-radical activity in cigarette smoke should only be evaluated on a "whole smoke" basis, unlike much of the research that had been conducted previously. Therefore, a reexamination of some of the toxicological data on free radicals would be prudent.

Chouchane et al. (27A17) recently studied the involvement of semiquinone radicals in the in vitro cytotoxicity of cigarette MSS. Prior to their study, it was known that dihydroxybenzenes can generate semiquinone radicals, QHs, and ROS in oxygenated physiological media in vitro, e.g., in the growth media used in cytotoxicity assays. It was believed that certain dihydroxybenzenes could possibly generate similar semiquinone radicals, QHs, and ROS in vivo in the epithelial lining fluid of the lungs of smokers. Brunmark and Cadenas (27A15) suggested that the cytotoxicity of quinols and QHs may be due to the concerted action of several processes that include redox cycling, alteration of thiols balance through oxidation or arylation, inhibition of cellular functions, alteration of Ca^{+2} homeostasis, and covalent binding to nucleic acids, proteins, and lipids. It is difficult to extrapolate in vitro data analysis to an in vivo system, especially if the in vitro experiments were not conducted under conditions close to physiological conditions. Moreover, few data are available on the cytotoxicity of pure dihydroxybenzenes to compare with the toxicity of a complex mixture containing dihydroxybenzenes, such as cigarette smoke. The dihydroxybenzenes in their study were constituents of the particulate phase of MSS and were found to exhibit significant cytotoxicity. The methyl-substituted dihydroxybenzenes were shown to have higher cytotoxicity than the unsubstituted compounds. The dihydroxybenzenes

were shown to generate semiquinone radicals in the medium used in the NRU cytotoxicity assay. Nevertheless, a correlation between the abundance of semiquinone radicals formed and their cytotoxicity was not found. The observed interaction between 2,6-dimethylhydroquinone and HQ in the cytotoxicity assay and EPR analysis demonstrates that the EC_{50} values in binary mixtures of the dihydroxybenzenes cannot, in general, be assumed to be additive. Consequently, the interpretation of the bioactivity of cigarette smoke evaluated by similar methods should consider the possible effects of the complex mixture of MSS on the activities of the individual constituents.

The most recent study of free radicals in tobacco smoke, published by Bartalis et al. (27A05), indicated that the analysis of whole smoke *vs.* vapor-phase and/or particulate-phase samples is not only important but absolutely necessary in evaluating the true chemistry of free radicals in tobacco smoke. Bartalis et al. measured and identified 7 acyl and 11 alkylaminocarbonyl radicals in fresh whole smoke from a single 2R4F cigarette. These 18 free radicals had a spin concentration of 1.4×10^{17} radicals/cig and accounted for nearly the entire ESR signal. They showed that the long-accepted steady-state mechanism for the formation of carbon-centered radicals in cigarette smoke involving NO_2 chemistry cannot account for these newly identified radicals, and that it does not in general appear to be a major source of carbon-centered radicals in fresh cigarette MSS. The fiberglass Cambridge filter pad conventionally employed to separate the vapor phase from MSS was found to reduce the yield of these radicals, introduced artifacts of measurement. The introduction of a Cambridge pad reduced the yield of the 18 free radicals measured and identified by 96%. In their experimental procedure, that does not use Cambridge pads or any spin traps; no NO_2 was detected in the smoke. (This finding parallels that of Cooper and Hege (816) who reported that, even under unfavorable conditions, the nitrogen oxides in cigarette MSS are predominantly NO.) NO_2 formation was shown to be an artifact of the smoke separation procedure. Bartalis et al. found no evidence of any type of free radicals containing a NO_2 group as previously proposed by Pryor and his associates (746, 2999, 27A88, 27A89) and Flicker and Green (27A37, 27A38). The proposed mechanism of the addition of NO_2 to dienes in cigarette smoke, cigarette pyrolysates, or model gas mixtures of NO, air, and isoprene was found to have no merit. The long-accepted steady-state mechanism for the formation of carbon-centered radicals in cigarette smoke involving NO_2 chemistry cannot account for these newly identified radicals; consequently, they suggested that the precise nature of radicals in cigarette smoke warrants a total reexamination.

Bartalis et al. stated:

> The widely accepted mechanism for the formation of both alkyl and alkoxyl radicals in cigarette was proposed by Pryor and co-workers and supported by persuasive, but primarily indirect, evidence was based on comparisons of gas-phase cigarette smoke and model gas mixtures.

Based on the work of Blakley et al. (27A11), Ingebrethsen and Lyman (27A48), Chouchane et al. (27A17, 27A18), Culcasi et al. (27A22), and Bartalis et al. (27A05), the proposed mechanisms of Pryor and his associates certainly need to be reexamined. Additionally, the previously made biological assertions need to be reevaluated since the free radicals presumably present in MSS may not actually exist. The clear evidence of artifacts formed by the separation of whole smoke into particulate and vapor phases supports the total reexamination of the chemistry and biology of free radicals in tobacco smoke proposed by Bartalis et al. (27A05).

In summary, it would appear that we have come full circle over the last 50 years. Lyons et al. (2429) initially examined free radicals in whole smoke without the use of Cambridge pads, and today, this appears to be the collection method of choice. Tremendous analytical advancements have occurred over the last 50 years, and now, the identification and quantification of free radicals in whole tobacco smoke are finally possible. Artifact formation is always possible in research and is not a weakness of the experimenter. As additional research continues on free radicals in tobacco smoke, we express the same concerns and hopes of Ishiguru and Sugawara (1884) in 1980:

It is hoped that further progress will be made in this field so that the formation routes of many smoke components can be understood and the composition of smoke components can be better controlled.

Table 27.1 is a catalog of free radicals identified to date in tobacco and tobacco smoke. The catalog contains only 50 entries, plus a general entry labeled Radicals, free. The vast majority of the entries in the table are tobacco smoke components, except for NO and oxygen that are also found in tobacco. Hydrogen peroxide was added for completeness since it was discussed several times in the chapter. It is anticipated that with the new analytical methods recently demonstrated by Bartalis et al. (27A05), Masselot et al. (27A68), and Rolando et al. (27A99, 27A100), many additional free radicals in tobacco smoke will soon be identified. It should be kept in mind that, in light of the recent discovery by Bartalis et al. (27A05), some of the previously identified free radicals in tobacco smoke may be artifacts.

Since the first edition of this book was published in 2008 several new presentations on free radicals have been given and several new articles have been published. As a result, the list of free radical found in Table 27.1 has grown as well as the total number of references located within that table. The following paragraphs will give short synopses of the most significant work reported since the first edition.

Late in 2007, Park et al. (4830) published the results of their study on the effect of additives (antioxidants for free radicals reduction) in cigarette filter treated with various antioxidants (three types of proanthocyanidins and ascorbic acid) and various concentrations of ascorbic acid and loaded with activated carbon on the delivery of free radicals of MS by ESR. Their results showed that cigarette filters treated with ascorbic acid delivered less HQ, isoprene, and quinoline

TABLE 27.1
Free Radicals in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
		Radicals, free [General discussion]	74, 329, 349, 369–372, 448, 746, 814, 828a, 960c, 1143, 1210, 1211, 1555c, 1861, 1862, 1884, 1957, 2379b, 2380a, 2429, 2432, 2435, 2466, 2625, 2677, 2786a, 2789a, 2998a, 2998b, 2998c, 2999, 2999a, 3000, 3001, 3129, 3134, 3687, 3797, 3862, 3864, 4220a, 4277, 4332, 4415, 5036, 5043, 5927, 5959, 5960. 5964, 5966, 27A05, 27A12, 27A33, 27A39, 27A44, 27A56, 27A62, 27A68, 27A69, 27A99, 27A100, 27A122		
1.		Acyl radical, butyl- {three isomers} $O{=}C{-}CH_2CH_2CH_2CH_3$	27A05		
2.		Acyl radical, ethenyl- {acrolein radical} $O{=}C{-}CH{=}CH_2$	5044		
3.		Acyl radical, ethyl- {propionyl radical} $O{=}C{-}CH_2CH_3$	5044, 5503, 5504, 27A05		
4.		Acyl radical, methyl- {acetyl} $O{=}C{-}CH_3$	5044, 5503, 5504, 27A05		
5.		Acyl radical, 2-propenyl- {crotonyl radical} $O{=}C{-}CH{=}CHCH_3$	5044, 5503, 5504,		
6.		Acyl radical, propyl- {two isomers} $O{=}C{-}CH_2CH_2CH_3$	27A05		
7.		Alkylaminocarbonyl radical, butyl- {two isomers} {butylaminocarbonyl} $O{=}C{-}NHCH_2CH_2CH_2CH_3$	5044, 5503, 5504, 27A05		
8.		Alkylaminocarbonyl radical, ethyl- {ethylaminocarbonyl} $O{=}C{-}NHCH_2CH_3$	5044, 5503, 5504, 27A05		
9.		Alkylaminocarbonyl radical, methyl- {methylaminocarbonyl} $O{=}C{-}NHCH_3$	5044, 5503, 5504, 27A05		
10.		Alkylaminocarbonyl radical, pentyl- {three isomers} {pentylaminocarbonyl} $O{=}C{-}NHCH_2CH_2CH_2CH_2CH_3$	5044, 5503, 5504, 27A05		
11.		Alkylaminocarbonyl radical, propyl- {two isomers} {propylaminocarbonyl} $O{=}C{-}NHCH_2CH_2CH_3$	5044, 5503, 5504, 27A05		
12.		Alkylaminocarbonyl radical (unsaturated) C_5H_8NO	27A05		
13.		Alkylaminocarbonyl radical (unsaturated) $C_7H_{12}NO$	27A05		
14.		Aminocarbonyl (amide) radical $O{=}C{-}NH_2$	5044, 5503, 5504		
15.		Benzenaminocarbonyl radical {anilinocarbonyl radical} $C_6H_5\text{-}NH{-}C{=}O$	5044, 5503, 5504		
16.		*o*-Benzosemiquinone radical	27A12		
17.	3225-29-4	*p*-Benzosemiquinone radical	27A122		

(*continued*)

TABLE 27.1 (continued)
Free Radicals in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
18.		1-Buten-1-aminocarbonyl- (1*E*)-{[(1*E*)-1-but-1-en-1-yl]aminocarbonyl-} CH_3CH_2-CH═CH-NH-C═O	5044, 5503, 5504		
19.		Butadiene radical	27A33		
20.		1,3-Butadiene, 2-methyl- radical {isoprene radical}	27A33		
21.	19062-98-7	Butoxyl radical $CH_3(CH_2)_3O$	5075, 27A56		
22.		*tert*-Butoxyl radical	27A44		
23.		Cyanide radical CN	27A68, 27A99, 27A100		
24.		Cyanide radical {acrylonitrile radical} C_3H_2N	27A68		
25.		Cyanide radical C_3H_4N	27A68		
26.	2154-50-9	Ethoxyl radical OH_2CH_3	5075, 27A56		
27.	2597-44-6	Formyl radical H-CO	5044, 5503, 5504, 27A100		
28.		Heptoxyl radical $O(CH_2)_6CH_3$	5075		
29.		1-Hexen-1-aminocarbonyl- (1*E*)-{[(1*E*)-1-hex-1-en-1-yl]aminocarbonyl-} $CH_3(CH_2)_3$-CH═CH-NH-C═O	5044, 5503, 5504		
30.		Hexoxyl radical $O(CH_2)_5CH_3$	5074, 5075		
31.	7722-84-1	Hydrogen peroxide	2677, 5026, 5076, 5086, 5571, 5870, 5960		
32.		Hydrogen peroxyl radical OOH	27A100		
33.		HQ/semiquinone/QH radical	5076, 27A08		
34.	3352-57-6	Hydroxide radical	828a, 5076, 27A62, 27A68, 27A99, 27A100		
35.	15438-31-0	Iron, ferrous ion Fe^{+2}	5076	20A20	
36.		Iron, ferric ion Fe^{+3}	5076		
37.	2143-68-2	Methoxy radical CH_3O	5075, 27A39		
38.		Methoxy, amido- NH_2-CO-CH_2O	5074, 5075		
39.		Methoxy, amino- NH_2-CH_2O	5074, 5075		
40.		Methoxy, phenyl- C_6H_5-CH_2O	5075		
41.	2229-07-4	Methyl radical CH_3	5044, 27A68, 27A69, 27A99, 27A100		
42.		Nitrite radical O-N═O	27A99, 27A100		

TABLE 27.1 (continued)
Free Radicals in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

			References		
	CAS No.	Name (per CA Collective Index)	Tobacco Smoke	Tobacco	Tobacco Substitute Smoke
43.	10102-43-9	Nitrogen oxide {nitric oxide} NO	21, 28, 199, 172, 173a, 189, 239, 386, 387, 401, 480, 499, 574, 603, 688, 753, 815, 816, 845, 855, 887, 960b, 988a, 1051, 1063–1074, 1089, 1140, 1331, 1373, 1375, 1375a, 1375b, 1377, 1378, 1386, 1388–1390, 1419, 1420, 1437, 1465, 1602, 1634, 1693, 1741, 1833, 1834, 1859, 1929, 1930, 1952, 1955, 1956, 1963, 2062, 2079, 2083–2085, 2122, 2133, 2134a, 2142, 2159, 2270, 2293, 2297, 2310, 2360, 2545, 2557a, 2634, 2690, 2724, 2738, 2782, 2800, 2801, 2803, 2804, 2806, 2878a, 2919, 2927, 2939, 3007, 3116, 3132, 3135–3137, 3139, 3149, 3255, 3300, 3302, 3308, 3370, 3441, 3491, 3557, 3587, 3655, 3671, 3691, 3694, 3720, 3818, 3862, 3907, 3952, 3973, 3993, 3997, 4005–4007, 4052, 4056, 4162, 4219, 4249, 4250, 4252, 4319, 4332, 4365, 5008, 5034, 5042, 5590, 5836, 5960	1175a, 4249	642, 1375a, 1377, 1378, 3192, 4052, 4056, 4249
44.	7782-44-7	Oxygen (diradical)	168, 172, 237, 239, 411, 421, 480, 621, 1140, 1284, 1306, 1373, 1375a, 1377, 1420, 1437, 1664, 1668, 1842, 1924, 1969, 2059, 2060, 2066, 2068, 2079, 2133, 2252, 2310, 2607, 2634, 2736, 2780, 2781, 2782, 2804, 2939, 3120, 3121, 3132, 3302, 3308, 3516, 3880, 3882, 3883, 4249, 27A62	1206a	1375A, 1377
45.		1-Penten-1-aminocarbonyl- (1*E*)-{[(1*E*)-1-pent-1-en-1-yl]aminocarbonyl-} $CH_3(CH_2)_2$-CH═CH-NH-C═O	5044, 5503, 5504		
46.		Pentoxyl radical $CH_3(CH_2)_4O$	5074, 5075, 27A56		
47.	2122-46-5	Phenoxyl radical C_6H_5O	5075		
48.	17374-79-7	Phenoxyl, methyl-radical CH_3-C_6H_4O	5075		
49.	16499-18-6	Propoxyl radical $CH_3(CH_2)_2O$	5074, 5075, 27A56		
50.	11062-77-4	Superoxide (anion radical)	2677, 4249, 27A56		

to MSS than those treated with the other antioxidants. They concluded that the antioxidants tested were useful for reducing free radicals in MSS because of the fast reaction rate between the antioxidant and free radicals.

In 2008, Moldoveanu and Borgerding (5008) reexamined the mechanism for the formation of tobacco-specific nitrosamines in MSS via the formation of N_2O_3 from NO and NO_2. Both secondary and tertiary amines can react with N_2O_3. Tertiary amine alkaloids can undergo free-radical reactions involving the formation of organic monodentate radicals and bidentate radicals via N_2O_3 to generate nitrosamines. Their proposed mechanism can be used to explain the formation of *N′*-nitrosonornicotine (NNN) and 4-(*N*-methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK) from nicotine by pyrosynthesis during smoking (and during different curing processes that expose tobacco to NO_x).

During 2009, several significant papers were published, and presentations given on free radicals. Adam and Mitschke (5034) conducted an investigation of tobacco pyrolysis gases and puff-by-puff resolved cigarette smoke by single-photon ionization (SPI)—time-of-flight MS. In their investigation, they found that the transit time of the smoke to the analyzer was greater in the presence of the Cambridge pad (*vs.* no pad) because of the tortuous path of the smoke through the filter pad. This allowed more time for various free-radical reactions of NO with assorted organics and resulted in the measurement of lower quantities of NO when the Cambridge filter pad is present. They stated that "it is experimentally convenient to

use a Cambridge pad in smoke analysis but it does not give an absolute separation of the two phases. The materials collected on the pad are affected by a host of factors, including moisture content, temperature, flow rate and specific chemical interaction between aerosol constituents and the fiber glass." They observed that different separation techniques, such as electrostatic precipitation and jet impaction traps, give different values for the vapor/aerosol composition.

At the *63rd TSRC*, no less than eight papers were presented that dealt with various aspects of free radicals:

- Bennett (5036) discussed the comparative quantification of oxygen and nitrogen free radicals induced by cigarette smoke in human lung cells in vitro.
- El-Mahdy et al. (5042) discussed the development of an in vivo mouse model for smoking-induced cardiovascular disease that was sensitive to various fixed and variable gases found in MSS including NO, NO_2, O_2, HCN, H_2S, NH_3, SO_2, and CO. White blood cells in smoke-exposed mice demonstrated significantly higher cell-specific ROS generation associated with free-radical reactions.
- Gerardi and Coleman, from RJRT Company, made two presentations at the 2009 TSRC. One was on new methodologies for quantitative and semiquantitative determination of carbon-centered free radicals in cigarette smoke using LC-MS and GC-MS (5043). Their method quantitated 14 different carbon-centered free radicals, both acyl and alkylaminocarbonyl type. Another was on qualitative and relative quantitative determination of carbon-centered free radicals in whole smoke from various cigarette types (5044). In the first presentation, several approaches were explored to develop a high-throughput procedure for relative determination of 14 different carbon-centered free radicals, both acyl and alkylaminocarbonyl type, in cigarette smoke. In the second presentation, a variety of commercial and reference cigarettes with "tar" yields from 5 to 14 mg/cigarette were smoked using two different smoking regimes to quantitate the level of multiple 3-CNP/radical adducts and several formyl and ethyl radical adducts. The range of carbon-centered free-radical concentration was related to "tar" delivery and was found to be 41–348 nmol/cigarette with the 35/60/2/0 regime and 349–647 nmol/cigarette with the 55/30/2/100 regime.
- Robinson and coworkers, from Lorillard, made three presentations at the 2009 TSRC (5074–5076). The first presentation examined the formation of radicals from cigarettes under different smoking conditions. The second concerned the identification of gas-phase radicals by tandem MS. The third gave results of modulating effects of Fe(II), Fe(III), and QH/HQ on tobacco smoke–mediated hydrogen peroxide formation.
- Takanami (5086) presented results from his study on the detection of ROS by DMPO spin-trapping method in aqueous extract of cigarette smoke and made a comparison of his results with other model reaction systems. These authors tried to detect superoxide anion radicals and hydroxyl radicals by ESR using a DMPO spin-trapping technique on aqueous extracts of cigarette smoke. Their results indicated that the signals of DMPO-OH originally found (but later eliminated by adding superoxide dismutase and not by adding catalase) were derived from degradation of DMPO-OOH, which is a reaction product of DMPO and superoxide anion radicals. Their data support the conclusion that aqueous extracts of cigarette smoke generate superoxide anion radicals and not hydroxyl radicals.

In 2009, McAdam et al. (5963a) delivered a presentation at the *42nd Annual International Meeting* of the Electron Spin Resonance Spectroscopy Group of the Royal Society of Chemistry that was a literature review of free radicals in cigarette smoke. It was a historical walk from 1958 to the present, containing much of the information in this chapter.

Continuing work on the effects of hydrogen peroxide in an aqueous extracts of cigarette smoke, Takanami et al. (5975) examined the effect of pH on the yield. An aqueous extract of the particulate phase of cigarette smoke was analyzed by HPLC with an electrochemical detector (ECD). The recovery of hydrogen peroxide by using an extract of the particulate phase of the cigarette smoke was more than 80%. An increase in the amount of hydrogen peroxide was observed during extraction with the phosphate buffer at higher pH values. In contrast, extraction with phosphoric acid did not increase the amount of hydrogen peroxide during extraction.

Gerardi and Coleman (5503) made presentations at the 2010 *CORESTA Congress* and the *64th TSRC*. The first presentation dealt with the use of high-resolution MS to confirm several previously proposed 3-CNP/radical adducts, the formyl and ethyl radical adducts that they had reported in 2009. The second talk which was made at the 2010 *CORESTA Congress* and subsequently published was on two methods for the detection and quantitation of free radicals. GC-MS was employed for the first time as an alternate means of detecting several relatively highly concentrated radical adducts. LC-MS/MS with either precursor ion monitoring (PIM), selected reaction monitoring (SRM), or selected ion monitoring (SIM) was used for detecting the large array of radicals, including several not previously reported: formyl, crotonyl, acrolein, aminocarbonyl, and anilinocarbonyl radicals. Relative quantitation was achieved using external calibration standards of 4-[1-pyrrolindino]benzaldehyde and nicotine. They determined that the yield of carbon-centered free radicals for reference cigarette 2R4F was approximately 265 nmol/cigarette at 35 cc puff/60 s interval/2 s duration smoking conditions.

In 2010, Takanami (5571) continued to present his work on aqueous extract of particulate-phase cigarette smoke. This presentation described the identification of hydrogen peroxide precursors by fractionation of the aqueous extract of particulate-phase cigarette smoke.

Zweier et al. (5590) made a presentation at the *64th TSRC* on the application of carbon fiber microelectrodes for measurement of kinetic constants of nitric oxide decay in blood.

In 2011, Takanami and Nakayama (5976) reported the generation of superoxide anion radicals generated from an aqueous extract of particulate-phase cigarette smoke by ESR using DMPO. The ESR signals of DMPO-OH were detected from the extract by using DMPO. These signals were eliminated by adding superoxide dismutase but hardly by catalase. These responses of the ESR signals to the scavengers were similar to those of a hypoxanthine–xanthine oxidase system. The results indicate that the signals of DMPO-OH from the extract were derived from a reaction product of DMPO with superoxide anion radicals and clarify the mechanism by which the extract generated superoxide anion radicals.

Finally, in 2011, a special edition of *Mini-Reviews in Organic Chemistry* was published that was dedicated to a better understanding of cigarette smoke free radicals and their relationship to smoking-related disease (5959). This special issue containing 11 review articles by experts in this area of research provides reader with an up-to-the-date overview of this evolving subject. Five review articles are particularly germane to this chapter of the book, namely, the reviews by Liu et al. (5960) on "Some recent topics in cigarette smoke science," by Menshov and Trofimov (5964) on hydrogen peroxide derived from cigarette smoke: "Pardon impossible, to be sent to Siberia"?, by Robinson and Johnson (5966) on "Methods for analysis of free radicals in cigarette smoke," by Wooten (5979) on "Gas-phase radicals in cigarette smoke: A re-evaluation of the steady-state model and the Cambridge filter pad," and by Dellinger et al. (5927) on "Free radicals in tobacco smoke."

28 Summary

In the Chapter 28 Summary of our 2008 cataloging of the chemical components of tobacco and tobacco smoke, Rodgman and Perfetti noted the following (5078):

> Since the mid-1950s, the combined referenced cataloging of the chemical components of tobacco and tobacco smoke may have been conducted in-house at various U.S. and foreign tobacco companies as well as by various governmental agencies but none has been published since the excellent 1968 review by R.L. Stedman of the U.S. Department of Agriculture (3797). Prior to that, there were only a few such publications, one in 1959 [Johnstone and Plimmer (1971)] and one in 1963 [Philip Morris, Inc. (2939)]. In subsequent years, several tobacco and tobacco smoke publications dealt with specific types of components, e.g., the 1977 review by Schmeltz and Hoffmann on the nitrogen-containing components in tobacco and tobacco smoke (3491). Several catalogs of the chemical components of only tobacco smoke have been published, but the most recent one was that of Ishiguro and Sugawara (1884) in 1980. Since the 1968 Stedman article, the number of identified tobacco and tobacco smoke components has increased sevenfold to more than 8600. No other commercial product has been so completely defined. This catalog is our attempt to categorize with references the identified and reported components in tobacco and tobacco smoke as of 2007.

Hundreds of scientific articles (many of them referenced in this text) have stated that tobacco and tobacco smoke are complex mixtures (5551). This is an accurate statement. But some have alluded to or emphasized that they are primarily complex, i.e., these mixtures of chemicals are just too multifarious, too difficult to completely understand, or so complicated and/or convoluted that the normal individual could not possibly comprehend the totality of the concept or composition of the mixture. This was never the intent of the definition of a complex mixture, but nevertheless, some have implied that this multifaceted conglomeration of chemical components in tobacco and tobacco smoke is too difficult to explain and understand. The tobacco industry has often stated that tobacco and tobacco smoke are complex mixtures, without providing a basis for the statement. This text illustrates the complexity of tobacco and tobacco smoke. It provides the reader with a historical perspective on the identification of thousands of chemical components in tobacco and tobacco smoke, it contains reviews of all known and identified classes of chemical components in tobacco and tobacco smoke, and it provides thousands of accessible references on identified chemical components in tobacco and tobacco smoke. Also provided in the preceding pages are references and discussions of one of the major problems with a complex mixture, i.e., the extrapolation of a biological property found in experimental studies with an individual compound in the mixture to the property of that component in a mixture which may contain components that either enhance or offset the experimentally observed biological property of the component. Even though tobacco and tobacco smoke are complex mixtures, they are not incomprehensible.

Tobacco and tobacco smoke are among the most extensively studied complex mixtures (5551). There are literally millions of protein fragments being cataloged as part of the tobacco genome projects. Over 30,000 enzymes are known to participate in plant growth and regulation. Oxidation, reduction, additions, hydrogenation, pyrolysis, decarboxylation, and dehydration are but a few of the many chemical reactions known to be involved in tobacco pyrolysis and combustion. These reactions are capable of producing hundreds of thousands of reaction products. The limiting factor in the discovery and identification of additional chemical components in tobacco and tobacco smoke was the early analytical technology, but this was changed significantly over the years by the development of new and ever-improved analytical technologies.

Since the 1954 listing of fewer than a hundred tobacco smoke components by Kosak (2170), various investigators have estimated from gas chromatographic scans that for each component identified in tobacco smoke, there are 5–20 components present at extremely low per cigarette yields that have not yet been identified. Thus, as noted by Wakeham (4103) in 1971 when the identified tobacco smoke components numbered about 1350:

> Gas chromatographic scans indicate there are many more, probably over ten thousand, possibly even a hundred thousand [tobacco smoke components].

Grob (1422), one of the pioneers of the use of glass capillary gas chromatography in tobacco smoke composition studies, as well as other tobacco smoke investigators, also noted that the number of peaks, each of which represented at least one component, in the chromatographic scans far exceeded the number of identified components.

If it were not for scientists' curiosity and the tremendous advances in analytical chemistry over the last 50–60 years, the need for this up-to-date catalog of compounds in tobacco and tobacco smoke would not be critical. As analytical technology advances, surely thousands of new chemical components in tobacco and tobacco smoke will be added to the listings found in this text.

In each chapter of this text, one or more tabulations were made that contained the distribution of the components (by chemical class) that were identified in tobacco, tobacco smoke or in both tobacco and tobacco smoke. Table 28.1 illustrates the total distribution of chemical components distributed between tobacco and tobacco smoke.

TABLE 28.1
Distribution of Chemical Components between Tobacco and Tobacco Smoke

Component	Table	Total[a]	Smoke	Tobacco	Smoke and Tobacco
Hydrocarbons					
Alkanes	1.10	136	116	100	80
Alkenes and alkynes	1.11	392	376	49	33
Alicyclics	1.12	164	117	70	23
Monocyclic aromatic	1.13	113	103	47	37
Polycyclic aromatic	1.20	511	501	102	92
Subtotals		1316	1213	368	265
		617[a]	607[a]	102	92
		1422[a]	1319[a]	368	265
Oxygen-Containing Components[b]					
Alcohols	2.5	1722	675	1360	313
Phytosterols and derivatives	2.7	134	54	123	43
Aldehydes	3.12	297	187	217	107
Ketones	3.13	1254	737	799	282
Carboxylic acids	4.3	787	380	656	249
Amino acids	4.10	117	36	117	36
Esters	5.3	1143	670	1026	553
Lactones	6.3	336	201	213	78
Anhydrides	7.1	24	17	16	9
Carbohydrates	8.3	316	44	310	38
Phenols	9.22	607	468	305	166
Quinones	9.24	50	38	19	7
Ethers	10.2	1243	654	847	258
Subtotals		8030	4161	6008	2139
Nitrogen-Containing Components[b]					
Nitriles	11.2	156	145	30	19
Amines	12.2	510	295	354	139
Amides	13.1	227	137	134	44
Imides	14.1	103	82	45	24
N-Nitrosamines	15.8	66	53	53	40
Nitroalkanes, nitroarenes, nitrophenols	16.1	77	57	23	3
Subtotals		1139	769	639	269
Nitrogen Heterocyclic Components					
Monocyclic four-membered *N*-containing ring compounds	17.1	5	1	5	1
Monocyclic five-membered *N*-containing ring compounds	17.4	358	289	151	82
Compounds with multiple monocyclic five-membered *N*-containing ring	17.5	22	1	22	1
Monocyclic six-membered *N*-containing ring compounds	17.7	T	490	228	137
Compounds with a six-membered *N*-containing ring and a second five-membered *N*-containing ring	17.9	111	70	72	31
Compounds with two or more six-membered *N*-containing rings	17.11	76	66	33	23
Lactams	17.13	138	116	58	36
Oxazoles	17.15	63	51	15	3
Aza-arenes	17.21	343	336	25	18
Aza-arenes derivatives[c]	17.23	88	29	65	6
N-heterocyclic amines	17.31	9	9	0	0
Subtotals		1794	1458	674	338
Miscellaneous Components					
Sulfur-containing	18.1	289	139	194	44
Halogen-containing	18.4	266	153	188	75
Fixed gases	19.5	36	34	26	24
Metal, nonmetals	20.5	160	123	154	117

TABLE 28.1 (continued)
Distribution of Chemical Components between Tobacco and Tobacco Smoke

Component	Table	Total[a]	Smoke	Tobacco	Smoke and Tobacco
Ions, etc.	20.6	195	33	180	18
Pesticides	21.3	308	114	302	108
Enzymes	22.2	580	0	580	0
"Hoffmann analytes"	23.5	105	105	76	76
Added tobacco ingredients	24.3	313	269	313	269
Anticarcinogens	26.9	60	57	54	51
Free radicals	27.1	50	50	3	3
Subtotals		2362	1077	2070	785
Summary of item entries		1422	1319	368	265
Hydrocarbons		8030	4161	6008	2139
Oxygen-containing components[b]		1139	769	639	269
Nitrogen-containing components[b]		1794	1458	674	338
Nitrogen hetrocyclic components		2362	1077	2070	785
Grand totals		14,747	8784	9759	3796

[a] This number includes the various isomers of alkyl-PAHs reported in which the position of the alkyl group or groups has not been precisely defined.
[b] Polyfunctional *O*-containing compounds are counted in each functional group, e.g., propanoic acid. 2-bydroxy- {lactic acid} appears in the alcohol catalog and the acid catalog; benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid} appears in the acid catalog, the phenol catalog, and the ether catalog.
[c] The number of aza-arene derivatives does not include the nine *N*-heterocyclic amines.

There are 27 chapters in the book (excluding this Summary). Table 28.1 contains summary data on the distribution of chemicals discussed in all but one chapter (Chapter 25 on Pyrolysis). The tobacco and tobacco smoke components discussed in Chapter 25 are all previously covered in the remaining chapters of the book. Table 28.1 is divided into five sections: Hydrocarbons (Tables in Chapter 1), Oxygen-Containing Components (Tables in Chapters 2 through 10), Nitrogen-Containing Components (Tables in Chapters 11 through 16), Nitrogen Heterocyclic Components (Tables in Chapter 17), and Miscellaneous Components (Tables in Chapters 18 through 24, 26, and 27). Below each section in Table 28.1 is a subtotal of the total of identified chemical components found in tobacco, tobacco smoke, or both tobacco and tobacco smoke.

As previously mentioned throughout the text, a great number of the individual identified components found in tobacco and/or tobacco smoke are multifunctional. Many contain two or more functionalities, and for that reason, they are located in multiple chapters. The current Alphabetical Index to Components Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke that follows the Reference section now contains 9390 components. The following is a summary of the overall change in the Index during the past 3 years:

Index Date	Tobacco Smoke	Tobacco	Tobacco and Tobacco Smoke	Subtotal	Smoke Isomers	Total
2012	6010	5595	2215	9390	192	9582
2008	5315	4994	1879	8430	192	8622

Between the 2008 assembly of the data on tobacco and tobacco smoke components and the current assembly of the revised edition, several meaningful procedures were utilized. A detailed review of the various major chapter tables and the Alphabetical Index in the 2008 Rodgman–Perfetti publication (5078) revealed the following:

- Several dozen components were duplicated in one or more of the major chapter tables and/or in the Alphabetical Index. The duplicates occurring in specific tables have been deleted. The following are several examples of such deletions from a chapter table and from the Index: In Table III-13 in (5078), cycloheptanone {suberone} was duplicated on pages 262 and 268. Because the page 268 item was out of sequence, it has been deleted. On page 1494 of the Index in (5078), the items 7-Azaindole and 7-Azaindole, *N*-methyl- were deleted because they were duplicated as 1*H*-Pyrrolo[2,3-*b*]pyridine and 1*H*-Pyrrolo[2,3-*b*]pyridine, 1-methyl- on pages 1761 and 1762, respectively. On page 1508 of the Index, the item 1,4-Benzenediol, monoacetate was duplicated several units apart; the second one has been deleted in the amended Index.
- Some components were inadvertently inserted in the wrong table. In Table III-12 (5078), three compounds were listed incorrectly as aldehydes. They are actually oxime derivatives of an aldehyde {propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino) carbonyl]oxime} {aldicarb sulfoxide}; propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino) carbonyl]oxime {Aldoxycarb®}; and propanal,

2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb®}. Such incorrect insertions have been deleted from Table 3.12. From Table III-13, 2*H*-1-benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*Z*)- was deleted because it is not a ketone.

- Over 900 newly reported tobacco and/or tobacco smoke components, many with CAS Nos., have been appropriately inserted in one or more of the major chapter tables and in the updated Alphabetical Index.
- Because of the availability of significant analytical data on a component identified in tobacco, the same analytical data were eventually used during the past 3 years to certify the same component in tobacco smoke. The reverse situation was also applicable, i.e., significant analytical data available for a smoke component was used to identify a tobacco component. This situation resulted in modest changes in the number of tobacco smoke and tobacco components, and the number of components identified in both.

These deletions and additions resulted in an overall increase in the number of cataloged components from the 8622 previously reported [see p. 1764 in (5078)] to the current number, 9077. Inclusion of these newly reported components in the Alphabetical Index and various major chapter tables was also accompanied by a substantial increase, almost 1000, in the number of references listed in the updated Bibliography. The new references also contributed to expansion of many of the major chapter tables because of the insertion of the reference numbers in the reference lists for many components.

The updated Alphabetical Index contains 9390 individually identified components and numerous isomers. Each component is tabulated to indicate its identification in smoke, tobacco, or both. The total number of isomers noted in the Index is 292, but 100 of them are accounted for in the 9390 listed components. Thus, the number of identified/partially identified components in tobacco and tobacco smoke listed in our recent Index totals 9582 = (9390 + 292 − 100). The total number of chemical component entries in the chapters tables listed in Table 28.1 is 14,747. There are 9759 entries for tobacco, 8785 entries for tobacco smoke, and 3797 entries for both tobacco and tobacco smoke. The difference between 14,747 and 9583 indicates that indeed many of the chemical components of tobacco and smoke are multifunctional and as such are listed in several chapters.

The oxygen-containing components (tables in Chapters 2 through 10) account for the largest number of compounds found in tobacco and tobacco smoke, i.e., 8029. These components are distributed as follows: 6008 in tobacco and 4161 in tobacco smoke, with 2139 reported in both tobacco and tobacco smoke. The components in Chapters 18 through 24, 26, and 27 listed under Miscellaneous Components number 2362. There are 2070 components identified in tobacco, 1077 components identified in tobacco smoke, and 785 found in both tobacco and tobacco smoke. The nitrogen heterocyclic components (tables in Chapter 17) represent the next largest class of compounds with 1794 components identified in tobacco and tobacco smoke. In this section, there are 674 components identified in tobacco, 1458 components identified in tobacco smoke, and 338 found in both tobacco and tobacco smoke. The hydrocarbons (the five major tables in Chapter 1) represent the next class of compounds identified in tobacco and tobacco smoke. This section of Table 28.1 contains 1316 compounds. There are 368 hydrocarbons identified in tobacco, 1213 hydrocarbons identified in tobacco smoke, and 265 found in both tobacco and tobacco smoke. The nitrogen-containing components (tables in Chapters 11 through 16) are the smallest and last group of compounds identified in tobacco and tobacco smoke. This group of compounds numbers 1139. There are 639 nitrogen-containing components identified in tobacco, 769 nitrogen-containing components identified in tobacco smoke, and 269 reported in both tobacco and tobacco smoke.

Because of the great interest in the components in tobacco and tobacco smoke by academic and governmental agencies, we prepared a second index of the identified components. It is a listing of the components in the sequence of their CAS Nos. It follows the Alphabetical Index.

In closing, the authors hope that this amended version will serve a useful purpose. The content of the book represents over 60 years of effort by the researchers attempting to build a framework about our understanding of the complex mixtures of tobacco and tobacco smoke. Much progress has been made during the last 60 years in terms of understanding of tobacco and tobacco smoke. During that time, the number of identified components in tobacco and tobacco smoke has increased more than sevenfold. This progress has been due, in large part, to the great strides that have been made in analytical technology, but more than that, these scientists have shown great perseverance in the face of uncertainty and controversy surrounding the roles of tobacco and tobacco smoke and health.

> Great works are performed, not by strength, but by perseverance. (Samuel Johnson, ca. 1740)

We hope that present and future scientists will persevere and use the information contained herein to answer new questions by looking back to history.

> If you want to understand today, you have to search yesterday. (Pearl Buck, 1892–1973)

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Note: Each of the following references that includes an electronic reference was accessed and found to be functional during the period July 12–17, 2012.

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2809. Number of identified tobacco smoke components—A comment: Since the mid-1980s, few newly identified tobacco and tobacco smoke components have been reported. Reasonable explanations for why the number of identified smoke components may exceed 3,900 include: (a) At the 38th TCRC, Arrendale et al. reported the identification of a series of long-chained aliphatic esters [Arrendale, R.F., R.F. Severson, O.T. Chortyk, and M.G. Stevenson: Isolation and identification of the wax esters from the cuticular waxes of green tobacco leaf; Beitr. Tabakforsch. Int. 14 (1988) 67–84]. Although many matched those reported by Rodgman et al. [Rodgman, A., L.C. Cook, S.A. Bellin, S.S. Mims, and G.W. Young: The composition of cigarette smoke. IX. The composition of an aliphatic ester fraction from tobacco and tobacco smoke; Tob. Sci. 6 (1962) 42–49], other esters with higher molecular weight acid and alcohol moieties plus *iso* and *anteiso* structures were found by Arrendale et al. Since each ester reported by Rodgman *et al*. was found in tobacco *and* smoke, logic dictates that each new tobacco ester found by Arrendale et al. is also present in smoke. (b) In the PAH studies by Snook et al. [Snook, M.E., R.F. Severson, H.C. Higman, R.F. Arrendale, and O.T. Chortyk: Polynuclear aromatic hydrocarbons of tobacco smoke: Isolation and identification; Beitr. Tabakforsch. 8 (1976) 250–272; Snook, M.E., R.F. Severson, R.F. Arrendale, H.C. Higman, and O.T. Chortyk: The identification of high molecular weight polynuclear aromatic hydrocarbons in a biologically active fraction of cigarette smoke condensate; Beitr. Tabakforsch. Int. 9 (1977) 79–101; Multi-alkylated polynuclear aromatic hydrocarbons of tobacco smoke: Separation and identification; Beitr. Tabakforsch. Int. 9 (1978) 222–247], numerous peaks are listed as being mixtures of two or more isomers, a fact ignored by many cataloguers of smoke components. (c) In tobacco smoke, several dozen secondary amines exist for which no corresponding NNAs have been reported. Because these NNAs are known and stable, they probably exist in smoke. (d) Similarly, the parent amines for several volatile NNAs in smoke have not been identified in tobacco smoke.

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The Alphabetical Index to Components Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

The forerunner of the Index was initiated in the mid-1950s (2270, 2292a, 3245) and subsequently updated periodically (3224, 3252, 3253, 3301–3304) as the identifications of more and more tobacco and tobacco smoke components were reported. The Index was originally created in its present form for two purposes. The first was to capture in one site all the basic information on the identified tobacco and tobacco smoke components subsequently discussed in the chapters of this book. The components in the Index are listed alphabetically. Secondly, the Index may permit the reader to easily retrieve or search for information on a specific tobacco and/or smoke component or class of components so that further study will be facilitated. To achieve these goals, the Index was constructed to include the following:

1. The CAS No. for many of the components.
2. An indication of the component identification in tobacco, tobacco smoke, or both.
3. The structure of many of the components.
4. The table number and chapter in which the component is not only referenced but its properties are described, particularly if they are considered adverse.
5. For multifunctional components, several chapters and table numbers are cited.

As with the First Edition, Taylor & Francis/CRC Press of Boca Raton, FL, has provided the index on a compact disc (read-only memory) (CD-ROM). Hopefully, the searchable format of the CD-ROM will aid the reader in retrieving any desired information.

The updated Index comprises almost 9600 components completely or partially identified in tobacco, tobacco smoke, and tobacco substitute smoke. It includes not only identified components but also several hundred compounds not identified in tobacco or tobacco smoke but reported by Doull et al. (1053) as tobacco ingredients used in the United States and by Baker et al. (172a, 174b) as tobacco ingredients used outside the United States and in a summary by Rodgman (3266) and in our Chapter 24. Because the transfer from a tobacco product to smoke of very few of the added ingredients has been examined, they primarily are listed as tobacco components. Exceptions include several humectants used in tobacco products for many years. However, it should be noted that the detailed pyrolysis study by Baker and Bishop (172a) indicated that many such added ingredients would transfer in part to MSS during the tobacco smoking process.

In some instances, the reader may wonder about the peculiar nature of the component listing. For example, a tobacco smoke component initially reported as 2-butene was later shown to be present in the smoke as *cis*- and *trans*-2-butene. Thus, three items are listed in the Index for 2-butene, namely, 2-butene (CAS No. 107-10-7), 2-butene, (*Z*)- (CAS No. 590-18-1), and 2-butene, (*E*)- (CAS No. 624-64-6). In the appropriate chapter and table, Chapter 1, Table 1.11, references to the identification of each are provided. 2-Butenedioic acid is similarly listed in Chapter 4, Table 4.3, as 2-butenedioic acid (CAS No. 6915-18-0), 2-butenedioic acid, (*Z*)- (maleic acid) (CAS No. 110-16-7), and 2-butenedioic ac id, (*E*)- (fumaric acid) (CAS No. 110-17-8).

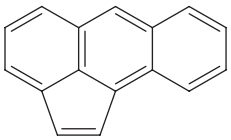
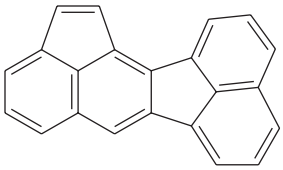
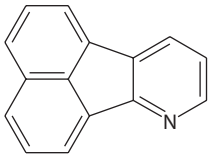
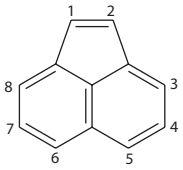
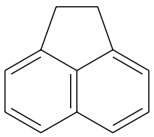
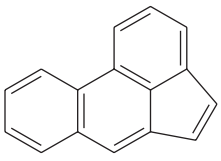
The reader will also find in the Index certain broad classifications of components, like oxidases and free radicals. These and similar examples in the Index are not there to confuse the reader, as many of the individual components in the broad classifications have specific CAS numbers.* Generally, the references associated with these classes of components (found within the chapters noted in the Index) will provide the reader with information of a common nature. In nearly all cases, individual components such as ascorbate oxidase, choline oxidase, cytochrome oxidase, and glycolate oxidase follow after the broadly classified component, oxidase. Likewise, specific free radicals such as methyl-acyl radical, ethyl-acyl radical, and propyl-acyl radical {two isomers} may be found in the Index. For some components in the Index, several partially identified isomers exist, their number noted, and included in the total number of components identified in tobacco and/or smoke.

While the number of enzymes, genes, and nucleotides listed in the Index is fewer than 600, their known number, as noted in Chapter 21, exceeds many thousands. The paltry number of enzymes, genes, and nucleotides listed in Table 21.2, was never intended to represent the total biological agents operating in the plant. Those selected for inclusion were from texts, research manuscripts, and patents where active research was conducted in the past in attempts to better understand the physiology and biochemistry of tobacco. As future genetic research develops, it is envisioned that the identity and function of hundreds of thousands of additional chemicals will be published.

The authors hope that the format of the Index and accompanying CD-ROM will help the reader to reach a better understanding of the components of tobacco and tobacco smoke.

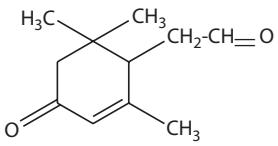
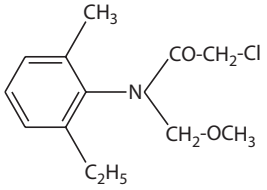
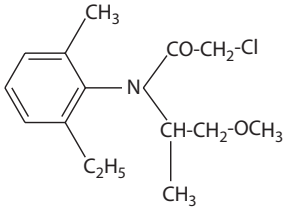
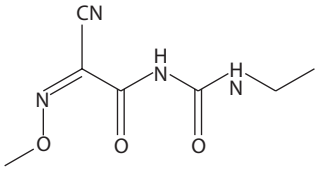
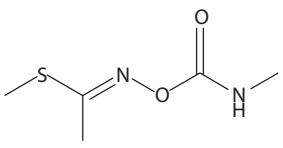
* Each CAS Registry Number used throughout the Alphabetical Components Index and the various preceding chapters is a Registered Trademark of the American Chemical Society.

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1.	202-03-9	1	0	0	Aceanthrylene		1.20
2.	641-48-5	1	0	0	Aceanthrylene, 1,2-dihydro-		1.20
3.	340-99-8	1	0	0	Acenaphth[1,2-*a*]acenaphthylene		1.20
4.	71265-26-4	1	0	0	Acenaphth[1,2-*a*]acenaphthylene,methyl-		1.20
5.	206-49-5	1	0	0	Acenaphtho[1,2-*b*]pyridine {7-azafluoranthene}		17.21
6.	208-96-8	1	1	1	Acenaphthylene		1.20
7.	83-32-9	1	1	1	Acenaphthylene, 1,2-dihydro- {acenaphthene}		1.20
8.	60684-29-9	1	0	0	Acenaphthylene, 1,2-dihydrodimethyl-		1.20
9.	36541-21-6	1	0	0	Acenaphthylene, 1,2-dihydromethyl-		1.20
10.	60826-72-4	1	0	0	Acenaphthylene,1,2-dihydrotetramethyl-		1.20
11.	60826-69-9	1	0	0	Acenaphthylene, 1,2-dihydrotrimethyl-		1.20
12.	60826-68-8	1	0	0	Acenaphthylene, dimethyl-		1.20
13.	19346-00-0	1	0	0	Acenaphthylene, 1,3-dimethyl-		1.20
14.	19346-02-2	1	0	0	Acenaphthylene, 1,5-dimethyl-		1.20
15.	58548-40-6	1	0	0	Acenaphthylene, diphenyl-		1.20
16.	58548-38-2	1	0	0	Acenaphthylene, methyl-		1.20
17.	19345-99-4	1	0	0	Acenaphthylene, 1-methyl-		1.20
18.	19345-94-9	1	0	0	Acenaphthylene, 3-methyl-		1.20
19.	19345-97-2	1	0	0	Acenaphthylene, 4-methyl-		1.20
20.	19345-91-6	1	0	0	Acenaphthylene, 5-methyl-		1.20
21.	60826-73-5	1	0	0	Acenaphthylene, tetramethyl-		1.20
22.	60826-70-2	1	0	0	Acenaphthylene, trimethyl-		1.20
23.	201-06-9	1	0	0	Acephenanthrylene		1.20
24.	6232-48-0	1	0	0	Acephenanthrylene, 4,5-dihydro-		1.20
25.	75-07-0	1	1	1	Acetaldehyde	$H_3C\text{-}CH{=}O$	0.4, 3.12, 23.5
26.	5371-49-3	1	0	0	Acetaldehyde, (acetyloxy)-	$H_3C\text{-}COO\text{-}CH_2\text{-}CH{=}O$	3.12, 5.3
27.	6542-88-7	1	0	0	Acetaldehyde, amino-	$H_2N\text{-}CH_2\text{-}CH{=}O$	3.12, 12.2
28.	141-46-8	1	0	0	Acetaldehyde, hydroxy- {glycolaldehyde}	$HO\text{-}CH_2\text{-}CH{=}O$	2.5, 3.12

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
29.	10312-83-1	1	0	0	Acetaldehyde, methoxy-	$H_3C\text{-}O\text{-}CH_2\text{-}CH{=}O$	3.12, 10.2
30.	16825-04-0	0	1	0	Acetaldehyde, (2,6,6-trimethyl-4-oxo-2-cyclohexen-1-ylidene)-		3.12, 3.13
31.	60-35-5	1	0	0	Acetamide	$H_3C\text{-}CO\text{-}NH_2$	3.1, 3.5
32.	1113-68-4	1	1	1	Acetamide, *N*-acetyl-*N*-methyl- {methanamine, *N,N*-diacetyl-}	$H_3C\text{-}CO\text{-}N{<}^{CH_3}_{CO\text{-}CH_3}$	13.1
33.	1119-49-9	1	0	0	Acetamide, *N*-butyl-	$H_3C\text{-}CO\text{-}NH\text{-}C_4H_9$	13.1
34.	15972-60-8	0	1	0	Acetamide, 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)- {Alachlor®}		10.2, 13.1, 18.4, 21.3
35.	51218-45-2	0	1	0	Acetamide, 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)- {Metolachlor®}		10.2, 13.1, 18.4, 21.3
36.	107-91-5	1	0	0	Acetamide, 2-cyano-	$NC\text{-}CH_2\text{-}CO\text{-}NH_2$	11.2, 13.1
37.	57966-95-7	0	1	0	Acetamide, 2-cyano-2-methoxyimino-*N*-(ethylcarbamoyl)- {Cymoxanil®}		10.2, 11.2, 13.1, 21.3
38.	685-91-6	1	0	0	Acetamide, *N,N*-diethyl-	$H_3C\text{-}CO\text{-}N{=}(C_2H_5)_2$	13.1
39.	127-19-5	1	1	1	Acetamide, *N,N*-dimethyl-	$H_3C\text{-}CO\text{-}N{=}(CH_3)_2$	13.1
40.	625-50-3	1	0	0	Acetamide, *N*-ethyl-	$H_3C\text{-}CO\text{-}NH\text{-}C_2H_5$	13.1
41.	38806-26-7	1	0	0	Acetamide, *N*-ethyl-*N*-methyl-	$H_3C\text{-}CO\text{-}N{<}^{CH_3}_{C_2\text{-}H_5}$	13.1
42.	5663-62-7	1	0	0	Acetamide, *N*-(2-furanylmethyl)-		10.2, 13.1
43.	621-42-1	0	1	0	Acetamide, 3-hydroxyphenyl-		9.22, 13.1
44.	4293-57-6	1	0	0	Acetamide, *N*-(2-hydroxypropyl)-	$H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CHOH\text{-}CH_3$	2.5, 13.1
45.	79-16-3	1	0	0	Acetamide, *N*-methyl-	$H_3C\text{-}CO\text{-}NH\text{-}CH_3$	13.1
46.	54824-90-7	1	0	0	Acetamide, *N*-(2-methylbutyl)-	$H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH(CH_3)\text{-}C_2H_5$	13.1
47.	13434-12-3	0	1	0	Acetamide, *N*-(3-methylbutyl)-	$H_3C\text{-}CO\text{-}NH\text{-}(CH_2)_2\text{-}CH{=}(CH_3)_2$	13.1
48.	1189-05-5	1	0	0	Acetamide, *N*-(1-methylpropyl)-	$H_3C\text{-}CO\text{-}NH\text{-}CH(CH_3)\text{-}C_2H_5$	13.1
49.	1540-94-9	1	1	1	Acetamide, *N*-(2-methylpropyl)-	$H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH{=}(CH_3)_2$	13.1
50.	7737-16-8	1	0	0	Acetamide, *N*-(2-oxopropyl)-	$H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CO\text{-}CH_3$	3.13, 13.1
51.	103-84-4	1	0	0	Acetamide, *N*-phenyl-	$H_3C\text{-}CO\text{-}NH\text{-}C_6H_5$	13.1
52.	877-95-2	1	0	0	Acetamide, *N*-(2-phenylethyl)-	$H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}C_6H_5$	13.1
53.	692-33-1	1	0	0	Acetamide, *N*-2-propenyl-	$H_3C\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH{=}CH_2$	13.1
54.	5331-48-6	1	0	0	Acetamide, *N*-propyl-	$H_3C\text{-}CO\text{-}NH\text{-}C_3H_7$	13.1
55.	354-38-1	1	0	0	Acetamide, 2,2,2-trifluoro-	$F_3C\text{-}CO\text{-}NH_2$	13.1, 18.4
56.	16752-77-5	0	1	0	Acetamidic acid, thio-, *N*-[(methylcarbamoyl)oxy]-, methyl ester {Methomyl®}		5.3, 13.1, 21.3

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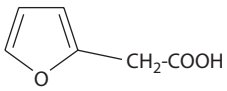
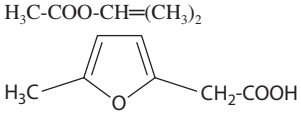
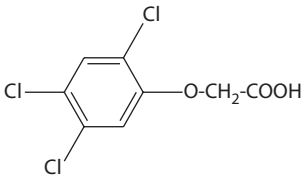
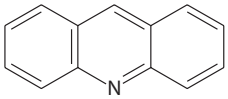
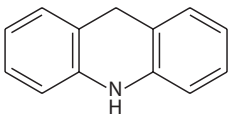
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
57.	71-50-1	1	0	0	Acetate	$H_3C\text{-}COO^-$	0.4, 20.6
58.	64-19-7	1	1	1	Acetic acid	$H_3C\text{-}COOH$	0.4, 4.3, 24.3, 25.29
59.	13831-30-6	1	1	1	Acetic acid, (acetyloxy)-	$H_3C\text{-}COO\text{-}CH_2\text{-}COOH$	4.3, 5.3
60.	108-24-7	1	0	0	Acetic acid, anhydride	$(H_3C\text{-}CO)_2O$	7.1
61.	162188-92-3	0	1	0	Acetic acid, bromo-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro[4.5]dec-7-yl ester, (±)-		5.3, 18.4
62.	123-86-4	1	1	1	Acetic acid, butyl ester {butyl acetate}	$H_3C\text{-}COO\text{-}C_4H_9$	5.3, 24.3, 25.29
63.	5743-26-0	0	1	0	Acetic acid, calcium salt, monohydrate		20.6
64.	79-43-6	0	1	0	Acetic acid, dichloro-	$Cl_2CH\text{-}COOH$	4.3, 18.4
65.	94-75-7	0	1	0	Acetic acid, 2,4-dichlorophenoxy- {2,4-D}		4.3, 10.2, 18.4, 21.3
66.	162188-93-4	0	1	0	Acetic acid, (diethoxyphosphinyl)-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro [4.5]dec-7-yl ester, (±)-		5.3, 10.2
67.	32833-96-8	0	1	0	Acetic acid, (dimethylamino)oxo-	$(H_3C)_2{=}N\text{-}CO\text{-}COOH$	4.3
68.	105-87-3	0	1	0	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl, (*E*)- ester {geranyl acetate}		5.3
69.	16409-44-2	0	1	0	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl acetate}		5.3
70.	141-12-8	0	1	0	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl, (*Z*)- ester {neryl acetate}		5.3
71.	150-84-5	0	1	0	Acetic acid, 3,7-dimethyl-6-octen-1-yl ester {citronellyl acetate}		5.3
72.	151-05-3	0	1	0	Acetic acid, 1,1-dimethyl-2-phenylethyl ester		5.3
73.	112-66-3	0	1	0	Acetic acid, 1-dodecyl ester	$CH_3\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	5.3
74.	108-05-4	1	0	0	Acetic acid, ethenyl ester {vinyl acetate}	$H_3C\text{-}COO\text{-}CH{=}CH_2$	5.3
75.	141-78-6	1	1	1	Acetic acid, ethyl ester {ethyl acetate}	$H_3C\text{-}COO\text{-}C_2H_5$	5.3, 24.3, 25.29
76.	123617-80-1	1	0	0	Acetic acid, 2-furanyl-		4.3, 10.2
77.	112-06-1	0	1	0	Acetic acid, heptyl ester	$H_3C\text{-}COO\text{-}(CH_2)_6\text{-}CH_3$	5.3
78.	629-70-9	0	1	0	Acetic acid, 1-hexadecyl ester	$H_3C\text{-}COO\text{-}(CH_2)_{15}\text{-}CH_3$	5.3
79.	142-92-7	0	1	0	Acetic acid, hexyl ester {hexyl acetate}	$H_3C\text{-}COO\text{-}(CH_2)_5\text{-}CH_3$	5.3, 24.3, 25.29
80.	79-14-1	1	1	1	Acetic acid, hydroxy- {glycolic acid}	$HOCH_2\text{-}COOH$	2.5, 4.3
81.	623-50-7	1	0	0	Acetic acid, hydroxy-, ethyl ester	$HOCH_2\text{-}COO\text{-}C_2H_5$	2.5, 5.3
82.	61892-60-2	1	1	1	Acetic acid, hydroxy-, 2-hydroxypropyl ester	$HOCH_2\text{-}COO\text{-}CH_2\text{-}CHOH\text{-}CH_3$	2.5, 5.3
83.	96-35-5	1	0	0	Acetic acid, hydroxy-, methyl ester	$HOCH_2\text{-}COO\text{-}CH_3$	2.5, 5.3
84.	1932-50-9	0	1	0	Acetic acid, hydroxy-, potassium salt		5.3, 20.6
85.	90357-58-7	1	1	1	Acetic acid, hydroxy-, propyl ester	$HOCH_2\text{-}COO\text{-}C_3H_7$	2.5, 5.3
86.		1	0	0	Acetic acid, hydroxymethyl ester	$H_3C\text{-}COO\text{-}CH_2OH$	2.5, 5.3
87.	142-72-3	0	1	0	Acetic acid, magnesium salt		20.6
88.	625-45-6	0	1	0	Acetic acid, methoxy-	$H_3CO\text{-}CH_2\text{-}COOH$	4.3, 10.2
89.	79-20-9	1	1	1	Acetic acid, methyl ester	$H_3C\text{-}COO\text{-}CH_3$	5.3
90.	624-41-9	0	1	0	Acetic acid, 2-methylbutyl ester	$H_3C\text{-}COO\text{-}CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	5.3
91.	123-92-2	0	1	0	Acetic acid, 3-methylbutyl ester	$H_3C\text{-}COO\text{-}(CH_2)_2\text{-}CH{=}(CH_3)_2$	5.3, 24.3, 25.29
92.	1191-16-8	0	1	0	Acetic acid, 3-methyl-2-butenyl ester	$H_3C\text{-}COO\text{-}CH_2\text{-}CH{=}C{=}(CH_3)_2$	5.3
93.	108-21-4	1	1	1	Acetic acid, 1-methylethyl ester	$H_3C\text{-}COO\text{-}CH{=}(CH_3)_2$	5.3
94.	72360-04-4	1	0	0	Acetic acid, 2-(5-methylfuranyl)-		4.3, 10.2
95.	35897-16-6	0	1	0	Acetic acid, 2-methyl-3-pentyl ester	$H_3C\text{-}COO\text{-}CH(C_2H_5)\text{-}CH{=}(CH_3)_2$	5.3
96.	110-19-0	0	1	0	Acetic acid, 2-methylpropyl ester {isobutyl acetate}	$H_3C\text{-}COO\text{-}CH_2\text{-}CH{=}(CH_3)_2$	5.3, 25.29

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
97.	373-02-4	0	1	0	Acetic acid, nickel salt		20.6
98.	143-13-5	0	1	0	Acetic acid, nonyl ester		5.3
99.	112-14-1	0	1	0	Acetic acid, octyl ester		5.3
100.	298-12-4	1	1	1	Acetic acid, oxo- {glyoxalic acid, glyoxylic acid}	O═CH-COOH	3.12, 4.3
101.	628-63-7	0	1	0	Acetic acid, pentyl ester	H_3C-COO-$(CH_2)_4$-CH_3	5.3
102.	24851-98-7	0	1	0	Acetic acid, 2-pentyl-3-oxo-1-cyclopentyl-, methyl ester {methyl dihydrojasmonate}		5.3
103.	103-45-7	1	1	1	Acetic acid, 2-phenylethyl ester {2-phenethyl acetate}	H_3C-COO-$(CH_2)_2$-C_6H_5	5.3, 24.3, 25.29
104.	140-11-4	1	1	1	Acetic acid, phenylmethyl ester {benzyl acetate}	H_3C-COO-CH_2-C_6H_5	5.3
105.	103-54-8	0	1	0	Acetic acid, 3-phenyl-2-propenyl ester {cinnamyl acetate}		5.3
106.	122-72-5	0	1	0	Acetic acid, phenylpropyl ester	H_3C-COO-$(CH_2)_3$-C_6H_5	5.3
107.	13147-57-4	0	1	0	Acetic acid, (phosphonoxy)-		4.3
108.	127-08-2	0	1	0	Acetic acid, potassium salt	H_3C-COO-K	20.6
109.	109-60-4	1	1	1	Acetic acid, propyl ester {propyl acetate}	H_3C-COO-$(CH_2)_2$-CH_3	5.3, 24.3, 25.29
110.	127-09-3	0	1	0	Acetic acid, sodium salt	H_3C-COO-Na	20.6, 25.29
111.	93-76-5	0	1	0	Acetic acid, 2,4,5-trichlorophenoxy- {2,4,5-T®}		4.3, 10.2, 18.4, 21.3
112.	76-49-3 5655-61-8	0	1	0	Acetic acid, *endo*-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl ester {bornyl acetate}		5.3
113.	75-05-8	1	0	0	Acetonitrile	H_3C-CN	11.2
114.	926-64-7	1	0	0	Acetonitrile, (dimethylamino)-	$(H_3C)_2$═N-CH_2-CN	11.2, 12.2
115.	107-16-4	1	0	0	Acetonitrile, hydroxy-	$HOCH_2$-CN	2.5, 11.2
116.	4471-47-0	1	0	0	Acetonitrile, oxo-	O═CH-CN	3.12, 11.2
117.	9012-33-3	0	1	0	β-Acetylglucosaminidase		22.2
118.	9040-07-7	0	1	0	Acetyltransferase, chloramphenicol		22.2
119.		0	1	0	*Acinetobacter*		22.2
120.	260-94-6	1	0	0	Acridine {benzo[*b*]quinoline}		17.21, 25.29
121.	92-81-9	1	0	0	Acridine, 9,10-dihydro- {acridan}		17.21
122.	6267-02-3	1	0	0	Acridine, 9,10-dihydro-9,9-dimethyl- {9,9-dimethylacridan}		17.21
123.	26914-16-9	1	0	0	Acridine, 9,10-dihydro-9,9-dimethyl-(1-methylethyl)-		17.21
124.	63451-42-3	1	0	0	Acridine, 9,10-dihydro-9,9-dimethyl-2-(1-methylethyl)-		17.21
125.	64828-44-0	1	0	0	Acridine, ethyl-		17.21
126.	54116-90-4	1	0	0	Acridine, methyl-		17.21
127.	64828-45-1	1	0	0	Acridine, propyl-		17.21
128.	55751-83-2	1	0	0	Acridine, 2-ethyl-		17.21

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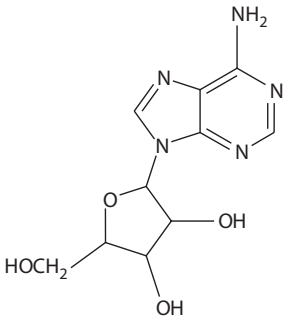
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
129.	65789-44-8	1	0	0	Acridine, 4-ethyl-		17.21
130.	4740-12-9	1	0	0	Acridine, 3-methyl-		17.21
131.	7440-34-8	1	1	1	Actinium	Ac	0.4, 20.5
132.	20379-10-6	0	1	0	Actinium, isotope of mass 226	^{226}Ac	20.5
133.	14331-83-0	0	1	0	Actinium, isotope of mass 228	^{228}Ac	20.5
134.		0	1	0	*Actinobacteria*, *Actinobacteria*		22.2
135.	50-76-0	0	1	0	Actinomycin D		21.3
136.		1	0	0	Acyl radical, butyl- {three isomers}	O═C-$CH_2CH_2CH_2CH_3$	27.1
137.		1	0	0	Acyl radical, ethenyl- {acrolein radical}	O═C-CH═CH_2	27.1
138.		1	0	0	Acyl radical, ethyl- {propionyl radical}	O═C-CH_2CH_3	27.1
139.		1	0	0	Acyl radical, methyl- {acetyl}	O═C-CH_3	27.1
140.		1	0	0	Acyl radical, 2-propenyl- {crotonyl radical}	O═C-CH═$CHCH_3$	27.1
141.		1	0	0	Acyl radical, propyl- {two isomers}	O═C-$CH_2CH_2CH_3$	27.1
142.	141733-40-6	0	1	0	Acyltransferase, glycerol phosphate (*Arabidopsis thaliana* clone BX3. 6/BB2.6 reduced)		22.2
143.	58-61-7	0	1	0	Adenosine		2.5, 8.3, 10.2, 12.2, 17.23
144.	60-92-4	0	1	0	Adenosine, cyclic 3′,5′-(hydrogen phosphate)		2.5, 17.23
145.	139636-55-8	0	1	0	Adenosine, 2′-deoxyadenylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxyadenylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxycytidylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxy-		2.5, 17.23
146.	146689-29-4	0	1	0	Adenosine, 2′-deoxycytidylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxyguanylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxyguanylyl-(5′→3′)-2′-deoxy-		2.5, 17.23
147.	28542-78-1	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-		2.5, 8.3, 17.23
148.	6025-53-2	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*E*)-		2.5, 8.3, 17.23
149.	15896-46-5	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*Z*)-		2.5, 8.3, 17.23
150.	26190-61-4	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-		2.5, 8.3, 17.23, 18.1

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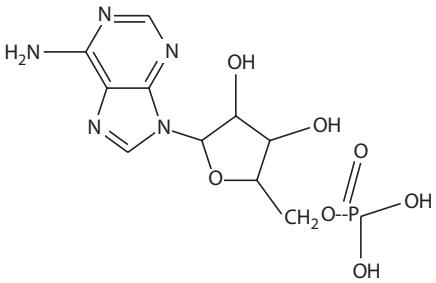
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
151.	53274-45-6	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*E*)-		2.5, 8.3, 17.23, 18.1
152.	52049-48-6	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*Z*)-		2.5, 8.3, 17.23, 18.1
153.	22663-55-4	0	1	0	Adenosine, *N*-(4-hydroxy-3-methylbutyl)-		2.5, 8.3, 17.23
154.	7724-76-7	0	1	0	Adenosine, *N*-(3-methyl-2-butenyl)-		2.5, 8.3, 17.23
155.	75081-82-2	0	1	0	Adenosine, *N*-[3-methyl-4-[(*O*-phosphono-β-*D*-glucopyranosyl) oxy]-2-butenyl]-, (*E*)-		2.5, 8.3, 17.23
156.	4294-16-0	0	1	0	Adenosine, *N*-(phenylmethyl)-		2.5, 8.3, 17.23
157.	56-65-5	0	1	0	Adenosine 5′-(tetrahydrogen triphosphate)		2.5, 2.5, 8.3,17.23
158.	40922-97-2	0	1	0	Adenosine 5′-(tetrahydrogen triphosphate), *N*-(phenylmethyl)-		2.5, 8.3, 17.23
159.	58-64-0	0	1	0	Adenosine 5′-(trihydrogen diphosphate)		2.5, 8.3, 17.23
160.	53-57-6	0	1	0	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		2.5, 5.3, 8.3, 13.1, 17.23
161.	53-59-8	0	1	0	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		2.5, 5.3, 8.3, 10.2, 12.2, 17.7, 17.23
162.	7298-93-3	0	1	0	Adenosine 5′-(trihydrogen diphosphate), 5′→5′-ester with 3-(aminocarbonyl)-1-α-*D*-ribofuranosylpyridinium hydroxide, inner salt		2.5, 5.3, 8.3, 10.2, 12.2, 17.7, 17.23
163.	55030-93-8	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *N*-(3-methyl-2-butenyl)-		2.5, 5.3, 17.23
164.	22732-83-8	0	1	0	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester		2.5, 5.3, 8.3, 17.23
165.	40811-89-0	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *N*-(phenylmethyl)-		2.5, 5.3, 8.3, 17.23
166.	58-68-4	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide		2.5, 5.3, 8.3, 13.1, 17.23
167.	53-84-9	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt		2.5, 5.3, 8.3, 13.1, 17.23
168.	9012-52-6	0	1	0	Adenosyltransferase, methionine		12.2
169.	84-21-9	0	1	0	3′-Adenylic acid		2.5, 10.2, 12.2, 17.23
170.	61-19-8	0	1	0	5′-Adenylic acid		2.5, 10.2, 12.2, 17.23

(*continued*)

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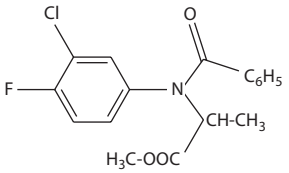
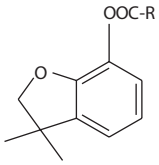
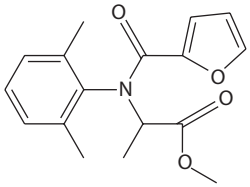
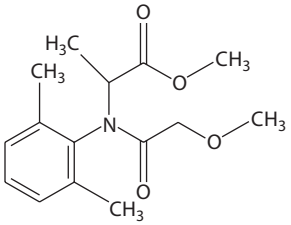
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
171.	20268-93-3	0	1	0	5′-Adenylic acid, *N*-(3-methyl-2-butenyl)-		2.5, 10.2, 12.2, 17.23
172.	13484-66-7	0	1	0	5′-Adenylic acid, *N*-(phenylmethyl)-		2.5, 10.2, 12.2, 17.23
173.	9012-39-9	0	1	0	Adenylyltransferase, sulfate		22.2
174.	6898-94-8	1	1	1	Alanine		4.3, 4.10, 12.2, 24.3
175.	62-57-7	0	1	0	Alanine, 2-methyl-	$(CH_3)_2{=}C(NH_2)$ COOH	4.3, 4.10, 12.2
176.	13100-82-8	0	1	0	Alanine, 3-sulfo-	$HO\text{-}SO_2\text{-}CH_2\text{-}C(NH_2)$ COOH	4.3, 4.10, 12.2
177.	107-95-9	1	1	1	β-Alanine	$H_2N\text{-}(CH_2)_2\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 24.3, 25.29
178.	79-83-4 137-08-8	0	1	0	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- {pantothenic acid}	$HO\text{-}CH_2\text{-}C(CH_3)_2\text{-}CHOH\text{-}CO\text{-}NH\text{-}(CH_2)_2\text{-}$ COOH	0.4, 2.5, 4.3, 4.10, 12.2
179.	10478-42-9	1	1	1	β-Alanine, *N*-methyl-*N*-nitroso- = propanoic acid, 3-(methylnitrosoamino)- {NMPA}	$H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOH$	4.3, 4.10, 12.2, 15.8, 25.29
180.	133201-38-4	1	1	1	β-Alanine, *N*-(nitrosomethyl)-		4.3, 4.10, 12.2, 15.8
181.		1	1	1	β-Alanine, *N*-methyl-*N*-nitroso-, methyl ester	$H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}COOCH_3$	4.3, 4.10, 5.3, 12.2, 15.8
182.	923-16-0	0	1	0	*D*-Alanine, *N*-*D*-alanyl-	$H_2N\text{-}(CH_2)_2\text{-}CO\text{-}NH\text{-}(CH_2)_2\text{-}COOH$	4.3, 4.10, 12.2
183.	56-41-7	1	1	1	*L*-α-Alanine	$H_3C\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 25.29
184.	52756-25-9	0	1	0	*DL*-Alanine, *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-, methyl ester {Flamprop-methyl®}		12.2, 13.1, 18.4, 21.3
185.	16124-24-6 25127-16-6	0	1	0	*L*-Alanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 12.2
186.	82560-54-1	0	1	0	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy)carbonyl) methylamino)thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}	 R = -NH-S-N[CH(CH$_3$)$_2$]-(CH$_2$)$_2$-COOC$_2$H$_5$	10.2, 12.2, 18.1, 21.3
187.	19701-89-4	1	0	0	*DL*-Alanine, *N,N*-dimethyl-		4.3, 4.10, 12.2
188.	57646-30-7	0	1	0	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(2-furanylcarbonyl)-, methyl ester {Furalaxyl®}		5.3, 10.2, 13.1, 21.3
189.	57837-19-1	0	1	0	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-, methyl ester {Ridomil®}		5.3, 10.2, 13.1, 21.3

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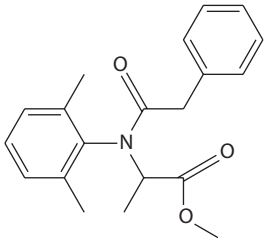
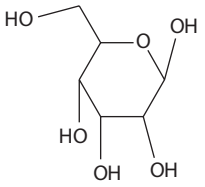
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
190.	71626-11-4	0	1	0	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)-, methyl ester {Benalaxyl®}		5.3, 13.1, 21.3
191.	9006-50-2	0	1	0	Albumin		22.2
192.	9048-46-8	0	1	0	Albumins, blood serum		22.2
193.	9024-52-6	0	1	0	Aldolase, fructose diphosphate		22.2
194.	9026-94-2	0	1	0	Aldolase, phospho-2-keto-3-deoxyheptonate		22.2
195.	145137-43-5	0	1	0	Aldolase, phospho-2-keto-3-deoxyheptonate (tobacco clone NtDAHPS-1 precursor reduced)		22.2
196.		1	0	0	Alkylaminocarbonyl radical, butyl- {two isomers} {butylaminocarbonyl}	$CONHCH_2CH_2CH_2CH_3$	27.1
197.		1	0	0	Alkylaminocarbonyl radical, ethyl- {ethylaminocarbonyl}	$CONHCH_2CH_3$	27.1
198.		1	0	0	Alkylaminocarbonyl radical, methyl- {methylaminocarbonyl}	$CONHCH_3$	27.1
199.		1	0	0	Alkylaminocarbonyl radical, pentyl- {three isomers} {pentylaminocarbonyl}	$CONHCH_2CH_2CH_2CH_2CH_3$	27.1
200.		1	0	0	Alkylaminocarbonyl radical, propyl- {two isomers} {propylaminocarbonyl}	$CONHCH_2CH_2CH_3$	27.1
201.		1	0	0	Alkylaminocarbonyl radical (unsaturated)	C_5H_8NO	27.1
202.		1	0	0	Alkylaminocarbonyl radical (unsaturated)	$C_7H_{12}NO$	27.1
203.	2595-97-3	0	1	0	*D*-Allose		2.5, 8.3
204.	7429-90-5	1	1	1	Aluminum	Al	0.4, 20.5
205.	1344-28-1	0	1	0	Aluminum oxide	Al_2O_3	20.6
206.	1335-30-4	1	1	1	Aluminum silicate	$Al_2(SiO_3)_3$	20.6
207.	9031-85-0	0	1	0	Aminoacyltransferase		22.2
208.		1	0	0	Aminocarbonyl (amide) radical	$O{=}C\text{-}NH_2$	27.1
209.	9031-94-1	0	1	0	Aminopeptidase		22.2
210.	9001-61-0	0	1	0	Aminopeptidase, cytosol		22.2
211.	9054-63-1	0	1	0	Aminopeptidase, leucine		22.2
212.	37277-82-0	0	1	0	Aminopropyltransferase, putrescine		22.2
213.	9031-66-7	0	1	0	Aminotransferase		22.2
214.	9000-86-6	0	1	0	Aminotransferase, alanine		22.2
215.	9000-97-9	0	1	0	Aminotransferase, aspartate		22.2
216.	50812-10-7	0	1	0	Aminotransferase, glutamate–glyoxylate		22.2
217.	9030-42-6	0	1	0	Aminotransferase, ornithine–keto acid		22.2
218.	37259-57-7	0	1	0	Aminotransferase, serine–glyoxylate		22.2
219.	7664-41-7	1	1	1	Ammonia	NH_3	0.4, 12.2, 19.5, 24.3, 23.5, 25.29

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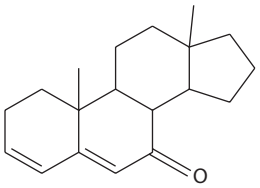
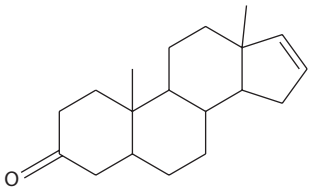
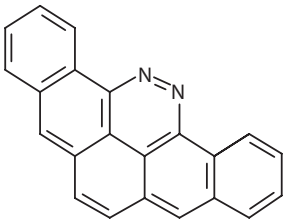
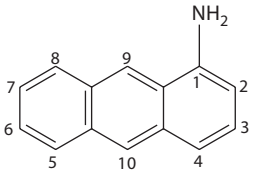
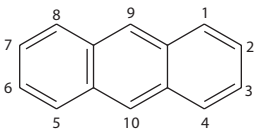
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
220.	9024-28-6	0	1	0	Ammonia-lyase, phenylalanine {tyrase}		22.2
221.	14798-03-9	1	1	1	Ammonium	NH_4^{+1}	20.6
222.	12125-02-9	1	0	0	Ammonium chloride	NH_4Cl	20.6
223.	53516-76-0	0	1	0	Ammonium chloride, alkyldimethylbenzyl- {Benzalkonium chloride®}		18.4, 21.3
224.	1336-21-6	0	1	0	Ammonium hydroxide	NH_4OH	20.6
225.	12135-76-1	0	1	0	Ammonium sulfide	$(NH_4)_2S$	18.1, 20.6
226.	9000-92-4	0	1	0	Amylase		0.4, 22.2
227.	9000-90-2	0	1	0	Amylase, α- {diastase}		22.2
228.	9000-91-3	0	1	0	Amylase, β-		22.2
229.	9067-73-6	0	1	0	Amylase, iso-		22.2
230.	9037-22-3	0	1	0	Amylopectin		8.3
231.	9005-82-7	0	1	0	Amylose		8.3
232.	32222-21-2	0	1	0	Androsta-3,5-dien-7-one		2.7, 3.13
233.	18339-16-7	0	1	0	5α-Androst-16-en-3-one {androstenone}		2.7, 3.13
234.	9001-03-0	0	1	0	Anhydrase, carbonate		22.2
235.	189-58-2	1	0	0	Anthra[9,1,2-*cde*]benzo[*h*]cinnoline		17.21
236.	62813-37-0	1	0	0	Anthracenamine		12.2
237.	610-49-1	1	1	1	1-Anthracenamine		12.2
238.	613-13-8	1	1	1	2-Anthracenamine		12.2
239.	779-03-3	1	0	0	9-Anthracenamine		12.2
240.	120-12-7	1	1	1	Anthracene		0.4, 1.20, 26.9
241.		1	1	1	9-^{14}C-Anthracene {anthracene-9-^{14}C}		1.20, 25.29
242.		1	0	0	Anthracene, alkyl-		1.20
243.	613-31-0	1	0	0	Anthracene, 9,10-dihydro-		1.20
244.	29063-00-1	1	0	0	Anthracene, dimethyl-		1.20
245.	781-43-1	1	0	0	Anthracene, 9,10-dimethyl-		1.20
246.	41637-86-9	1	0	0	Anthracene, ethyl-		1.20

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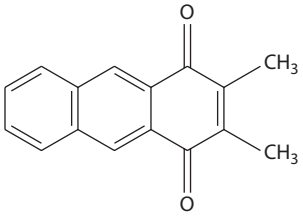
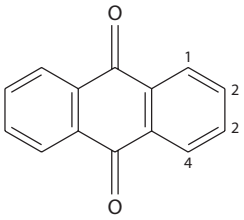
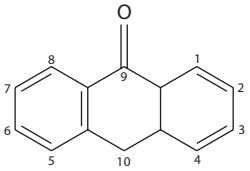
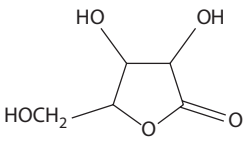
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
247.	605-83-4	1	0	0	Anthracene, 9-ethyl-		1.20
248.	71265-29-7	1	0	0	Anthracene, ethylmethyl-		1.20
249.	26914-18-1	1	0	0	Anthracene, methyl-		1.20
250.	610-48-0	1	0	0	Anthracene, 1-methyl-		1.20
251.	613-12-7	1	0	0	Anthracene, 2-methyl-		1.20
252.	779-02-2	1	0	0	Anthracene, 9-methyl-		1.20
253.	71265-30-0	1	0	0	Anthracene, propyl-		1.20
254.	27358-28-7	1	0	0	Anthracene, trimethyl-		1.20
255.		0	1	0	1,4-Anthracenedione, 2,3-dimethyl-		9.24
256.	84-65-1	1	1	1	9,10-Anthracenedione {9,10-anthraquinone}		9.24, 21.3
257.	20724-30-5	1	0	0	9,10-Anthracenedione, 1,2-diethyl-		9.24
258.	117-12-4	1	0	0	9,10-Anthracenedione, 1,5-dihydroxy-		9.22, 9.24
259.	71265-31-1	1	0	0	9,10-Anthracenedione, dimethyl-		9.24
260.	6531-35-7	1	0	0	9,10-Anthracenedione, 2,3-dimethyl-		9.24
261.	27936-34-1	1	0	0	9,10-Anthracenedione, methyl-		9.24
262.	84-54-8	1	1	1	9,10-Anthracenedione, 2-methyl-		9.24
263.		1	0	0	9,10-Anthracenedione, trimethyl-		9.24
264.	90-44-8	1	0	0	9(10*H*)-Anthracenone {anthrone}		3.13
265.	7440-36-0	1	1	1	Antimony	Sb	0.4, 20.5
266.	14683-10-4	1	1	1	Antimony, isotope of mass 124	^{124}Sb	20.5
267.	14331-88-5	0	1	0	Antimony, isotope of mass 129	^{129}Sb	20.5
268.	9000-95-7	0	1	0	Apyrase		22.2
269.	11078-27-6	0	1	0	Arabinan		2.5, 8.3
270.	20261-96-5	1	1	1	Arabinohexonic acid, 3-deoxy-, γ-lactone		2.5, 6.3, 8.3
271.	42400-32-8	0	1	0	*D*-Arabinohexonic acid, 2-deoxy-, γ-lactone		2.5, 6.3, 8.3
272.	23675-06-1	0	1	0	α-*D*-Arabinohexopyranoside, 2-deoxy- α-*D*-arabino-hexopyranosyl 2-deoxy-		2.5, 8.3
273.	154-17-6	0	1	0	*D*-Arabinohexose, 2-deoxy- {2-deoxy-*D*-glucose}		2.5, 8.3, 10.2
274.	16449-30-2	0	1	0	*D*-Arabinohexose, 2-deoxy- 4-*O*-β-*D*-glucopyranosyl-		2.5, 8.3, 10.2
275.	13752-83-5	0	1	0	Arabinonic acid	$HO\text{-}CH_2\text{-}(CHOH)_3\text{-}COOH$	2.5, 4.3
276.	13280-76-7	1	0	0	Arabinonic acid, γ-lactone		2.5, 6.3, 8.3

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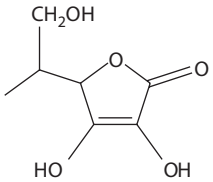
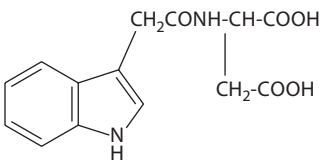
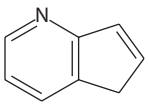
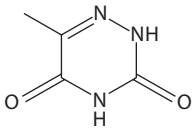
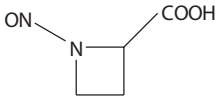
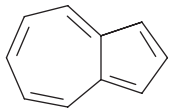
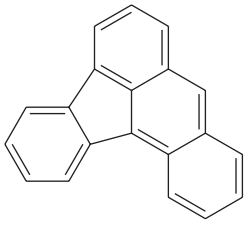
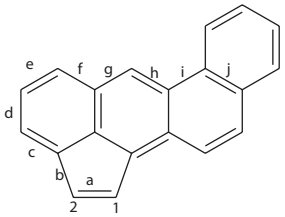
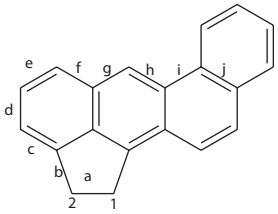
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
277.	87-72-9 5328-37-0	1	1	1	*L*-Arabinose	$HO\text{-}CH_2\text{-}(CHOH)_3\text{-}CH{=}O$	2.5, 3.12, 8.3, 25.29
278.	147-81-9	1	1	1	*DL*-Arabinose		0.4, 2.5, 3.12, 8.3, 25.29
279.	9040-27-1	0	1	0	Arabinoxylan		2.5, 8.3
280.	7643-75-6	1	1	1	Arabitinol	$HO\text{-}CH_2\text{-}(CHOH)_3\text{-}CH_3$	2.5
281.		0	1	0	Arabitinol, 2,3-di-*O*-methyl-	$HO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$	2.5, 8.3, 10.2
282.		0	1	0	Arabitinol, 2,5-di-*O*-methyl-	$H_3CO\text{-}CH_2\text{-}(CHOH)_2\text{-}(CHOCH_3)\text{-}CH_3$	2.5, 8.3, 10.2
283.		0	1	0	Arabitinol, 3,5-di-*O*-methyl-	$H_3CO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)\text{-}CHOH\text{-}CH_3$	2.5, 8.3, 10.2
284.		0	1	0	Arabitinol, 2,3,4-tri-*O*-methyl-	$HO\text{-}CH_2\text{-}(CHOCH_3)_3\text{-}CH_3$	2.5, 8.3, 10.2
285.		0	1	0	Arabitinol, 2,3,5-tri-*O*-methyl-	$H_3CO\text{-}CH_2\text{-}CHOH\text{-}(CHOCH_3)_2\text{-}CH_3$	2.5, 8.3, 10.2
286.	98530-09-7	0	1	0	Arabogalactan		2.5, 3.12, 8.3
287.	7004-12-8	0	1	0	Arginine	$H_2N\text{-}C(=NH)\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2
288.	1069-09-6 34522-32-2	0	1	0	Arginine, *N*2-(1-carboxyethyl)-		4.3, 4.10, 12.2
289.	74-79-3	0	1	0	*L*-Arginine	$H_2N\text{-}C(=NH)\text{-}NH\text{-}(CH_2)_3\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 12.2, 24.3
290.	7440-37-1	1	0	0	Argon	A	20.5
291.	7440-38-2	1	1	1	Arsenic	As	0.4, 20.5, 21.3, 23.5
292.	22541-54-4	1	1	1	Arsenic, arsenious state	As^{+3}	20.5, 21.3
293.		1	1	1	Arsenic, arsenic state	As^{+5}	20.5, 21.3
294.	15575-20-9	0	1	0	Arsenic, isotope of mass 76	^{76}As	20.5
295.	7778-44-1	0	1	0	Arsenic acid, calcium salt	$Ca_3(AsO_4)_2$	20.6, 21.3
296.	7645-25-2	0	1	0	Arsenic acid, lead salt	$Pb_3(AsO_4)_2$	20.6, 21.3
297.	7784-40-9	0	1	0	Arsenic acid, lead salt	$PbHAsO_4$	20.6, 21.3
298.	1327-53-3	0	1	0	Arsenic oxide {arsenious oxide}	As_2O_3	0.4, 20.6
299.	7784-42-1	1	0	0	Arsine	H_3As	20.6
300.	603-32-7	1	0	0	Arsine, triphenyl-	$As(C_6H_5)_3$	20.6
301.	50-81-7	1	1	1	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-}		0.4, 2.5, 6.3, 8.3, 24.3, 25.29, 26.9
302.	7006-34-0	1	1	1	Asparagine	$H_2N\text{-}CO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 13.1, 24.3
303.	70-47-3	0	1	0	*L*-Asparagine		4.3, 4.10, 12.2, 13.1
304.	5794-13-8	0	1	0	*L*-Asparagine monohydrate		4.3, 4.10, 12.2, 13.1
305.	6899-03-2	1	1	1	Aspartic acid		4.3, 4.10, 12.2
306.	56-84-8	1	1	1	*L*-Aspartic acid	$HOOC\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 24.3
307.	31105-02-9	0	1	0	*L*-Aspartic acid *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 12.2
308.	2456-73-7	0	1	0	*L*-Asparticacid, *N*-(1*H*-indol-3-ylacetyl)-		4.3, 4.10, 13.1
309.		0	1	0	*Atopobium*		22.2
310.		0	1	0	*Aurantimonas altamirensis*		22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
311.	89126-45-4	1	0	0	Azafluoranthene		17.21
312.	8047-67-4	1	0	0	Azaindene		17.21
313.	89126-46-5	1	0	0	Azapyrene		17.21
314.	932-53-6	0	1	0	6-Azathymine		14.1, 17.7
315.	503-29-7	1	1	1	Azetidine		17.1
316.	34441-14-0	0	1	0	1-Azetidinebutanoic acid, α-[(3-amino-3-carboxypropyl)amino]-2-carboxy-, [2S-[1[αR*(R*)],2R*]]- {nicotianamine}		4.3, 12.2, 17.1
317.	2517-04-6	0	1	0	2-Azetidinecarboxylic acid		4.3, 12.2, 17.1
318.	55556-98-4	0	1	0	2-Azetidinecarboxylic acid, 1-nitroso-		4.3, 15.8, 17.1
319.	275-51-4	1	0	0	Azulene {cyclopentacycloheptene}		0.4, 1.20
320.	529-05-5	1	0	0	Azulene, 1,4-dimethyl-7-ethyl-		1.20
321.	9024-08-2	0	1	0	*Bacillus pumilus* {racemase, glutamate}		22.2
322.	68038-71-1	0	1	0	*Bacillus thuringiensis* {Dipel®}		21.3, 22.2
323.		0	1	0	*Bacteroidetes*, *Bacteroidetes*		22.2
324.		0	1	0	*Bacteroidetes*, *Sphingobacteria*		22.2
325.	7440-39-3	1	1	1	Barium	Ba	0.4, 20.5
326.	203-33-8	1	0	0	Benz[*a*]aceanthrylene {benzo[*a*]fluoranthene}		1.20
327.	202-33-5	1	0	0	Benz[*j*]aceanthrylene {cholanthrylene}		1.20
328.	479-23-2	1	0	0	Benz[*j*]aceanthrylene, 1,2-dihydro- {cholanthrene}		1.20

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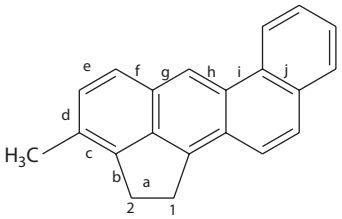
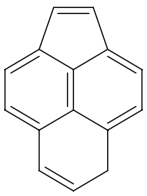
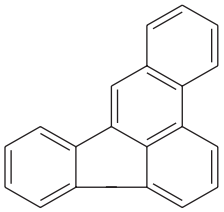
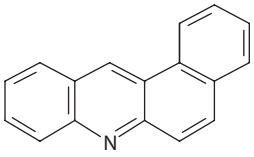
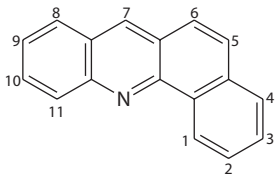
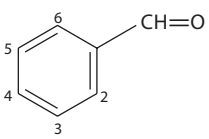
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
329.	56-49-5	1	0	0	Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl- {3-methylcholanthrene}		1.20
330.	76774-50-0	1	0	0	Benz[*fg*]acenaphthylene		1.20
331.	205-99-2	1	1	1	Benz[*e*]acephenanthrylene {benzo[*b*]fluoranthene}		1.20, 23.5
332.	41637-94-9	1	0	0	Benz[*e*]acephenanthrylene, methyl-		1.20
333.	149021-93-2	1	0	0	Benz[*e*]acephenanthrylene, 10-methyl-		1.20
334.	225-11-6	1	0	0	Benz[*a*]acridine		17.21
335.	53-69-0	1	0	0	Benz[*a*]acridine, 8,10-dimethyl-		17.21
336.	17401-48-8	1	0	0	Benz[*a*]acridine, 9,12-dimethyl-		17.21
337.	225-51-4	1	0	0	Benz[*c*]acridine		17.21
338.	10567-95-0	1	0	0	Benz[*c*]acridine, 5,7-dimethyl-		17.21
339.	71265-19-5	1	0	0	Benz[*c*]acridine, 6,9-dimethyl-		17.21
340.	963-89-3	1	0	0	Benz[*c*]acridine, 7,9-dimethyl-		17.21
341.	2381-40-0	1	0	0	Benz[*c*]acridine, 7,10-dimethyl-		17.21
342.	32740-01-5	1	0	0	Benz[*c*]acridine, 7,11-dimethyl-		17.21
343.	3340-94-1	1	0	0	Benz[*c*]acridine, 7-methyl-		17.21
344.	14319-90-5	1	0	0	Benz[*c*]acridine, 8-methyl-		17.21
345.	33942-93-7	1	0	0	Benz[*c*]acridine, 9-methyl-		17.21
346.	7230-71-9	1	0	0	Benz[*c*]acridine, 10-methyl-		17.21
347.	67028-20-0	1	0	0	Benz[*c*]acridine, 11-methyl-		17.21
348.	58430-01-6	1	0	0	Benz[*c*]acridine, 7,9,10-trimethyl-		17.21
349.	51787-42-9	1	0	0	Benz[*c*]acridine, 7,9,11-trimethyl-		17.21
350.	100-52-7	1	1	1	Benzaldehyde		0.4, 3.12, 24.3, 25.29

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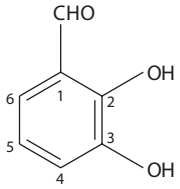
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
351.	1620-98-0	0	1	0	Benzaldehyde, 3,5-di(1,1-dimethylethyl)-4-hydroxy-		3.12, 9.22
352.	33774-71-9	1	1	1	Benzaldehyde, dihydroxy-		3.12, 9.22
353.	24677-78-9	1	1	1	Benzaldehyde, 2,3-dihydroxy-		3.12, 9.22
354.	95-01-2	1	0	0	Benzaldehyde, 2,4-dihydroxy-		3.12, 9.22
355.	1194-98-5	1	0	0	Benzaldehyde, 2,5-dihydroxy-		3.12, 9.22
356.	139-85-5	1	1	1	Benzaldehyde, 3,4-dihydroxy- {protocatechualdehyde}		3.12, 9.22
357.	86-51-1	1	1	1	Benzaldehyde, 2,3-dimethoxy-		3.12, 10.2
358.	613-45-6	0	1	0	Benzaldehyde, 2,4-dimethoxy-		3.12, 10.2
359.	93-02-7	1	1	1	Benzaldehyde, 2,5-dimethoxy-		3.12, 10.2
360.	4925-88-6	1	0	0	Benzaldehyde, 2,5-dimethoxy-4-methyl-		3.12, 10.2
361.	3392-97-0	1	1	1	Benzaldehyde, 2,6-dimethoxy-		3.12, 10.2
362.	120-14-9	1	1	1	Benzaldehyde, 3,4-dimethoxy- {veratraldehyde}		3.12, 10.2, 24.3, 25.29
363.	7311-34-4	1	1	1	Benzaldehyde, 3,5-dimethoxy-		3.12, 10.2
364.	134-96-3	1	1	1	Benzaldehyde, 3,5-dimethoxy-4-hydroxy- {syringaldehyde}		3.12, 9.22
365.	708-76-9	1	1	1	Benzaldehyde, 4,6-dimethoxy-2-hydroxy-		3.12, 9.22, 10.2
366.	15764-16-6	1	0	0	Benzaldehyde, 2,4-dimethyl-		3.12
367.	5779-94-2	1	0	0	Benzaldehyde, 2,5-dimethyl-		3.12
368.	100-10-7	1	0	0	Benzaldehyde, 4-(dimethylamino)-		3.12, 12.2
369.	121-32-4	1	1	1	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}		3.12, 9.22, 10.2, 24.3, 25.29
370.	10031-82-0	0	1	0	Benzaldehyde, 4-ethoxy-		3.12, 10.2
371.	2539-53-9	0	1	0	Benzaldehyde, 4-ethoxy-3-hydroxy-		3.12, 9.22, 10.2
372.	53951-50-1	0	1	0	Benzaldehyde, ethyl-		3.12
373.	4748-78-1	0	1	0	Benzaldehyde, 4-ethyl-		3.12, 25.29
374.		1	0	0	Benzaldehyde, hydroxy-		3.12, 9.22, 24.3, 25.29
375.	90-02-8	1	1	1	Benzaldehyde, 2-hydroxy- {salicylaldehyde}		3.12, 9.22, 24.3, 25.29
376.	148-53-8	1	1	1	Benzaldehyde, 2-hydroxy-3-methoxy-		3.12, 9.22, 10.2
377.	698-27-1	0	1	0	Benzaldehyde, 2-hydroxy-4-methyl-		3.12, 9.22
378.	100-83-4	0	1	0	Benzaldehyde, 3-hydroxy-		3.12, 9.22
379.	123-08-0	1	1	1	Benzaldehyde, 4-hydroxy-		3.12, 9.22
380.	106799-60-4	0	1	0	Benzaldehyde, hydroxymethoxy-		3.12, 9.22, 10.2
381.	121-33-5	1	1	1	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}		3.12, 9.22, 10.2, 24.3, 25.29
382.		1	1	1	Benzaldehyde, 4-hydroxy-3-methoxy-, labeled with ^{14}C {vanillin-^{14}C}		3.12, 9.22, 10.2, 25.29
383.		1	0	0	Benzaldehyde, hydroxymethyl-		3.12, 9.22
384.	97122-27-5	1	0	0	Benzaldehyde, hydroxy-3-methyl-		3.12, 9.22
385.	57295-30-4	1	0	0	Benzaldehyde, 3-hydroxy-4-methyl-		3.12, 9.22
386.	15174-69-3	1	0	0	Benzaldehyde, 4-hydroxy-3-methyl-		3.12, 9.22
387.		1	0	0	Benzaldehyde, methoxy-		3.12, 10.2

(*continued*)

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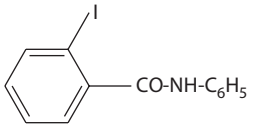
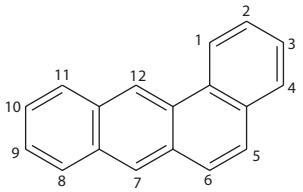
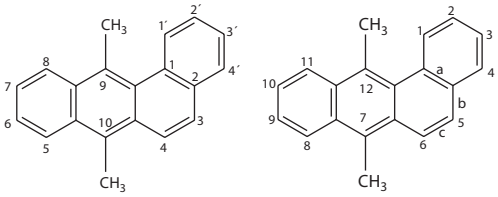
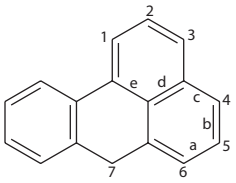
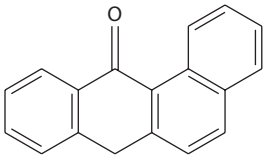
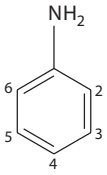
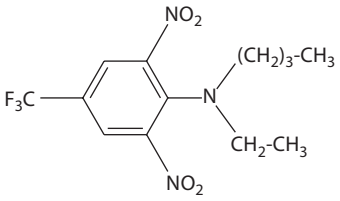
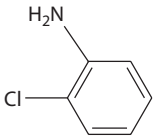
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
388.	135-02-4	1	0	0	Benzaldehyde, 2-methoxy-		3.12, 10.2
389.	591-31-1	1	0	0	Benzaldehyde, 3-methoxy-		3.12, 10.2
390.	123-11-5	1	1	1	Benzaldehyde, 4-methoxy- {*p*-anisaldehyde}		3.12, 10.2, 24.3, 25.29
391.	1334-78-7	1	0	0	Benzaldehyde, methyl-		3.12
392.	529-20-4	1	1	1	Benzaldehyde, 2-methyl- {*o*-tolualdehyde}		3.12, 24.3, 25.29
393.	620-23-5	1	1	1	Benzaldehyde, 3-methyl- {*m*-tolualdehyde}		3.12, 24.3, 25.29
394.	104-87-0	1	1	1	Benzaldehyde, 4-methyl- {*p*-tolualdehyde}		3.12, 24.3, 25.29
395.	122-03-2	1	1	1	Benzaldehyde, 4-(1-methylethyl)- {cuminaldehyde}		3.12, 24.3, 25.29
396.	29344-95-4	0	1	0	Benzaldehyde, 2,3,4,5-tetramethyl-		3.12
397.	487-68-3	1	0	0	Benzaldehyde, 2,4,6-trimethyl-		3.12
398.	55-21-0	1	1	1	Benzamide	C_6H_5-CO-NH_2	13.1
399.	15310-01-7	0	1	0	Benzamide, 2-iodo-*N*-phenyl- {Benodanil®}		13.1, 18.4, 21.3
400.		1	0	0	Benzanthracene		1.20
401.	63194-18-3	1	0	0	Benzanthracene, methyl-		1.20
402.	56-55-3	1	1	1	Benz[*a*]anthracene {B*a*A or B[*a*]A}		1.20, 23.5, 26.9
403.		1	0	0	Benz[*a*]anthracene, alkyl-		1.20
404.	43178-07-0	1	0	0	Benz[*a*]anthracene, dimethyl-		1.20
405.	57-97-6	1	0	0	Benz[*a*]anthracene, 7,12-dimethyl- {DMBA} *Note*: Benz[*a*]anthracene, 9,10-dimethyl- There can be no such compound as 7,12-dimethyl-1,2-benzanthracene because, according to the now obsolete nomenclature shown, there was never a 12 position in the 1,2-benzanthracene molecule. Also shown is 7,12-dimethylbenz[*a*]anthracene named according to the current nomenclature		1.20
406.	31632-62-9	1	0	0	Benz[*a*]anthracene, ethyl-		1.20
407.	71265-32-2	1	0	0	Benz[*a*]anthracene, ethylmethyl-		1.20
408.	43178-22-9	1	0	0	Benz[*a*]anthracene, methyl-		1.20
409.	2498-77-3	1	0	0	Benz[*a*]anthracene, 1-methyl-		1.20
410.	2498-76-2	1	0	0	Benz[*a*]anthracene, 2-methyl-		1.20
411.	2498-75-1	1	0	0	Benz[*a*]anthracene, 3-methyl-		1.20
412.	316-49-4	1	0	0	Benz[*a*]anthracene, 4-methyl-		1.20
413.	2319-96-2	1	0	0	Benz[*a*]anthracene, 5-methyl-		1.20
414.	316-14-3	1	0	0	Benz[*a*]anthracene, 6-methyl-		1.20

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
415.	2381-31-9	1	0	0	Benz[*a*]anthracene, 8-methyl-		1.20
416.	2381-16-0	1	0	0	Benz[*a*]anthracene, 9-methyl-		1.20
417.	2381-15-9	1	0	0	Benz[*a*]anthracene, 10-methyl-		1.20
418.	2422-79-9	1	0	0	Benz[*a*]anthracene, 12-methyl-		1.20
419.		1	0	0	Benz[*a*]anthracene, methylene-		1.20
420.	71265-33-3	1	0	0	Benz[*a*]anthracene, propyl-		1.20
421.		1	0	0	Benz[*a*]anthracene, tetramethyl-		1.20
422.	60826-78-0	1	0	0	Benz[*a*]anthracene, trimethyl-		1.20
423.	199-94-0	1	0	0	7*H*-Benz[*de*]anthracene		1.20
424.		1	0	0	Benz[*a*]anthrone		3.13
425.	62-53-3	1	1	1	Benzenamine {aniline}		12.2
426.	106-40-1	1	0	0	Benzenamine, 4-bromo-		12.2, 18.4
427.	1861-40-1	0	1	0	Benzenamine, *N*-butyl-2,6-dinitro-*N*-ethyl-4-(trifluoromethyl)- {Benefin®, Benfluralin®}		12.2, 16.1, 18.4, 21.3
428.	95-51-2	1	1	1	Benzenamine, 2-chloro- {2-chloroaniline}		12.2, 18.4, 21.3
429.	106-47-8	1	0	0	Benzenamine, 4-chloro-		12.2, 18.4
430.	46175-80-8	0	1	0	Benzenamine, 2-(cyclohexen-1-yl)-		12.2
431.	95-76-1	0	1	0	Benzenamine, 3,4-dichloro-		12.2, 18.4
432.	99-30-9	0	1	0	Benzenamine, 2,6-dichloro-4-nitro- {Dicloran®}		12.2, 16.1, 18.4, 21.3
433.		1	0	0	Benzenamine, dimethyl-		12.2
434.	87-59-2	1	1	1	Benzenamine, 2,3-dimethyl- {2,3-xylidine}		12.2
435.	95-68-1	1	1	1	Benzenamine, 2,4-dimethyl- {2,4-xylidine}		12.2
436.	95-78-3	1	1	1	Benzenamine, 2,5-dimethyl- {2,5-xylidine}		12.2
437.	87-62-7	1	1	1	Benzenamine, 2,6-dimethyl- {2,6-xylidine}		12.2, 23.5

(*continued*)

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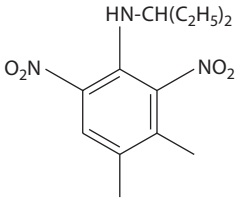
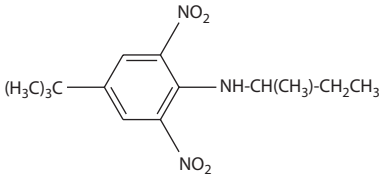
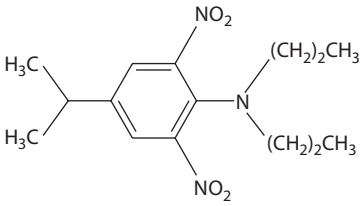
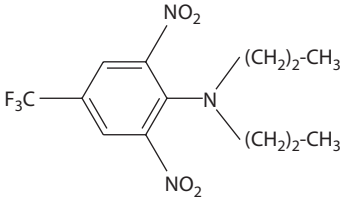
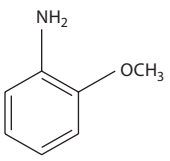
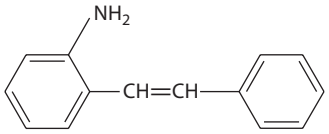
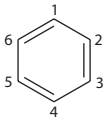
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
438.	95-64-7	1	1	1	Benzenamine, 3,4-dimethyl- {3,4-xylidine}		12.2
439.	40487-42-1	0	1	0	Benzenamine, 3,4-dimethyl-2,6-dinitro-*N*-(1-ethylpropyl)- {Pendimethalin®}		12.2, 16.1, 21.3
440.	108-69-0	1	1	1	Benzenamine, 3,5-dimethyl- {3,5-xylidine}		12.2
441.	611-21-2	1	0	0	Benzenamine, *N*,2-dimethyl-		12.2
442.	623-08-5	1	0	0	Benzenamine, *N*,4-dimethyl-		12.2
443.	121-69-7	1	0	0	Benzenamine, *N*,*N*-dimethyl-		12.2
444.	769-92-6	0	1	0	Benzenamine, 4-(1,1-dimethylethyl)- {parvoline}		0.4, 12.2
445.	33629-47-9	0	1	0	Benzenamine, 4-(1,1-dimethylethyl)-2,6-dinitro-*N*-(1-methylpropyl)- {Butralin®}		12.2, 16.1, 21.3, 25.29
446.	579-66-8	1	1	1	Benzenamine, 2,6-diethyl-		12.2
447.	33820-53-0	0	1	0	Benzenamine, 2,6-dinitro-*N*, *N*-dipropyl-4-(1-methylethyl)- {Isopropalin®}		12.2, 16.1, 21.3
448.	1582-09-8	0	1	0	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)- {Trifluralin®}		12.2, 16.1, 18.4, 21.3
449.	1520-21-4	1	1	1	Benzenamine, 4-ethenyl- {4-aminostyrene}		12.2
450.	578-54-1	1	1	1	Benzenamine, 2-ethyl-		12.2
451.	587-02-0	1	0	0	Benzenamine, 3-ethyl-		12.2
452.	589-16-2	1	0	0	Benzenamine, 4-ethyl-		12.2
453.	103-69-5	1	0	0	Benzenamine, *N*-ethyl- {*N*-ethylaniline}	C_6H_5-NH-CH_2-CH_3	12.2
454.	1821-38-1	1	1	1	Benzenamine, 2-ethyl-*N*-methyl-		12.2
455.	71265-20-8	1	0	0	Benzenamine, 3-ethyl-*N*-methyl-		12.2
456.	37846-06-3	1	0	0	Benzenamine, 4-ethyl-*N*-methyl-		12.2
457.	94-68-8	1	0	0	Benzenamine, *N*-ethyl-2-methyl-		12.2
458.	102-27-2	0	1	0	Benzenamine, *N*-ethyl-3-methyl-		12.2
459.	71265-27-5	1	0	0	Benzenamine, ar-ethyl-ar-methyl-		12.2
460.	90-04-0	1	1	1	Benzenamine, 2-methoxy- {*o*-anisidine}		10.2, 12.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
461.	50868-72-9	1	1	1	Benzenamine, 2-methoxy-5-methyl-		10.2, 12.2
462.	536-90-3	1	1	1	Benzenamine, 3-methoxy- {*m*-anisidine}		10.2, 12.2
463.	104-94-9	1	1	1	Benzenamine, 4-methoxy- {*p*-anisidine}		10.2, 12.2
464.		1	0	0	Benzenamine, methyl-		12.2
465.	26915-12-8	1	0	0	Benzenamine, ar-methyl-		12.2
466.	95-53-4	1	1	1	Benzenamine, 2-methyl- {*o*-toluidine, 2-toluidine}		12.2, 23.5
467.	108-44-1	1	0	0	Benzenamine, 3-methyl- {*m*-toluidine 3-toluidine}		12.2
468.	106-49-0	1	0	0	Benzenamine, 4-methyl- {*p*-toluidine, 4-toluidine}		12.2
469.	100-61-8	1	1	1	Benzenamine, *N*-methyl- {*N*-methylaniline}	C_6H_5-NH-CH_3	12.2
470.	5266-85-3	0	1	0	Benzenamine, 2-methyl-6-(1-methylethyl)-		12.2
471.	614-00-6	1	1	1	Benzenamine, *N*-methyl-*N*-nitroso-		12.2, 15.8
472.		1	0	0	Benzenamine, (1-methylethyl)-*N*-(1-methylethylphenyl)-		12.2
473.	5650-10-2	1	0	0	Benzenamine,4-(1-methylethyl)-*N*-phenyl-		12.2
474.	552-82-9	1	0	0	Benzenamine, *N*-methyl-*N*-phenyl-		12.2
475.	86-30-6	1	0	0	Benzenamine, *N*-nitroso-*N*-phenyl-		12.2, 15.8
476.	122-39-4	1	0	0	Benzenamine, *N*-phenyl- {diphenylamine}	C_6H_5-NH-C_6H_5	12.2, 25.29
477.	13066-19-8	1	1	1	Benzenamine, 2-(2-phenylethenyl)- {2-aminostilbene}		12.2
478.	14064-37-0	1	0	0	Benzenamine, 3-(2-phenylethenyl)-, (*Z*)-		12.2
479.	834-24-2	1	0	0	Benzenamine, 4-(2-phenylethenyl)-		12.2
480.	28059-64-5	1	0	0	Benzenamine, ?-phenylmethyl-		12.2
481.	71265-28-6	1	0	0	Benzenamine, ar,ar,ar,ar-tetramethyl-		12.2
482.	31093-11-5	1	0	0	Benzenamine, ar,ar,ar-trimethyl-		12.2
483.	88-05-1	1	1	1	Benzenamine, 2,4,6-trimethyl- {mesitylamine}		12.2
484.		1	0	0	Benzenaminocarbonyl radical {anilinocarbonyl radical}	C_6H_5-NH-C=O	27.1
485.	71-43-2	1	1	1	Benzene		1.13, 23.5, 25.29, 26.9
486.		1	0	0	Benzene, C_3-alkyl-		1.13
487.		1	0	0	Benzene, C_4-alkyl-		1.13
488.		1	0	0	Benzene, C_5-alkyl-		1.13
489.	103-33-3	0	1	0	Benzene, azobis- {azobenzene}	C_6H_5-N=N-C_6H_5	16.1
490.	1014-60-4	1	1	1	Benzene, 1,3-bis(1.1-dimethylethyl)-		1.13
491.	1012-72-2	1	1	1	Benzene, 1,4-bis(1.1-dimethylethyl)-		1.13
492.	100-18-5	1	1	1	Benzene, 1,4-bis(1-methylethyl)-		1.13
493.	886-66-8	1	0	0	Benzene,1,1′-(1,3-butadiyne-1,4-diyl)bis-	C_6H_5-C≡C-C≡C-C_6H_5	1.13
494.	824-90-8	1	0	0	Benzene, 1-butenyl-	C_6H_5-CH=CH-$(CH_2)_2$-CH_3	1.13
495.	104-51-8	1	0	0	Benzene, butyl-	C_6H_5-$(CH_2)_3$-CH_3	1.13, 25.29
496.	108-90-7	1	0	0	Benzene, chloro-	C_6H_5-Cl	18.4, 21.3
497.	104-83-6	1	0	0	Benzene, 1-chloro-4-(chloromethyl)-		18.4

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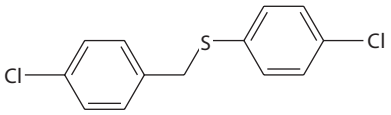
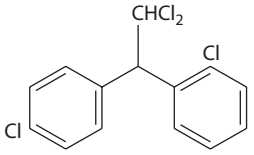
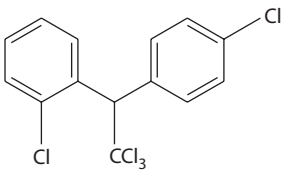
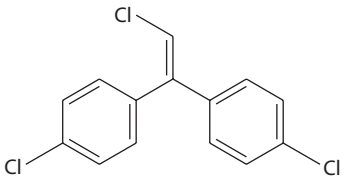
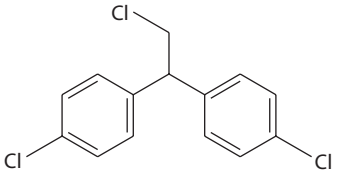
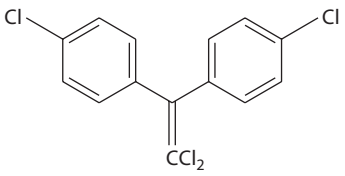
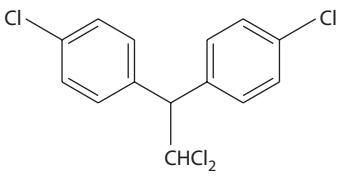
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
498.	22349-74-2	1	0	0	Benzene, 1-chloro-4-(2-chloro-1-phenylethenyl)-		18.4
499.	103-17-3	0	1	0	Benzene, 1-chloro-4-((4-chlorophenyl) methyl)thio- {Chlorobenside®}		18.4, 18.1, 21.3
500.	3424-82-6	1	0	0	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethenyl]-		18.4
501.	53-19-0	1	1	1	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDD, *o.p′*-TDE}		0.4, 18.4, 21.3, 25.29
502.	4329-12-8	1	1	1	Benzene, 1-chloro-3-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*m,p′*-DDD}		0.4, 18.4, 21.3
503.	789-02-6	1	1	1	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDT}		0.4, 18.4, 21.3, 23.5
504.	4541-89-3	1	0	0	Benzene, 1,1′-(chloroethenylidene)bis-		18.4
505.	1022-22-6	1	1	1	Benzene, 1,1′-(chloroethenylidene) bis[4-chloro-{DDM}		18.4, 21.3
506.	2642-80-0	1	1	1	Benzene, 1,1′-(2-chloroethylidene) bis[4-chloro-{DDMS}		18.4, 21.3
507.	622-24-2	0	1	0	Benzene, 2-chloroethyl-	C_6H_5-$(CH_2)_2$-Cl	18.4
508.		0	1	0	Benzene, chloromethoxy- {chloroanisole}		10.2, 18.4
509.	27987-13-9	1	0	0	Benzene, chloromethyl-	C_6H_5-CH_2-Cl	18.4
510.	95-50-1	1	1	1	Benzene, 1,2-dichloro-		18.4
511.	541-73-1	1	0	0	Benzene, 1,3-dichloro-		18.4
512.	106-46-7	1	0	0	Benzene, 1,4-dichloro-		18.4
513.	72-55-9	1	1	1	Benzene, 1,1′-(dichloroethenylidene) bis[4-chloro-{*p,p′*-DDE}		18.4, 21.3, 23.5
514.	27013-25-8	1	0	0	Benzene, 1,1′-(2,2-dichloroethylidene) bis[chloro-		18.4, 21.3

(continued)

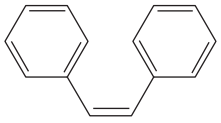
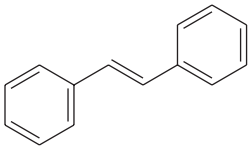
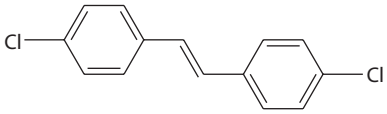
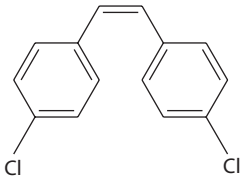
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
515.	72-54-8	1	1	1	Benzene, 1,1′-(2,2-dichloroethylidene) bis[4-chloro-{*p,p′*-DDD, *p,p′*-TDE}		18.4, 21.3
516.	25340-17-4	1	1	1	Benzene, diethyl-		1.13
517.	135-01-3	1	0	0	Benzene, 1,2-diethyl-		1.13
518.	141-93-5	1	0	0	Benzene, 1,3-diethyl-		1.13
519.	105-05-5	1	0	0	Benzene, 1,4-diethyl-		1.13
520.	25550-13-4	1	0	0	Benzene, diethylmethyl-		1.13
521.	27598-81-8	1	0	0	Benzene, dimethoxy-		10.2
522.	1125-88-8	1	0	0	Benzene, dimethoxy-methyl-		10.2
523.	91-16-7	1	1	1	Benzene, 1,2-dimethoxy- {veratrole}		10.2
524.		1	1	1	Benzene, 1,2-dimethoxy-4-ethenyl-		10.2
525.	494-99-5	1	0	0	Benzene, 1,2-dimethoxy-4-methyl-		10.2
526.	93-16-3	1	1	1	Benzene, 1,2-dimethoxy-4-(1-propenyl)-		10.2
527.	151-10-0	0	1	0	Benzene, 1,3-dimethoxy-		10.2
528.	150-78-7	1	1	1	Benzene, 1,4-dimethoxy-		10.2, 24.3, 25.29
529.	14753-08-3	0	1	0	Benzene, 1,4-dimethoxy-2-methyl-5-(1-methylethyl)-		10.2
530.	1330-20-7	1	1	1	Benzene, dimethyl- {xylene}		1.13
531.	29224-55-3	1	0	0	Benzene, dimethylethyl-		1.13
532.	95-47-6	1	1	1	Benzene, 1,2-dimethyl- {*o*-xylene}		1.13
533.	108-38-3	1	1	1	Benzene, 1,3-dimethyl- {*m*-xylene}		1.13
534.	2234-20-0	1	0	0	Benzene, 1,3-dimethyl-2-ethenyl- {2,4-dimethylstyrene}		1.13
535.	1004-66-6	1	0	0	Benzene, 1,3-dimethyl-2-methoxy-		10.2
536.	106-42-3	1	1	1	Benzene, 1,4-dimethyl- {*p*-xylene}		1.13
537.	2039-89-6	1	1	1	Benzene, 1,4-dimethyl-2-ethenyl- {2,5-dimethylstyrene}		1.13
538.	934-80-5	1	0	0	Benzene, 1,2-dimethyl-4-ethyl-		1.13
539.	874-41-9	1	0	0	Benzene, 1,3-dimethyl-4-ethyl-		1.13
540.	1758-88-9	1	0	0	Benzene, 1,4-dimethyl-2-ethyl-		1.13
541.	3459-80-1	0	1	0	Benzene, [(1,1-dimethylethoxy)methyl]-		10.2
542.	98-06-6	1	1	1	Benzene, (1,1-dimethylethyl)-	C_6H_5-$C(CH_3)_3$	1.13
543.	2049-95-8	1	0	0	Benzene, (1,1-dimethylpropyl)-		1.13
544.	81-15-2	0	1	0	Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro- {musk xylene}		16.1
545.	14411-56-4	1	0	0	Benzene, 1-(1,1-dimethylethyl)-3-ethyl-		1.13
546.	83-66-9	0	1	0	Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro-{musk ambrette}		10.2, 16.1
547.	1075-38-3	1	0	0	Benzene,1-(1,1-dimethylethyl)-3-methyl-		1.13
548.		1	0	0	Benzene, 3,5-bis(1,1-dimethylethyl)-1-methyl-		1.13
549.	874-63-5	1	0	0	Benzene, 3,5-dimethyl-1-methoxy-		10.2
550.	644-30-4	0	1	0	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-		1.13
551.	4176-17-4	0	1	0	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-, (R)-		1.13
552.	99-51-4	1	0	0	Benzene, 1,2-dimethyl-4-nitro-		16.1

(*continued*)

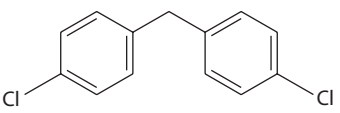
(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
553.	89-58-7	1	0	0	Benzene, 1,4-dimethyl-2-nitro- {2,5-dimethyl-1-nitrobenzene}		16.1
554.	89-87-2	1	0	0	Benzene, 2,4-dimethyl-1-nitro-		16.1
555.	1007-26-7	0	1	0	Benzene, (2,2-dimethylpropyl)-	C_6H_5-CH_2-$C(CH_3)_3$	16.1
556.	103-29-7	1	0	0	Benzene, 1,1′-(1,2-ethanediyl) bis- {bibenzyl}	C_6H_5-CH_2-CH_2-C_6H_5	1.13
557.	588-59-0	1	1	1	Benzene, 1,1′-(1,2-ethenediyl)bis- {stilbene}	C_6H_5-CH═CH-C_6H_5	1.13
558.	645-49-8	1	0	0	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*Z*)-		1.13, 25.29
559.	103-30-0	1	0	0	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*E*)-		1.13, 25.29
560.	5121-74-4	1	1	1	Benzene, 1,1′-(1,2-ethenediyl) bis[4-chloro- {DCS = dichlorostilbene}		18.4, 21.3
561.	1657-56-3	1	1	1	Benzene, 1,1′-(1,2-ethenediyl) bis[4-chloro-, (*E*)- {*trans*-DCS}		18.4, 21.3
562.	2510-74-9	1	0	0	Benzene, 1,1′-(1,2-ethenediyl) bis[4-chloro-, (*Z*)- {*cis*-DCS}		18.4, 21.3
563.	100-42-5	1	1	1	Benzene, ethenyl- {styrene}	C_6H_5-CH═CH_2	1.13, 23.5, 25.29
564.	6380-23-0	1	1	1	Benzene, 4-ethenyl-1,2-dimethoxy-		10.2
565.	27576-03-0	1	0	0	Benzene, ethenyldimethyl-		1.13
566.	28106-30-1	1	0	0	Benzene, ethenylethyl-		1.13
567.	71607-81-3 77227-00-0	1	0	0	Benzene, ethenylethyldimethyl-		1.13
568.	27138-10-9 77220-33-8	1	0	0	Benzene, ethenylethylmethyl-		1.13
569.	637-69-4	1	0	0	Benzene, 1-ethenyl-4-methoxy-		10.2
570.		1	0	0	Benzene, ethenylmethyl-		1.13
571.	611-15-4	1	0	0	Benzene, 1-ethenyl-2-methyl-		1.13
572.	100-80-1	1	0	0	Benzene, 1-ethenyl-3-methyl-		1.13
573.	622-97-9	1	0	0	Benzene, 1-ethenyl-4-methyl-		1.13
574.	71607-82-4 77226-99-4	1	0	0	Benzene, ethenyltetramethyl-		1.13
575.	50976-21-1 77220-32-7	1	0	0	Benzene, ethenyltrimethyl-		1.13
576.	103-73-1	1	0	0	Benzene, ethoxy-	C_6H_5-O-CH_2-CH_3	10.2
577.	5076-72-2	1	0	0	Benzene, 1-ethoxy-4-methoxy-		10.2
578.	100-41-4	1	1	1	Benzene, ethyl-	C_6H_5-CH_2-CH_3	1.13, 25.29
579.	25550-14-5	1	0	0	Benzene, ethylmethyl-		1.13
580.	611-14-3	1	1	1	Benzene, 1-ethyl-2-methyl-		1.13
581.	620-14-4	1	1	1	Benzene, 1-ethyl-3-methyl-		1.13
582.	622-96-8	1	1	1	Benzene, 1-ethyl-4-methyl-		1.13

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
583.	18908-70-8	0	1	0	Benzene, 1-ethyl-2-(1-phenylethyl)-		1.13
584.	18640-62-5	1	0	0	Benzene, 1-ethyl-4-(2-propenyl)-		1.13
585.	536-74-3	1	0	0	Benzene, ethynyl- {phenylacetylene}		1.13
586.		1	0	0	Benzene, 1-(2-hepten-6-yl)-4-methyl-		1.13
587.	118-74-1	0	1	0	Benzene, hexachloro-		18.4, 21.3
588.	1077-16-3	1	0	0	Benzene, hexyl-	C_6H_5-$(CH_2)_5$-CH_3	1.13
589.	622-78-6	0	1	0	Benzene, (isothiocyanatomethyl)-		18.1, 26.9
590.	2257-09-2	0	1	0	Benzene, (2-isothiocyanatoethyl)-		18.1
591.	100-66-3	1	1	1	Benzene, methoxy- {anisole}	C_6H_5-O-CH_3	10.2, 24.3, 25.29
592.	21730-66-5	1	1	1	Benzene, methoxy-, 1-^{14}C, labeled with ^{14}C {anisole-1-^{14}C}		10.2
593.	26897-24-5	0	1	0	Benzene, methoxymethyl- {two isomers detected}		10.2
594.	538-86-3	0	1	0	Benzene, (methoxymethyl)- {benzyl methyl ether}		10.2
595.	578-58-5	1	0	0	Benzene, 1-methoxy-2-methyl- {*o*-methylanisole}		10.2
596.	100-84-5	1	0	0	Benzene, 1-methoxy-3-methyl- {*m*-methylanisole}		10.2
597.	104-93-8	1	1	1	Benzene, 1-methoxy-4-methyl- {*p*-methylanisole}		10.2, 24.3, 25.29
598.	104-46-1	1	1	1	Benzene, 1-methoxy-4-(1-propenyl)- {anethole}		10.2, 24.3
599.	140-67-0	1	0	0	Benzene, 1-methoxy-4-(2-propenyl)- {estragole}		10.2
600.	104-45-0	0	1	0	Benzene, 1-methoxy-4-propyl- {dihydroanethole}		10.2
601.	20469-61-8	1	0	0	Benzene, 1-methoxy-2,3,5-trimethyl-		10.2
602.	3794-96-5	0	1	0	Benzene, 2-methoxy-1-methyl-4-(1-methylethenyl)-		10.2
603.	6379-73-3	0	1	0	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-		10.2
604.	1076-56-8	0	1	0	Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-		10.2
605.	40793-85-9	1	0	0	Benzene, 2-methoxy-1-methyl-4-(1-propenyl)-		10.2
606.	4028-66-4	1	0	0	Benzene, 2-methoxy-1,3,5-trimethyl-		10.2
607.	16277-67-1	0	1	0	Benzene, (3-methoxy-1-propenyl)-		10.2
608.	108-88-3	1	1	1	Benzene, methyl- {toluene}	C_6H_5-CH_3	1.13, 23.5, 25.29
609.	26444-18-8	1	0	0	Benzene, methyl (1-methylethenyl)-		1.13
610.		0	1	0	Benzene, ^{14}C-methyl- {toluene-^{14}C-methyl}		1.13, 25.29
611.	101-81-5	1	0	0	Benzene, 1,1′-methylenebis- {diphenylmethane}	C_6H_5-CH_2-C_6H_5	1.13
612.	101-76-8	1	0	0	Benzene, 1,1′-methylenebis[4-chloro-		18.4
613.	98-83-9	1	0	0	Benzene, (1-methylethenyl)- {α-methylstyrene}	C_6H_5-$C(CH_3)$=CH_2	1.13
614.	98-82-8	1	1	1	Benzene, (1-methylethyl)- {cumene}	C_6H_5-CH=$(CH_3)_2$	1.13

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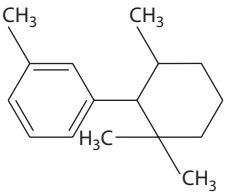
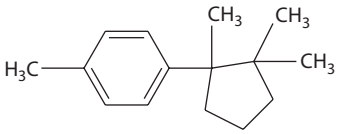
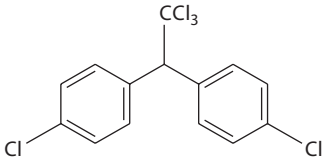
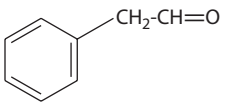
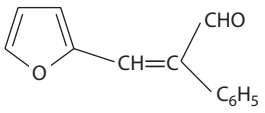
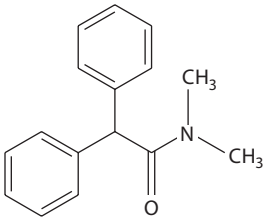
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
615.	1817-47-6	1	0	0	Benzene, 1-(1-methylethyl)-4-nitro- {4-nitrocumene}		16.1
616.	1124-20-5	1	0	0	Benzene, 1-methyl-3-(1-methylethenyl)-		1.13
617.	1195-32-0	1	0	0	Benzene, 1-methyl-4-(1-methylethenyl)- {*p*,α-dimethylstyrene}		1.13
618.	535-77-3	1	1	1	Benzene, 1-methyl-3-(1-methylethyl)- {*m*-cymene}		1.13
619.	99-87-6	1	1	1	Benzene, 1-methyl-4-(1-methylethyl)- {*p*-cymene}		1.13, 24.3, 25.29
620.	88-72-2	1	0	0	Benzene, 1-methyl-2-nitro-		16.1
621.	99-08-1	1	0	0	Benzene, 1-methyl-3-nitro-		16.1
622.	99-99-0	1	0	0	Benzene, 1-methyl-4-nitro-		16.1
623.		1	0	0	Benzene, methylpropenyl-		1.13
624.	17271-70-4	1	0	0	Benzene, 1-methyl-3-(1-propenyl)-		1.13
625.	1074-43-7	1	0	0	Benzene, 1-methyl-3-propyl-		1.13
626.	1074-55-1	1	0	0	Benzene, 1-methyl-4-propyl-		1.13
627.	538-93-2 28729-54-6	1	0	0	Benzene, (2-methylpropyl)-	C_6H_5-CH_2-$CH(CH_3)_2$	1.13
628.	1139-49-7	1	0	0	Benzene, 1-methyl-3-(2,2,6-trimethylcyclohexyl)- {toluene, *m*-(2,2,6-trimethylcyclohexyl)}		1.13
629.	16982-00-6	0	1	0	Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)-		1.13
630.	98-95-3	1	0	0	Benzene, nitro-	C_6H_5-NO_2	16.1, 23.5
631.	15457-05-3	0	1	0	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)-{Fluorodifen®}		16.1, 18.4, 21.3
632.	82-68-8	0	1	0	Benzene, nitropentachloro- {Quintocen®}		16.1, 18.4, 21.3
633.	2189-60-8 71607-64-2	1	0	0	Benzene, octyl- {phenyloctane}	C_6H_5-$(CH_2)_7$-CH_3	1.13
634.	101-84-8	0	1	0	Benzene, 1,1′-oxybis- {diphenyl ether}	C_6H_5-O-C_6H_5	10.2
635.	1579-40-4	1	0	0	Benzene, 1.1′-oxybis[4-methyl- {4-methylphenyl ether}		10.2
636.	103-50-4	1	0	0	Benzene, 1,1′-[oxybis(methylene)] bis- {dibenzyl ether}	C_6H_5-CH_2-O-CH_2-C_6H_5	10.2
637.	55044-97-8	1	0	0	Benzene, 1,1′-[oxybis(methylene)][4-ethyl-		10.2
638.	538-68-1	1	1	1	Benzene, pentyl-	C_6H_5-$(CH_2)_4$-CH_3	1.13
639.	637-50-3	1	1	1	Benzene, 1-propenyl-	C_6H_5-CH═CH-CH_3	1.13
640.	300-57-2	1	0	0	Benzene, 2-propenyl- {allyl benzene}	C_6H_5-CH_2-CH═CH_2	1.13
641.	937-61-1	1	0	0	Benzene, propoxymethyl- {benzyl propyl ether}	C_6H_5-CH_2-O-$CH_2CH_2CH_3$	10.2
642.	103-65-1	1	1	1	Benzene, propyl-	C_6H_5-$(CH_2)_2$-CH_3	1.13, 25.29
643.	673-32-5	1	0	0	Benzene, 1-propynyl-	C_6H_5-C≡C-CH_3	1.13
644.	10147-11-2	1	0	0	Benzene, 2-propynyl-		1.13
645.	938-22-7	0	1	0	Benzene, 1,2,3,5-tetrachloro-4-methoxy-		10.2, 18.4
646.	25619-60-7	1	1	1	Benzene, tetramethyl-		1.13

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
647.	488-23-3	1	0	0	Benzene, 1,2,3,4-tetramethyl-		1.13
648.	527-53-7	1	0	0	Benzene, 1,2,3,5-tetramethyl-		1.13
649.	95-93-2	1	1	1	Benzene, 1,2,4,5-tetramethyl-		1.13
650.	116-29-0	0	1	0	Benzene, 1,2,4-trichloro-5-((4-chlorophenyl) sulfonyl)- {Tetradifon®}		18.1, 18.4, 21.3
651.	50-29-3	1	1	1	Benzene, 1,1′-(2,2,2-trichloroethylidene) bis[4-chloro- {*p,p′*-DDT}		0.4, 18.4, 21.3, 23.5, 25.29
652.	87-40-1	0	1	0	Benzene, 1,3,5-trichloro-2-methoxy-		10.2, 18.4
653.	634-36-6	1	1	1	Benzene, 1,2,3-trimethoxy-		10.2
654.	135-77-3	1	0	0	Benzene, 1,2,4-trimethoxy-		10.2
655.	621-23-8	1	0	0	Benzene, 1,3,5-trimethoxy-		10.2
656.	487-11-6	0	1	0	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-		10.2
657.	2883-98-9	0	1	0	Benzene, 1,2,4-trimethoxy-5-(2-propenyl)-, (*Z*)- {α-Asarone®}		10.2
658.	5273-86-9	0	1	0	Benzene, 1,2,4-trimethoxy-5-(2-propenyl)-, (*E*)- {β-Asarone®}		10.2
659.	25551-13-7	1	1	1	Benzene, trimethyl-		1.13
660.	526-73-8	1	1	1	Benzene, 1,2,3-trimethyl-		1.13
661.	95-63-6	1	1	1	Benzene, 1,2,4-trimethyl- {pseudocumene}		1.13
662.	108-67-8	1	1	1	Benzene, 1,3,5-trimethyl- {mesitylene}		1.13
663.	122-78-1	1	1	1	Benzeneacetaldehyde {phenylacetaldehyde}		3.12, 24.3, 25.29
664.	4411-89-6 55088-52-3	1	1	1	Benzeneacetaldehyde, α-ethylidene- {2-phenyl-2-butenal}		3.12, 24.3, 25.29
665.	57568-60-2	0	1	0	Benzeneacetaldehyde, α-(2-furanylmethylene)-		3.12, 10.2
666.	65545-81-5	0	1	0	Benzeneacetaldehyde, α-(2-furanylmethylene)-, (*E*)-		3.13, 10.2
667.	5031-83-4	0	1	0	Benzeneacetaldehyde, α-(2-phenylethylidene)-		3.12
668.	104-09-6	0	1	0	Benzeneacetaldehyde, 4-methyl-		3.12
669.	103-81-1	1	1	1	Benzeneacetamide {phenylacetamide}	C_6H_5-CH_2-CO-NH_2	13.1
670.	4695-13-0	0	1	0	Benzeneacetamide, α-phenyl-	$(C_6H_5)_2$=CH-CO-NH_2	13.1
671.	957-51-7	1	1	1	Benzeneacetamide, *N,N*-dimethyl-α-phenyl- {diphenamid, Enide®}		13.1, 21.3

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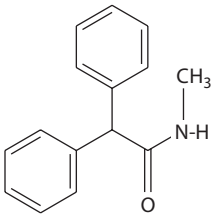
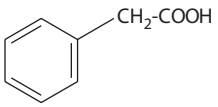
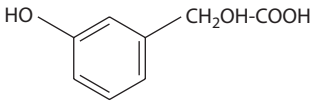
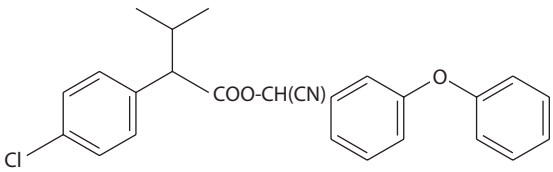
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
672.	954-21-2	1	1	1	Benzeneacetamide, *N*-methyl-α-phenyl- {desmethyl diphenamid}		13.1
673.	103-82-2	1	1	1	Benzeneacetic acid {phenylacetic acid}		4.3, 21.3, 24.3, 25.29
674.		1	1	1	Benzeneacetic acid, labeled with ^{14}C {phenylacetic acid-^{14}C}		4.3, 25.29
675.	122-43-0	0	1	0	Benzeneacetic acid, butyl ester	C_6H_5-CH_2-COO-$(CH_2)_3$-CH_3	5.3
676.	17119-15-2	1	0	0	Benzeneacetic acid, α,3-dihydroxy-		2.5, 4.3, 9.22
677.	1198-84-1	1	0	0	Benzeneacetic acid, α,4-dihydroxy-		2.5, 4.3, 9.22
678.		1	0	0	Benzeneacetic acid, α,?-dihydroxy-ethyl-		2.5, 4.3, 9.22
679.	4412-10-6	0	1	0	Benzeneacetic acid, α-ethylidene-		4.3
680.	20432-26-2	0	1	0	Benzeneacetic acid, α-ethylidene-, (*E*)-		4.3
681.	90-64-2	0	1	0	Benzeneacetic acid, α-hydroxy- {mandelic acid}		2.5, 4.3
682.	51-55-8	0	1	0	Benzeneacetic acid, α-(hydroxymethyl)- (3-endo)-8-methyl-8-azabicyclo[3.2.1] oct-3-yl ester {atropine}		2.5, 5.3
683.	492-37-5	1	0	0	Benzeneacetic acid, α-methyl- {hydratropic acid}		4.3
684.	19988-45-5	1	0	0	Benzeneacetic acid, 2,3-dihydroxy-		4.3, 9.22
685.	614-82-4	1	0	0	Benzeneacetic acid, 2,4-dihydroxy-		4.3, 9.22
686.	451-13-8	1	0	0	Benzeneacetic acid, 2,5-dihydroxy-		4.3, 9.22
687.	102-32-9	1	1	1	Benzeneacetic acid, 3,4-dihydroxy-		4.3, 9.22
688.	4670-09-1	1	0	0	Benzeneacetic acid, 3,5-dihydroxy-		4.3, 9.22
689.	96937-42-7	1	0	0	Benzeneacetic acid, ar,ar-dihydroxy-ar, ar-dimethyl-		4.3, 9.22
690.	96937-37-0	1	0	0	Benzeneacetic acid, ar,α-dihydroxy- ar-ethyl-		2.5, 4.3, 9.22
691.	96937-48-3	1	0	0	Benzeneacetic acid, ar,ar-dihydroxy- ar-methyl-		4.3, 9.22
692.	96937-41-6	1	0	0	Benzeneacetic acid, 3,4-dihydroxy- ar-methyl-		4.3, 9.22
693.	614-75-5	1	1	1	Benzeneacetic acid, 2-hydroxy-		4.3, 9.22
694.	621-37-4	1	1	1	Benzeneacetic acid, 3-hydroxy-		4.3, 9.22
695.	51630-58-1	1	1	1	Benzeneacetic acid, 4-chloro-α- (1-methylethyl)-, cyano (3-phenoxyphenyl)methyl ester {Fenvalerate®}		5.3, 10.2, 11.2, 18.4, 21.3, 25.29

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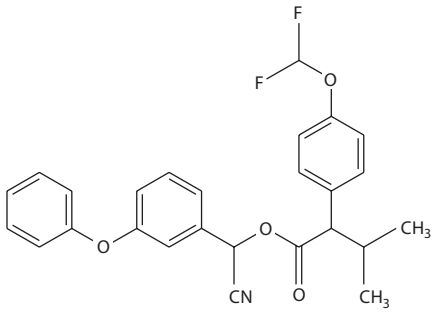
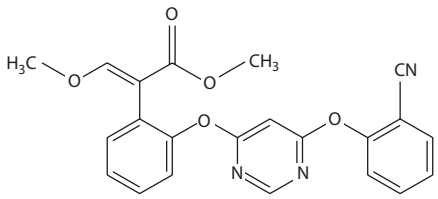
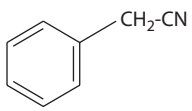
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
696.	70124-77-5	0	1	0	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Flucythrinate®}		5.3, 10.2, 11.2, 18.4, 21.3
697.	156-38-7	1	1	1	Benzeneacetic acid, 4-hydroxy-		4.3, 9.22
698.	306-08-1	1	0	0	Benzeneaceticacid, 4-hydroxy-3-methoxy- {homovanillic acid}		4.3, 9.22, 10.2
699.	102-22-7	0	1	0	Benzeneacetic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl phenylacetate}		5.3
700.	101-97-3	1	1	1	Benzeneacetic acid, ethyl ester {ethyl phenylacetate}	C_6H_5-CH_2-COO-CH_2-CH_3	5.3, 24.3, 25.29
701.	131860-33-8	0	1	0	Benzeneacetic acid, methyl (α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl] oxy]-α-(methoxymethylene)- {Azoxystrobin®}		5.3, 10.2, 11.2, 17.7, 21.3
702.	5421-17-0	0	1	0	Benzeneacetic acid, hexyl ester	C_6H_5-CH_2-COO-$(CH_2)_5$-CH_3	5.3
703.	7782-24-3	1	0	0	Benzeneacetic acid, α-methyl-, (S)-(+)-		4.3
704.	7782-26-5	1	0	0	Benzeneacetic acid, α-methyl-, (R)-(–)-		4.3
705.	101-41-7	1	1	1	Benzeneacetic acid, methyl ester {methyl phenylacetate}	C_6H_5-CH_2-COO-CH_3	5.3, 24.3, 25.29
706.	102-19-2	1	1	1	Benzeneacetic acid, 3-methylbutyl ester		5.3, 24.3, 25.29
707.	101-94-0	0	1	0	Benzeneacetic acid, 4-methylphenyl ester {*p*-tolyl phenylacetate}		5.3
708.	102-13-6	0	1	0	Benzeneacetic acid, 2-methylpropyl ester		5.3
709.	122-45-2	0	1	0	Benzeneacetic acid, octyl ester		5.3
710.1	102-20-5	1	1	1	Benzeneacetic acid, 2-phenylethyl ester	C_6H_5-CH_2-COO-$(CH_2)_2$-C_6H_5	5.3, 24.3, 25.29
711.	102-16-9	0	1	0	Benzeneacetic acid, phenylmethyl ester {benzyl phenylacetate}	C_6H_5-CH_2-COO-CH_2-C_6H_5	5.3
712.	140-29-4	1	1	1	Benzeneacetonitrile {benzyl cyanide}		11.2
713.	14191-95-8	1	0	0	Benzeneacetonitrile, 4-hydroxy-		9.22, 11.2
714.	21850-61-3	1	0	0	Benzeneacetonitrile, 4-hydroxy-α-methyl-		9.22, 11.2
715.		1	0	0	Benzeneacetonitrile, methyl-		11.2
716.	22364-68-7	1	0	0	Benzeneacetonitrile, 2-methyl-		11.2
717.	2947-61-7	1	0	0	Benzeneacetonitrile, 4-methyl-		11.2

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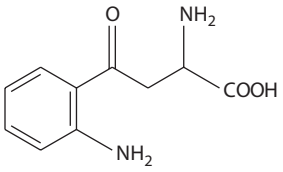
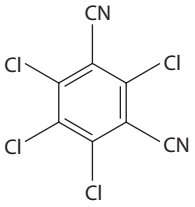
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
718.	343-65-7	0	1	0	Benzenebutanoic acid, α,2-diamino-γ-oxo- {kynurenine}		3.13, 4.3, 12.2
719.	53392-07-7	1	0	0	Benzenebutanol, 4-methyl-		2.5
720.	71607-71-1	1	0	0	Benzenediamine, *N*-methyl-		12.2
721.	95-54-5	1	0	0	1,2-Benzenediamine {*o*-phenylenediamine}		12.2
722.	3171-45-7	1	0	0	1,2-Benzenediamine, 4,5-dimethyl-		12.2
723.	496-72-0	1	0	0	1,2-Benzenediamine, ethyl-		12.2
724.	4760-34-3	1	0	0	1,2-Benzenediamine, *N*-methyl-		12.2
725.	823-40-5	1	0	0	1,3-Benzenediamine, 2-methyl-		12.2
726.	95-80-7	1	0	0	1,3-Benzenediamine, 4-methyl-		12.2
727.	25376-45-8	1	0	0	1,3-Benzenediamine, ar-methyl-		12.2
728.	106-50-3	1	0	0	1,4-Benzenediamine		12.2
729.	623-09-6	1	0	0	1,4-Benzenediamine, *N*-methyl-		12.2
730.	101-54-2	1	0	0	1,4-Benzenediamine, *N*-phenyl-		12.2
731.	140-56-7	0	1	0	Benzenediazosulfonate, dimethylamino-, sodium salt {Fenaminosulf®}		12.2, 18.1, 20.6, 21.3
732.	91-15-6	1	0	0	1,2-Benzenedicarbonitrile		11.2
733.	626-17-5	1	0	0	1,3-Benzenedicarbonitrile		11.2
734.	1897-45-6	0	1	0	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro {Chlorothalonil®}		11.2, 18.4, 21.3, 25.29
735.	623-26-7	1	0	0	1,4-Benzenedicarbonitrile		11.2
736.	88-99-3	1	1	1	1,2-Benzenedicarboxylic acid {phthalic acid}		4.3
737.	121-91-5	1	0	0	1,3-Benzenedicarboxylic acid {isophthalic acid}		4.3
738.	100-21-0	1	1	1	1,4-Benzenedicarboxylic acid {terephthalic acid}		0.4, 4.3
739.	7299-89-0	1	0	0	1,2-Benzenedicarboxylic acid, bis(2-ethylbutyl) ester		5.3
740.	117-81-7	1	1	1	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester		5.3, 23.5
741.	131-20-4 27554-26-3	1	1	1	1,2-Benzenedicarboxylic acid, bis(6-methylheptyl) ester {diisooctyl phthalate}		5.3
742.	84-69-5	0	1	0	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester		5.3
743.	85-69-8	1	1	1	1,2-Benzenedicarboxylic acid, butyl, 2-ethylhexyl ester		5.3
744.		0	1	0	1,2-Benzenedicarboxylic acid, butyl, 2-methylbutyl ester		5.3
745.		0	1	0	1,2-Benzenedicarboxylic acid, butyl, 3-methylbutyl ester		5.3
746.	85-68-7	0	1	0	1,2-Benzenedicarboxylic acid, butyl, phenylmethyl ester		5.3

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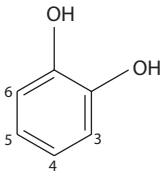
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
747.		1	0	0	1,2-Benzenedicarboxylic acid, dialkyl ester {four isomers detected}		5.3
748.	84-74-2	1	1	1	1,2-Benzenedicarboxylic acid, dibutyl ester {dibutyl phthalate}		5.3, 25.29
749.	84-66-2	1	1	1	1,2-Benzenedicarboxylic acid, diethyl ester {diethyl phthalate}		5.3
750.	3648-21-3	0	1	0	1,2-Benzenedicarboxylic acid, diheptyl {diheptyl phthalate}		5.3
751.	84-75-3	0	1	0	1,2-Benzenedicarboxylic acid, dihexyl ester		5.3
752.	131-11-3	1	1	1	1,2-Benzenedicarboxylic acid, dimethyl ester {dimethyl phthalate}		5.3
753.	117-84-0	1	1	1	1,2-Benzenedicarboxylic acid, dioctyl ester		5.3
754.	131-16-8	1	1	1	1,2-Benzenedicarboxylic acid, dipropyl ester		5.3
755.	1861-32-1	0	1	0	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester {Dichlorthal-dimethyl®, DCPA®}		5.3, 18.4, 21.3
756.		1	0	0	Benzenediol, C_2-alkyl-		9.22
757.		1	0	0	Benzenediol, C_3-alkyl-		9.22
758.	71630-70-1	1	0	0	Benzenediol, ethyl-nitro-		9.22, 16.1
759.	80934-44-7	1	1	1	Benzenediol, methyl-		9.22
760.		1	0	0	Benzenediol, 3-methyl-		9.22
761.		1	0	0	Benzenediol, methyl-nitro-		9.22, 16.1
762.	62726-14-1	1	0	0	Benzenediol, nitro- {at least four isomers were detected}		9.22, 16.1
763.	120-80-9	1	1	1	1,2-Benzenediol {catechol, pyrocatechol}		0.4, 9.22, 23.5
764.	69845-49-4	1	0	0	1,2-Benzenediol, dimethyl-		9.22
765.	2785-75-3	1	0	0	1,2-Benzenediol, 3,5-dimethyl-		9.22
766.	2785-78-6	1	0	0	1,2-Benzenediol, 3,6-dimethyl-		9.22
767.	98-29-3	1	0	0	1,2-Benzenediol, 4-(1,1-dimethylethyl)-		9.22
768.		1	0	0	1,2-Benzenediol, 3-ethenyl-		9.22
769.	6053-02-7	1	1	1	1,2-Benzenediol, 4-ethenyl-		9.22
770.	28930-20-3	1	0	0	1,2-Benzenediol, ethyl-		9.22
771.	933-99-3	1	0	0	1,2-Benzenediol, 3-ethyl-		9.22
772.	1124-39-6	1	0	0	1,2-Benzenediol, 4-ethyl-		9.22
773.	71608-02-1	1	0	0	1,2-Benzenediol, 5-ethyl-3-nitro-		9.22, 16.1
774.	934-00-9	1	1	1	1,2-Benzenediol, 3-methoxy-		9.22, 10.2
775.	28930-19-0	1	0	0	1,2-Benzenediol, methyl-		9.22
776.	488-17-5	1	0	0	1,2-Benzenediol, 3-methyl-		9.22
777.	452-86-8	1	0	0	1,2-Benzenediol, 4-methyl-		9.22
778.	2138-48-9	1	0	0	1,2-Benzenediol, 3-(1-methylethyl)-		9.22
779.	2138-43-4	1	0	0	1,2-Benzenediol, 4-(1-methylethyl)-		9.22
780.	102-29-4	1	0	0	1,2-Benzenediol, monoacetate		5.3, 9.22
781.	6665-98-1	1	0	0	1,2-Benzenediol, 3-nitro-		9.22, 16.1
782.	3316-09-4	1	0	0	1,2-Benzenediol, 4-nitro-		9.22, 16.1
783.	1126-61-0	1	1	1	1,2-Benzenediol, 4-(2-propenyl)-		9.22

(*continued*)

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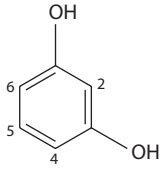
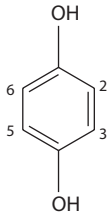
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
784.	29031-84-3	1	0	0	1,2-Benzenediol, propyl-		9.22
785.	2896-63-1	1	0	0	1,2-Benzenediol, 3-propyl-		9.22
786.	2525-02-2	1	0	0	1,2-Benzenediol, 4-propyl-		9.22
787.	108-46-3	1	1	1	1,3-Benzenediol {resorcinol}		9.22, 23.5
788.	25377-27-9	1	0	0	1,3-Benzenediol, dimethyl-		9.22
789.	488-87-9	1	0	0	1,3-Benzenediol, 2,5-dimethyl-		9.22
790.	67965-47-3	1	0	0	1,3-Benzenediol, ethenyl-		9.22
791.		1	0	0	1,3-Benzenediol, ethyl-		9.22
792.	2896-60-8	1	0	0	1,3-Benzenediol, 4-ethyl-		9.22
793.		1	0	0	1,3-Benzenediol, methyl-		9.22
794.	608-25-3	1	0	0	1,3-Benzenediol, 2-methyl-		9.22
795.	504-15-4	1	0	0	1,3-Benzenediol, 5-methyl- {orcinol}		9.22
796.		1	0	0	1,3-Benzenediol, (1-methylethyl)-		9.22
797.	71608-03-2	1	0	0	1,3-Benzenediol, 4-methyl-6-nitro-		9.22, 16.1
798.		1	0	0	1,3-Benzenediol, monoacetate		5.3, 9.22
799.	3163-07-3	1	0	0	1,3-Benzenediol, 4-nitro-		9.22, 16.1
800.	68146-94-1	1	0	0	1,3-Benzenediol, propyl-		9.22
801.	123-31-9	1	1	1	1,4-Benzenediol {hydroquinone}		0.4, 9.22, 23.5
802.		1	0	0	1,4-Benzenediol, dimethyl-		9.22
803.	3233-32-7	1	0	0	1,4-Benzenediol, monoacetate		5.3, 9.22
804.		1	0	0	1,4-Benzenediol, monopropanoate		5.3, 9.22
805.	497-76-7	0	1	0	1,4-Benzenediol, β-*D*-glucopyranoside {arbutin}		2.5, 9.22, 10.2
806.	608-43-5	1	0	0	1,4-Benzenediol, 2,3-dimethyl-		9.22
807.	615-90-7	1	0	0	1,4-Benzenediol, 2,5-dimethyl-		9.22
808.	2349-70-4	1	0	0	1,4-Benzenediol, 2-ethyl- = 1,4-benzenediol, ethyl-		9.22
809.	72693-14-2	1	0	0	1,4-Benzenediol, 2-ethyl-6-methyl-		9.22
810.	824-46-4	1	1	1	1,4-Benzenediol, 2-methoxy-		9.22, 10.2
811.	95-71-6	1	1	1	1,4-Benzenediol, 2-methyl- = 1,4-benzenediol, methyl-		9.22
812.	2349-71-5	0	1	0	1,4-Benzenediol, 2-(1-methylethyl)-		9.22
813.	4693-31-6	1	0	0	1,4-Benzenediol, 2-propyl-		9.22
814.	700-13-0	1	0	0	1,4-Benzenediol, 2,3,5-trimethyl-		9.22
815.	64-04-0	1	1	1	Benzeneethanamine	C_6H_5-CH_2-CH_2-NH_2	12.2, 25.29
816.	582-22-9	1	0	0	Benzeneethanamine, β-methyl-	C_6H_5-$CH(CH_3)$-CH_2-NH_2	12.2
817.	589-08-2	1	1	1	Benzeneethanamine, *N*-methyl-	C_6H_5-CH_2-CH_2-NH-CH_3	12.2
818.	60-12-8	1	1	1	Benzeneethanol {phenethyl alcohol} Occasionally listed as 1321-27-3 Ethanol, phenyl-	C_6H_5-CH_2CH_2-OH	2.5, 24.3, 25.29
819.	5040-23-3	1	0	0	Benzeneethanol, α,4-dimethyl-		2.5
820.	7779-78-4	0	1	0	Benzeneethanol, α-(2-methylpropyl)-		2.5

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
821.	13398-94-2	1	1	1	Benzeneethanol, 3-hydroxy-		2.5, 9.22
822.	501-94-0	1	1	1	Benzeneethanol, 4-hydroxy-		2.5, 9.22
823.	2380-78-1	1	1	1	Benzeneethanol, 4-hydroxy-3-methoxy-		2.5, 9.22, 10.2
824.	699-02-5	0	1	0	Benzeneethanol, 4-methyl-		2.5
825.	100-46-9	1	1	1	Benzenemethanamine {benzylamine}	C_6H_5-CH_2-NH_2	12.2
826.	62924-70-3	0	1	0	Benzenemethanamine, 2-chloro-*N*-(2,6-dinitro-4-(trifluoromethyl) phenyl)-*N*-ethyl-6-fluoro- {Flumetralin®}		12.2, 16.1, 18.4, 21.3
827.	100-51-6	1	1	1	Benzenemethanol {benzyl alcohol}	C_6H_5-CH_2OH	0.4, 2.5, 24.3, 25.29
828.	1197-01-9	1	1	1	Benzenemethanol, α,α,4-trimethyl- {*p*,α,α-trimethylbenzyl alcohol}		2.5, 24.3
829.	617-94-7	1	1	1	Benzenemethanol, α,α-dimethyl-	C_6H_5-$C(CH_3)_2OH$	2.5
830.	536-50-5	0	1	0	Benzenemethanol, α,4-dimethyl-		2.5, 24.3
831.	4393-06-0	0	1	0	Benzenemethanol, α-ethenyl-	C_6H_5-$CH(CH{=}CH_2)OH$	2.5
832.	93-54-9	0	1	0	Benzenemethanol, α-ethyl- {1-phenyl-1-propanol}	C_6H_5-$CH(C_2H_5)OH$	2.5
833.	5349-60-0	0	1	0	Benzenemethanol, α-ethyl-4-methoxy- {1-(4-methoxyphenyl)-1-propanol}		2.5, 10.2
834.	98-85-1	1	1	1	Benzenemethanol, α-methyl-	C_6H_5-$CH(CH_3)OH$	2.5, 24.3
835.	93-92-5	0	1	0	Benzenemethanol, α-methyl-, acetate		5.3
836.	93-03-8	0	1	0	Benzenemethanol, 3,4-dimethoxy-		2.5, 10.2
837.	13651-14-4	1	0	0	Benzenemethanol, 2,3-dimethyl-		2.5
838.	30923-59-2	0	1	0	Benzenemethanol, 2-hydroxy-, α-benzoate		2.5, 5.3
839.	89-95-2	1	1	1	Benzenemethanol, 2-methyl-		2.5
840.	620-24-6	1	1	1	Benzenemethanol, 3-hydroxy-		2.5, 9.22
841.	623-05-2	1	1	1	Benzenemethanol, 4-hydroxy-		2.5, 9.22
842.	498-00-0	1	1	1	Benzenemethanol, 4-hydroxy-3-methoxy-		2.5, 9.22, 10.2
843.	105-13-5	0	1	0	Benzenemethanol, 4-methoxy- {anisyl alcohol}		2.5, 10.2, 24.3
844.	104-21-2	1	1	1	Benzenemethanol, 4-methoxy-, acetate {anisyl acetate}		5.3, 10.2, 24.3, 25.29
845.	122-91-8	0	1	0	Benzenemethanol, 4-methoxy-, formate		5.3, 10.2
846.	102-17-0	0	1	0	Benzenemethanol, 4-methoxy-, phenylacetate		5.3, 10.2
847.	7549-33-9	0	1	0	Benzenemethanol, 4-methoxy-, propanoate		5.3, 10.2
848.	589-18-4	0	1	0	Benzenemethanol, 4-methyl-		2.5
849.	6282-37-7	1	0	0	Benzenemethanol, 4-methyl-α-propyl-		2.5
850.	1331-81-3	0	1	0	Benzenemethanol, ar-methoxy-		2.5, 10.2
851.	27043-34-1	1	0	0	Benzenemethanol, methyl-		2.5
852.	104-53-0	0	1	0	Benzenepropanal	C_6H_5-CH_2CH_2-CH═O	3.12
853.	80638-48-8	1	1	1	Benzenepropanal, 4-hydroxy-3-methoxy-		3.12, 9.22, 10.2
854.	103-95-7	0	1	0	Benzenepropanal, α-methyl-4-(1-methylethyl)- {cyclamen aldehyde}		3.12
855.	102-93-2	1	1	1	Benzenepropanamide	C_6H_5-CH_2CH_2-$CONH_2$	13.1
856.	121850-61-1	0	1	0	Benzenepropanamide, *N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl] amino]butyl]amino]propyl]-3,4-dihydroxy-		9.22, 12.2, 13.1
857.	645-59-0	1	0	0	Benzenepropanenitrile	C_6H_5-CH_2CH_2-CN	11.2

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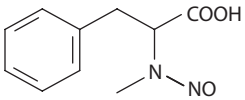
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
858.	501-52-0	1	1	1	Benzenepropanoic acid {3-phenylpropionic acid or hydrocinnamic acid}	C_6H_5-CH_2CH_2-COOH	4.3, 24.3, 25.29
859.	156-05-8	0	1	0	Benzenepropanoic acid, α-hydroxy- {phenyllactic acid}	C_6H_5-CH_2-CH_2OH-COOH	2.5, 4.3
860.	7326-19-4	0	1	0	Benzenepropanoic acid, α-hydroxy-, (R)-		2.5, 4.3
861.	4593-90-2	1	0	0	Benzenepropanoic acid, β-methyl-		4.3
862.	156-06-9	0	1	0	Benzenepropanoic acid, α-oxo- {phenylpyruvic acid}	C_6H_5-CH_2-CO-COOH	4.3
863.	24696-05-7	0	1	0	Benzenepropanoic acid, 2-(β-*D*-glucopyranosyloxy)-		2.5, 4.3, 10.2
864.		1	0	0	Benzenepropanoic acid, dihydroxy-methoxy-		4.3, 9.22, 10.2
865.		1	1	1	Benzenepropanoic acid, 2-(methylnitrosoamino)-		4.3, 12.2, 15.8
866.	3714-73-6	1	0	0	Benzenepropanoic acid, 2,3-dihydroxy-		4.3, 9.22
867.	96937-38-1	1	0	0	Benzenepropanoic acid, 2,3-dihydroxy-ar-methyl-		4.3, 9.22
868.	5631-68-5	1	0	0	Benzenepropanoic acid, 2,4-dihydroxy-		4.3, 9.22
869.	10538-47-3	1	1	1	Benzenepropanoic acid, 2,5-dihydroxy-		4.3, 9.22
870.	96937-34-7	1	0	0	Benzenepropanoic acid, 2,5-dihydroxy-ar-methyl-		4.3, 9.22
871.	98114-50-2	1	0	0	Benzenepropanoic acid, 2,6-dihydroxy-		4.3, 9.22
872.	495-78-3	1	1	1	Benzenepropanoic acid, 2-hydroxy-		4.3, 9.22
873.	1078-61-1	1	1	1	Benzenepropanoic acid, 3,4-dihydroxy- {dihydrocaffeic acid}		4.3, 9.22
874.	96961-47-6	1	0	0	Benzenepropanoic acid, 3,4-dihydroxy-2,5,6-trimethyl-		4.3, 9.22
875.	96937-33-6	1	0	0	Benzenepropanoic acid, 3,4-dihydroxy-ar-methyl-		4.3, 9.22
876.	26539-01-5	1	0	0	Benzenepropanoic acid, 3,5-dihydroxy-		4.3, 9.22
877.	621-54-5	1	1	1	Benzenepropanoic acid, 3-hydroxy-		4.3, 9.22
878.	501-97-3	1	1	1	Benzenepropanoic acid, 4-hydroxy-		4.3, 9.22
879.	156-39-8	1	0	0	Benzenepropanoicacid, 4-hydroxy-α-oxo-		4.3, 9.22
880.	5597-50-2	1	0	0	Benzenepropanoic acid, 4-hydroxy-, methyl ester		5.3, 9.22
881.	1135-23-5	1	0	0	Benzenepropanoic acid, 4-hydroxy-3-methoxy- {hydroferulic acid}		4.3, 9.22, 10.2
882.	96937-36-9	1	0	0	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methoxy-		4.3, 9.22, 10.2
883.	96937-35-8	1	0	0	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methyl-		4.3, 9.22
884.	122-97-4	1	1	1	Benzenepropanol {3-phenyl-1-propanol}	C_6H_5-CH_2-CH_2-CH_2OH	2.5, 24.3, 25.29
885.	1992-50-3	1	0	0	Benzenepropanol, α-ethyl-	C_6H_5-CH_2-CH_2-CH(C_2H_5)OH	2.5
886.	2845-25-2	1	0	0	Benzenepropanol, γ-ethyl-, (S)-	C_6H_5-CH(C_2H_5)-CH_2-CH_2OH	2.5
887.	10210-17-0	1	0	0	Benzenepropanol, 4-hydroxy-		2.5, 9.22
888.	19044-88-3	0	1	0	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro- {Oryzalin®}		12.2, 16.1, 18.1, 21.3

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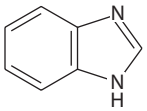
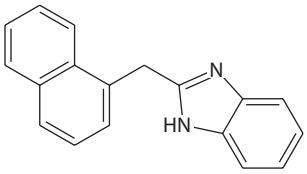
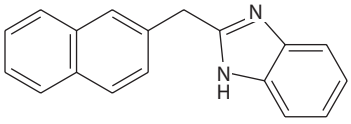
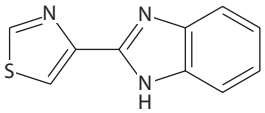
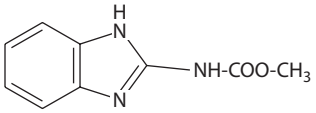
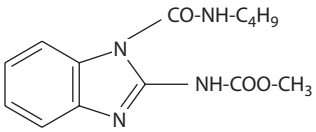
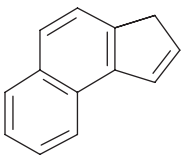
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
889.	108-98-5	1	0	0	Benzenethiol {phenyl mercaptan}	C_6H_5-SH	18.1
890.	87-66-1	1	1	1	1,2,3-Benzenetriol {pyrogallol}		9.22
891.	533-73-3	1	0	0	1,2,4-Benzenetriol {hydroxyhydroquinone}		9.22
892.		1	0	0	1,2,4-Benzenetriol, methyl-		9.22
893.	51-17-2	1	0	0	1*H*-Benzimidazole		17.21
894.		1	0	0	1*H*-Benzimidazole, C_2-alkyl-		17.21
895.	5851-44-5	1	0	0	1*H*-Benzimidazole, 2-butyl-		17.21
896.	72692-74-1	1	0	0	1*H*-Benzimidazole, dimethyl-		17.21
897.	2876-08-6	1	0	0	1*H*-Benzimidazole, 1,2-dimethyl-		17.21
898.	582-60-5	1	0	0	1*H*-Benzimidazole, 5,6-dimethyl-		17.21
899.	72692-75-2	1	0	0	1*H*-Benzimidazole, ethyl-		17.21
900.	30304-58-6	1	0	0	1*H*-Benzimidazole, methyl-		17.21
901.	7035-68-9	1	0	0	1*H*-Benzimidazole, 1-ethyl-		17.21
902.	1848-84-6	1	0	0	1*H*-Benzimidazole, 2-ethyl-		17.21
903.		1	0	0	1*H*-Benzimidazole, 2-(2-ethylphenylmethyl)-		17.21
904.	1632-83-3	1	0	0	1*H*-Benzimidazole, 1-methyl-		17.21
905.	615-15-6	1	0	0	1*H*-Benzimidazole, 2-methyl-		17.21
906.	946-18-9	1	0	0	1*H*-Benzimidazole, 2-(3-methylbutyl)-		17.21
907.	42268-60-0	1	0	0	1*H*-Benzimidazole, 2-(1-naphthalenylmethyl)-		17.21
908.	82326-40-7	1	0	0	1*H*-Benzimidazole, 2-(2-naphthalenylmethyl)-		17.21
909.	5851-46-7	1	0	0	1*H*-Benzimidazole, 2-pentyl-		17.21
910.	148-79-8	1	1	1	1*H*-Benzimidazole, 2-(4-thiazolyl)- {Thiabendazole®}		17.23, 18.1, 21.3, 25.29
911.	3363-56-2	0	1	0	1*H*-Benzimidazole, 2,5,6-trimethyl-		17.21
912.	10605-21-7	0	1	0	1*H*-Benzimidazole-2-carbamic acid, methyl ester {Carbendazim®}		5.3, 21.3, 25.29
913.	17804-35-2	0	1	0	1*H*-Benzimidazole-2-carbamic acid, 1-(butylcarbamoyl)-, methyl ester {Benomyl®}		5.3, 21.3, 25.29
914.	232-54-2	1	0	0	1*H*-Benz[*e*]indene		1.20

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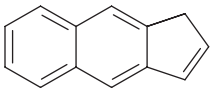
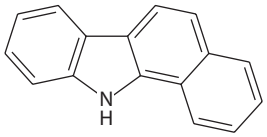
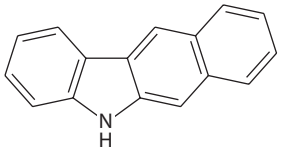
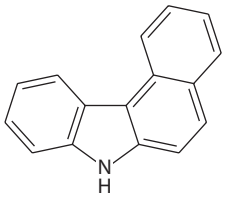
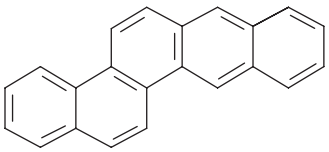
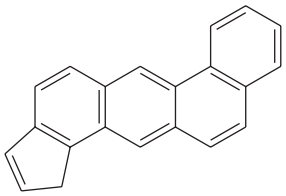
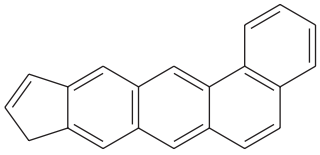
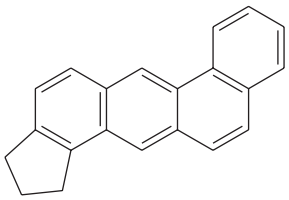
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
915.		1	0	0	1*H*-Benz[*e*]indene, dimethyl-		1.20
916.		1	0	0	1*H*-Benz[*e*]indene, ethylmethyl-		1.20
917.	64031-90-9	1	0	0	1*H*-Benz[*e*]indene, methyl-		1.20
918.	268-40-6	1	0	0	1*H*-Benz[*f*]indene		1.20
919.	60826-71-3	1	0	0	1*H*-Benz[*f*]indene, dimethyl-		1.20
920.	71265-34-4	1	0	0	1*H*-Benz[*f*]indene, ethylmethyl-		1.20
921.	60826-63-3	1	0	0	1*H*-Benz[*f*]indene, methyl-		1.20
922.	67526-84-5	1	0	0	Benzocarbazole		17.21
923.	64859-55-8	1	0	0	Benzocarbazole, dimethyl-		17.21
924.	64859-54-7	1	0	0	Benzocarbazole, methyl-		17.21
925.	239-01-0	1	0	0	11*H*-Benzo[*a*]carbazole		17.21
926.	243-28-7	1	0	0	5*H*-Benzo[*b*]carbazole		17.21
927.	205-25-4	1	0	0	7*H*-Benzo[*c*]carbazole		17.21
928.	57827-84-6	1	0	0	Benzochrysene		17.21
929.	214-17-5	1	0	0	Benzo[*b*]chrysene {dibenzo[*b,h*] phenanthrene}		1.20
930.	146506-80-1	1	0	0	Benzo[*g*]chrysene, methyl-		1.20
931.	240-44-8	1	0	0	1*H*-Benzo[*a*]cyclopent[*h*]anthracene		1.20
932.	226-78-8	1	0	0	9*H* Benzo[*a*]cyclopenta[*i*]anthracene		1.20
933.	7099-43-6	1	0	0	1*H*-Benzo[*a*]cyclopent[*h*]anthracene, 2,3-dihydro- {5,6-cyclopentano-1,2-benzanthracene, 2,3-dihydro-}		1.20

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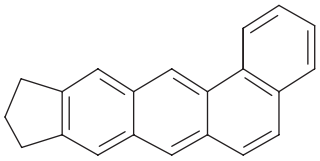
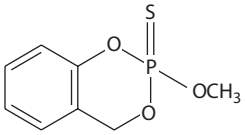
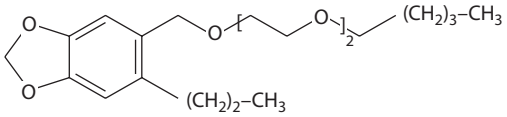
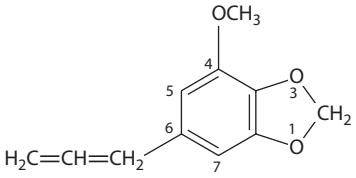
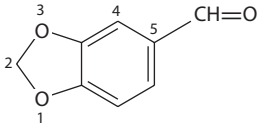
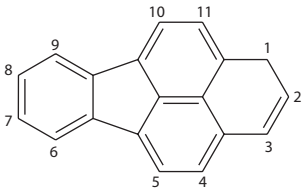
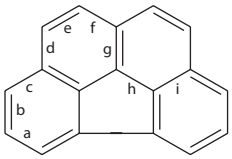
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
934.	7099-42-5	1	0	0	9*H*-Benzo[*a*]cyclopent[*i*]anthracene, 10,11-dihydro- {6,7-cyclopentano-1, 2-benzanthracene, 9,10-dihydro-}		1.20
935.	3811-49-2	0	1	0	4*H*-1,3,2-Benzodioxaphosphorin-2-sulfide, 2-methoxy- {Salithion®}		10.2, 18.1, 21.3
936.	51-03-6	0	1	0	1,3-Benzodioxole, 5-[[2-(2-butoxyethoxy) ethoxy]methyl]-6-propyl- {piperonyl butoxide}		10.2, 21.3
937.	607-91-0	1	1	1	1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)- {myristicin}		10.2
938.	94-59-7	0	1	0	1,3-Benzodioxole, 5-(2-propenyl)- {safrole}		10.2
939.	120-57-0	1	1	1	1,3-Benzodioxole-5-carboxaldehyde {piperonal, heliotropin}		3.12, 10.2, 24.3, 25.29
940.	56832-73-6	1	0	0	Benzofluoranthene		1.20
941.		1	0	0	Benzofluoranthene, dimethyl-		1.20
942.		1	0	0	Benzofluoranthene, ethyl-		1.20
943.	73020-30-1	1	0	0	Benzofluoranthene, methyl-		1.20
944.	16135-81-2 42126-84-1	1	0	0	11*H*-Benzo[*cd*]fluoranthene		1.20
945.	203-12-3	1	0	0	Benzo[*ghi*]fluoranthene		1.20
946.	64760-14-1	1	0	0	Benzo[*ghi*]fluoranthene, dimethyl-		1.20
947.	71265-35-5	1	0	0	Benzo[*ghi*]fluoranthene, ethyl-		1.20
948.	51001-44-6	1	0	0	Benzo[*ghi*]fluoranthene, methyl-		1.20
949.	71265-21-9	1	0	0	Benzo[*ghi*]fluoranthene, 1-methyl-		1.20
950.	71265-22-0	1	0	0	Benzo[*ghi*]fluoranthene, 2-methyl-		1.20
951.	71265-23-1	1	0	0	Benzo[*ghi*]fluoranthene, 3-methyl-		1.20

(*continued*)

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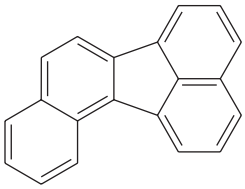
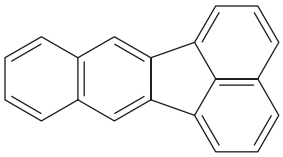
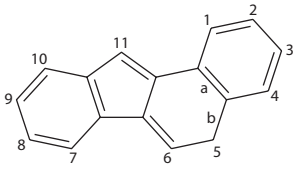
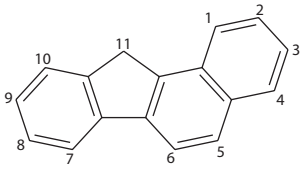
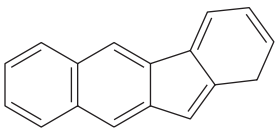
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
952.	71265-24-2	1	0	0	Benzo[*ghi*]fluoranthene, 4-methyl- {also known as 7-methylbenzo[*ghi*] fluoranthene}		1.20
953.	205-82-3	1	1	1	Benzo[*j*]fluoranthene		1.20, 23.5
954.	60826-67-7	1	0	0	Benzo[*j*]fluoranthene, methyl-		1.20
955.	207-08-9	1	1	1	Benzo[*k*]fluoranthene		1.20, 23.5
956.	41637-93-8	1	0	0	Benzo[*k*]fluoranthene, methyl-		1.20
957.	61089-87-0	1	0	0	Benzofluorene		1.20
958.		1	0	0	Benzofluorene, alkyl-		1.20
959.	77271-50-2	1	0	0	Benzofluorene, dimethyl- {at least threeisomers in MSS}		1.20
960.	60918-47-0	1	0	0	Benzofluorene, methyl- {at least four isomers in MSS}		1.20
961.	77271-51-3	1	0	0	Benzofluorene, tetramethyl- {at least two isomers in MSS}		1.20
962.	77271-52-4	1	0	0	Benzofluorene, trimethyl-		1.20
963.	30777-18-5	1	0	0	Benzo[*a*]fluorene		1.20
964.	238-82-4	1	0	0	1*H*-Benzo[*a*]fluorene		1.20
965.	238-79-9	1	0	0	5*H*-Benzo[*a*]fluorene		1.20
966.	238-84-6	1	0	0	11*H*-Benzo[*a*]fluorene		1.20
967.		1	0	0	11*H*-Benzo[*a*]fluorene, dimethyl-		1.20
968.	60826-64-4	1	0	0	11*H*-Benzo[*a*]fluorene, methyl-		1.20
969.	54811-53-9	1	0	0	11*H*-Benzo[*a*]fluorene, 9-methyl-		1.20
970.	71265-25-3	1	0	0	11*H*-Benzo[*a*]fluorene, 11-methyl-		1.20
971.	71607-85-7	1	0	0	11*H*-Benzo[*a*]fluorene, trimethyl- {at least three isomers in MSS}		1.20
972.	14458-76-5	1	0	0	1*H*-Benzo[*b*]fluorene		1.20
973.	30777-19-6	1	0	0	5*H*-Benzo[*b*]fluorene		1.20

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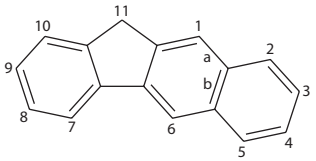
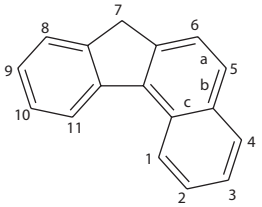
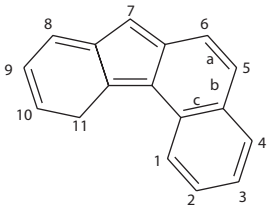
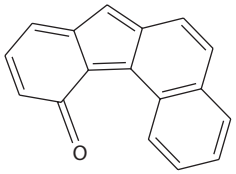
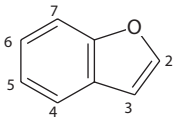
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
974.	243-17-4	1	0	0	11*H*-Benzo[*b*]fluorene		1.20
975.	60826-65-5	1	0	0	11*H*-Benzo[*b*]fluorene, methyl-		1.20
976.		1	0	0	11*H*-Benzo[*b*]fluorene, 9-methyl-		1.20
977.	77271-81-0	1	0	0	Benzo[*c*]fluorene, methyl-		1.20
978.	205-12-9	1	0	0	7*H*-Benzo[*c*]fluorene		1.20
979.	60826-66-6	1	0	0	7*H*-Benzo[*c*]fluorene, methyl-		1.20
980.	73492-01-0	1	0	0	11*H*-Benzo[*c*]fluorene		1.20
981.	479-79-8	1	0	0	11*H*-Benzo[*c*]fluoren-11-one		3.13
982.	271-89-6	1	1	1	Benzofuran {benzo[*b*]furan, coumarone}		10.2, 23.5
983.	25586-39-4	1	0	0	Benzofuran, dimethyl- {three isomers detected}		10.2
984.	58924-34-8	1	0	0	Benzofuran, ethyl-		10.2
985.	71265-37-7	1	0	0	Benzofuran, ethyldimethyl-		10.2
986.	25586-38-3	1	0	0	Benzofuran, methyl- {three isomers detected}		10.2
987.	13054-97-2	1	0	0	Benzofuran, octahydro-		10.2
988.	71265-38-8	1	0	0	Benzofuran, pentamethyl-		10.2
989.	36618-49-2	1	0	0	Benzofuran, tetramethyl-		10.2
990.	36541-17-0	1	0	0	Benzofuran, trimethyl-		10.2
991.	496-16-2	1	1	1	Benzofuran, 2,3-dihydro- {coumaran}		10.2
992.	71265-36-6	1	0	0	Benzofuran, 2,3-dihydromethyl-		10.2
993.	1746-11-8	0	1	0	Benzofuran, 2,3-dihydro-2-methyl-		10.2
994.	3782-00-1 28715-26-6	1	0	0	Benzofuran, 2,3-dimethyl-		10.2
995.	3131-63-3	1	0	0	Benzofuran, 2-ethyl-		10.2

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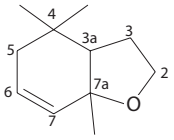
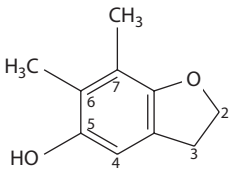
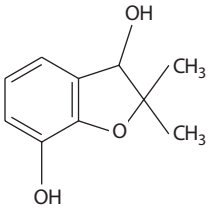
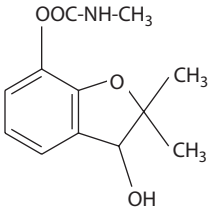
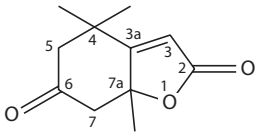
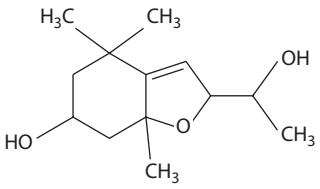
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
996.		1	0	0	Benzofuran, 2,3,3a,4,5,7a-hexahydro-4,4,7a-trimethyl-		10.2
997.	4265-25-2	1	0	0	Benzofuran, 2-methyl-		10.2
998.	36724-24-0	1	0	0	Benzofuran, 3-ethyl-		10.2
999.	21535-97-7	1	0	0	Benzofuran, 3-methyl-		10.2
1000.	17059-52-8	1	0	0	Benzofuran, 5-methyl-		10.2
1001.	494-90-6	1	0	0	Benzofuran, 4,5,6,7-tetrahydro-3,6-dimethyl-		10.2
1002.		1	0	0	Benzofuran, 4-hydroxy-5,6-dimethyl-		9.22, 10.2
1003.	60026-12-2	1	1	1	Benzofuran, 5-hydroxy-6,7-dimethyl-		9.22, 10.2
1004.	35355-35-2	0	1	0	Benzofuran, 5-methoxy-6,7-dimethyl-		10.2
1005.	4265-16-1	1	0	0	2-Benzofurancarboxaldehyde		3.12, 10.2
1006.	17781-15-6	0	1	0	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-		2.5, 9.22, 10.2
1007.	16655-82-6	1	1	1	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate) {3-hydroxycarbofuran®}		2.5, 5.3, 10.2, 13.1, 21.3
1008.		1	0	0	1,3-Benzofurandione, 5-(1,1-dimethylheptyl)-		3.13, 7.1
1009.	31297-30-0	1	0	0	2,3-Benzofurandione, 2,3-dihydro-4,7-dimethyl-		3.13, 6.3
1010.	19355-58-9	0	1	0	2,6-Benzofurandione, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-		3.13, 6.3
1011.	73051-72-6	0	1	0	2-Benzofuranmethanol, 2,4,5,6,7,7a-hexahydro-6-hydroxy-α,4,4,7a-tetramethyl-		2.5, 10.2
1012.		0	1	0	2-Benzofuranmethanol, 2,4,5,7a-tetrahydro-4,4,7a-trimethyl-		2.5, 10.2
1013.		0	1	0	6-Benzofuranol, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl-		2.5, 10.2

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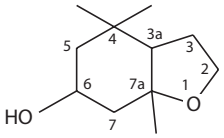
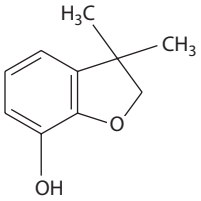
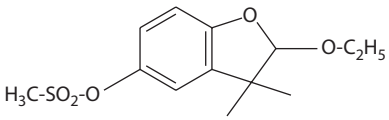
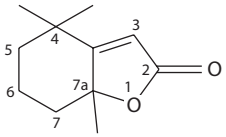
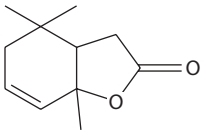
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1014.	39815-67-3	0	1	0	6-Benzofuranol,octahydro-4,4,7a-trimethyl-		2.5, 10.2
1015.	1563-38-8	0	1	0	7-Benzofuranol,2,3-dihydro-2,2-dimethyl-		9.22, 10.2
1016.	26225-79-6	0	1	0	7-Benzofuranol, 2,3-dihydro-3,3-dimethyl-2-ethoxy-, methanesulfonate {Ethofumesate®}		10.2, 18.1, 21.3
1017.	13341-72-5	0	1	0	Benzofuranone, dimethyltetrahydro-		6.3
1018.		1	0	0	Benzofuranone, methyl-		6.3
1019.	553-86-6	1	0	0	2(3*H*)-Benzofuranone		6.3
1020.	6051-03-2	1	0	0	2(3*H*)-Benzofuranone, hexahydro-		6.3
1021.	61892-48-6	1	0	0	2(3*H*)-Benzofuranone, hexahydro-3a-hydroxy-		2.5, 6.3
1022.	54911-63-6	1	0	0	2(3*H*)-Benzofuranone, hexahydro-4-hydroxy-		2.5, 6.3
1023.	16778-27-1	1	1	1	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl- {mariolide, dihydroactinidiolide}		6.3
1024.	37531-06-9	0	1	0	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-, (*Z*)-		6.3
1025.	37531-07-0	0	1	0	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-, (*E*)-		6.3
1026.	19432-10-1	0	1	0	2(3*H*)-Benzofuranone, octahydro-4,4,7a-trimethyl- {tetrahydroactinidiolide}		6.3
1027.	19432-09-8	1	1	1	2(3*H*)-Benzofuranone, 3a,4,5,7a-tetrahydro-4,4,7a-trimethyl-, *cis*-		6.3
1028.	75840-26-5	0	1	0	2(4*H*)-Benzofuranone, 5,6-dihydro-3,6-dimethyl-		6.3
1029.	17063-17-1	0	1	0	2(4*H*)-Benzofuranone, 5,7a-dihydro-4,4,7a-trimethyl-, (R)-		6.3
1030.	82395-89-9	0	1	0	2(4*H*)-Benzofuranone, 6-(β-*D*-glucopyranosyloxy)-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-		1.5, 6.3, 8.3
1031.	1133-03-5	0	1	0	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-		2.5, 6.3
1032.	10481-90-0	0	1	0	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, *Z*-(±)- {loliolide}		2.5, 6.3
1033.	5989-02-6	1	1	1	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-,(6S-*Z*)-		2.5, 6.3

(*continued*)

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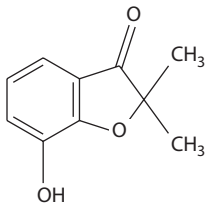
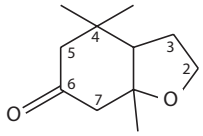
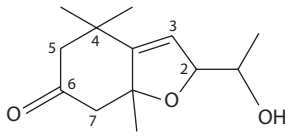
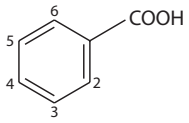
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1034.	19432-05-4 38725-47-2	0	1	0	2(4*H*)-Benzofuranone, tetrahydro-4,4,7a-trimethyl-		6.3
1035.	15356-74-8	1	1	1	2(4*H*)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-		6.3
1036.	17092-92-1	1	1	1	2(4*H*)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-,(R)-		6.3
1037.	124052-02-4	0	1	0	3(2*H*)-Benzofuranone, 2-(3,4-dihydroxyphenyl)-2,4,6-trihydroxy-		3.13, 9.22
1038.	17781-16-7	0	1	0	3(2*H*)-Benzofuranone, 7-hydroxy-2,2-dimethyl-		3.13, 9.22, 10.2
1039.	117769-21-8	0	1	0	5(4*H*)-Benzofuranone, 2,7a-dihydro-2-(1-hydroxyethyl)-4,4-dimethyl-		2.5, 3.13, 10.2
1040.	39815-70-8	0	1	0	6(2*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-		3.13, 10.2
1041.	70875-03-5	0	1	0	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl-		2.5, 3.13, 10.2
1042.	39815-73-1	0	1	0	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-		3.13, 10.2
1043.	65-85-0	1	1	1	Benzoic acid {benzenecarboxylic acid}		0.4, 4.3, 24.3, 25.29
1044.	50-78-2	0	1	0	Benzoic acid, 2-acetoxy-		4.3, 5.3
1045.	136-60-7	1	0	0	Benzoic acid, butyl ester	C_6H_5-COO-$(CH_2)_3$-CH_3	5.3
1046.	96937-46-1	1	0	0	Benzoic acid, dihydroxy-dimethyl-		4.3, 9.22
1047.	96937-47-2	1	0	0	Benzoic acid, dihydroxyethyl-		4.3, 9.22
1048.	96937-44-9	1	0	0	Benzoic acid, dimethyl-hydroxy-		4.3, 9.22
1049.	93-89-0	1	0	0	Benzoic acid, ethyl ester {ethyl benzoate}	C_6H_5-COO-CH_2-CH_3	5.3, 24.3, 25.29
1050.	96937-43-8	1	0	0	Benzoic acid, ethyl-hydroxy-		4.3, 9.22
1051.	6789-88-4	0	1	0	Benzoic acid, hexyl ester	C_6H_5-COO-$(CH_2)_5$-CH_3	5.3
1052.	87323-67-9	1	0	0	Benzoic acid, hydroxymethoxy-		4.3, 9.22, 10.2
1053.	28965-86-8	1	0	0	Benzoic acid, hydroxymethyl-		4.3, 9.22
1054.	25567-10-6	1	0	0	Benzoic acid, methyl- {toluic acid}		4.3
1055.	93-58-3	1	1	1	Benzoic acid, methyl ester {methyl benzoate}	C_6H_5-COO-CH_3	5.3, 24.3, 25.29
1056.	2049-96-9	1	0	0	Benzoic acid, pentyl ester {amyl benzoate}	C_6H_5-COO-$(CH_2)_4$-CH_3	5.3

(continued)

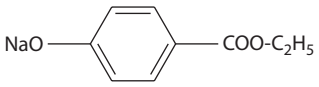
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1057.	93-99-2	0	1	0	Benzoic acid, phenyl ester	C_6H_5-COO-C_6H_5	5.3
1058.	120-51-4	1	1	1	Benzoic acid, phenylmethyl ester {benzyl benzoate}	C_6H_5-COO-CH_2-C_6H_5	5.3, 24.3, 25.29
1059.	2315-68-6	1	1	1	Benzoic acid, propyl ester	C_6H_5-COO-$(CH_2)_2$-CH_3	5.3
1060.	532-32-1	0	1	0	Benzoic acid, sodium salt		20.6
1061.	118-92-3	0	1	0	Benzoic acid, 2-amino- {anthranilic acid}		4.3, 12.2
1062.	7756-96-9	0	1	0	Benzoic acid, 2-amino-, butyl ester		5.3, 12.2
1063.	87-25-2	0	1	0	Benzoic acid, 2-amino-, ethyl ester		5.3, 12.2
1064.	134-20-3	0	1	0	Benzoic acid, 2-amino-, methyl ester {methyl anthranilate}		5.3, 12.2, 24.3
1065.	612-19-1	1	0	0	Benzoic acid, 2-ethyl-		4.3
1066.	10366-91-3	0	1	0	Benzoicacid, 2-(β-*D*-glucopyranosyloxy)-		2.5, 4.3, 8.3, 10.2
1067.	612-20-4	1	0	0	Benzoic acid, 2-(hydroxymethyl)-		2.5, 4.3
1068.	85-91-6	0	1	0	Benzoic acid, 2-(methylamino)-, methyl ester		5.3, 12.2
1069.	69-72-7	1	1	1	Benzoic acid, 2-hydroxy-{salicylic acid}		4.3, 9.22
1070.	2052-14-4	0	1	0	Benzoic acid, 2-hydroxy-, butyl ester		5.3, 9.22
1071.	118-61-6	0	1	0	Benzoic acid, 2-hydroxy-, ethyl ester {ethyl salicylate}		5.3, 9.22, 24.3, 25.29
1072.	6259-76-3	0	1	0	Benzoic acid, 2-hydroxy-, hexyl ester		5.3, 9.22
1073.	119-36-8	1	1	1	Benzoic acid, 2-hydroxy-, methyl ester {methyl salicylate}		5.3, 9.22, 24.3, 25.29
1074.	87-20-7	0	1	0	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester {isoamyl salicylate}		5.3, 9.22, 24.3, 25.29
1075.	87-19-4	0	1	0	Benzoic acid, 2-hydroxy-, 2-methylpropyl ester {isobutyl salicylate}		5.3, 9.22
1076.	87-22-9	0	1	0	Benzoic acid, 2-hydroxy-, 2-phenylethyl ester {phenethyl salicylate}		5.3, 9.22
1077.	118-58-1	0	1	0	Benzoic acid, 2-hydroxy-, phenylmethyl ester {benzyl salicylate}		5.3, 9.22
1078.	50-85-1	1	0	0	Benzoic acid, 2-hydroxy-4-methyl-		4.3, 9.22
1079.	579-75-9	0	1	0	Benzoic acid, 2-methoxy- {*o*-anisic acid}		4.3, 10.2
1080.	118-90-1	1	1	1	Benzoic acid, 2-methyl- {*o*-toluic acid}		4.3
1081.	94-47-3	0	1	0	Benzoic acid, 2-phenylethyl ester {2-phenylethyl benzoate}		5.3
1082.	583-04-0	0	1	0	Benzoic acid, 2-propenyl ester		5.3
1083.	303-38-8	1	1	1	Benzoic acid, 2,3-dihydroxy-		4.3, 9.22
1084.	3934-81-4	1	0	0	Benzoic acid, 2,3-dihydroxy-4-methoxy-		4.3, 9.22, 10.2
1085.	3929-89-3	1	0	0	Benzoic acid, 2,3-dihydroxy-4-methyl-		4.3, 9.22
1086.	603-79-2	1	0	0	Benzoic acid, 2,3-dimethyl-		4.3
1087.	610-02-6	1	0	0	Benzoic acid, 2,3,4-trihydroxy-		4.3, 9.22
1088.	89-86-1	1	0	0	Benzoic acid, 2,4-dihydroxy- {β-resorcylic acid}		4.3, 9.22
1089.	490-79-9	1	1	1	Benzoic acid, 2,5-dihydroxy- {gentisic acid}		4.3, 9.22, 21.3
1090.	96937-49-4	1	0	0	Benzoic acid, 2,5-dihydroxy-methyl-		4.3, 9.22

(*continued*)

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1091.	610-72-0	1	0	0	Benzoic acid, 2,5-dimethyl-		4.3
1092.	303-07-1	1	1	1	Benzoic acid, 2,6-dihydroxy-		4.3, 9.22
1093.	619-20-5	1	0	0	Benzoic acid, 3-ethyl-		4.3
1094.	99-06-9	1	1	1	Benzoic acid, 3-hydroxy-		4.3, 9.22
1095.	19438-10-9	1	0	0	Benzoic acid, 3-hydroxy-, methyl ester		5.3, 9.22
1096.	645-08-9	1	0	0	Benzoic acid, 3-hydroxy-4-methoxy- {isovanillic acid}		4.3, 9.22, 10.2
1097.	87513-63-1	0	1	0	Benzoic acid, 3-hydroxy-6-methoxy-, methyl ester		5.3, 9.22, 10.2
1098.	586-30-1	1	1	1	Benzoic acid, 3-hydroxy-4-methyl-		4.3, 9.22
1099.	586-38-9	1	1	1	Benzoic acid, 3-methoxy-		4.3, 10.2
1100.	99-04-7	1	1	1	Benzoic acid, 3-methyl- {*m*-toluic acid}		4.3
1101.	54846-63-8	0	1	0	Benzoic acid, 3-methylbutyl ester		5.3
1102.	99-50-3	1	1	1	Benzoic acid, 3,4-dihydroxy- {protocatechuic acid}		0.4, 4.3, 9.22
1103.	96937-39-2	1	0	0	Benzoic acid, 3,4-dihydroxy-dimethyl-		4.3, 9.22
1104.	96937-40-5	1	0	0	Benzoic acid, 3,4-dihydroxy-methyl-		4.3, 9.22
1105.		1	0	0	Benzoicacid, 3,4-dihydroxy-C_4-alkyl-methyl-		4.3, 9.22
1106.	93-07-2	0	1	0	Benzoic acid, 3,4-dimethoxy-		4.3, 10.2
1107.	619-04-5	1	0	0	Benzoic acid, 3,4-dimethyl-		4.3
1108.	149-91-7	1	1	1	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}		0.4, 4.3, 9.22, 26.9
1109.	121-79-9	1	1	1	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}		5.3, 9.22, 26.9
1110.	99-10-5	1	0	0	Benzoic acid, 3,5-dihydroxy-		4.3, 9.22
1111.	499-06-9	0	1	0	Benzoic acid, 3,5-dimethyl-		4.3
1112.	1918-00-9	1	1	1	Benzoic acid, 3,6-dichloro-2-methoxy- {Dicamba®}		4.3, 10.2, 18.4, 21.3
1113.	126-64-7	0	1	0	Benzoic acid, 3,7-dimethyl-1,6-octadien-6-yl ester {linalyl benzoate}		5.3
1114.	619-64-7	1	0	0	Benzoic acid, 4-ethyl-		4.3
1115.	32142-31-7	0	1	0	Benzoic acid, 4-(β-*D*-glucopyranosyloxy)-3-methoxy-		2.5, 4.3, 8.3, 10.2
1116.	99-96-7	1	1	1	Benzoic acid, 4-hydroxy- {*p*-salicylic acid}		4.3, 9.22
1117.	94-26-8 1322-01-6	0	1	0	Benzoic acid, 4-hydroxy-, butyl ester		5.3, 9.22
1118.	35285-68-8	0	1	0	Benzoic acid, 4-hydroxy-, ethyl ester, sodium salt		5.3, 20.6
1119.	99-76-3	1	0	0	Benzoic acid, 4-hydroxy-, methyl ester		5.3, 9.22
1120.	5026-62-0	0	1	0	Benzoic acid, 4-hydroxy-, methyl ester, sodium salt		5.3, 20.6
1121.	94-13-3	1	0	0	Benzoic acid, 4-hydroxy-, propyl ester		5.3, 9.22
1122.	35285-69-9	0	1	0	Benzoic acid, 4-hydroxy-, propyl ester, sodium salt		5.3, 20.6
1123.	530-57-4	1	1	1	Benzoic acid, 4-hydroxy-3,5-dimethoxy- {syringic acid}		4.3, 9.22, 10.2
1124.	121-34-6	1	1	1	Benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid}		4.3, 9.22, 10.2, 21.3
1125.	617-05-0	0	1	0	Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester		5.3, 9.22, 10.2
1126.	3943-74-6	1	1	1	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester		5.3, 9.22, 10.2

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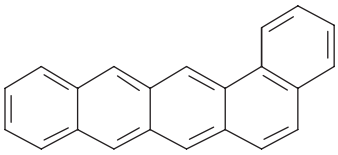
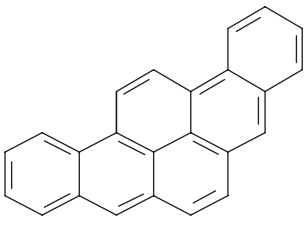
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1127.	96937-45-0	1	0	0	Benzoic acid, 4-hydroxymethyl-		4.3, 9.22
1128.	121-98-2	0	1	0	Benzoic acid, 4-methoxy-, methyl ester {methyl anisate}		5.3, 10.2
1129.	99-94-5	0	1	0	Benzoic acid, 4-methyl- {*p*-toluic acid}		4.3
1130.	3619-22-5	1	0	0	Benzoic acid, 4-methyl-, hydrazide	C_6H_5-CO-NH-NH_2	13.1
1131.		1	0	0	Benzoisoquinoline		17.21
1132.		1	0	0	Benzoisoquinoline, dimethyl-		17.21
1133.		1	0	0	Benzoisoquinoline, methyl-		17.21
1134.		1	0	0	Benzoisoquinoline, tetramethyl-		17.21
1135.		1	0	0	Benzoisoquinoline, trimethyl-		17.21
1136.	226-88-0	1	0	0	Benzo[*a*]naphthacene		1.20
1137.	239-30-5	1	0	0	Benzo[*b*]naphtho[2,1-*d*]furan		10.2
1138.	243-42-5	1	0	0	Benzo[*b*]naphtho[2,3-*d*]furan		10.2
1139.	239-35-0	1	0	0	Benzo[*b*]naphtho[2,1-*d*]thiophene		18.1
1140.	100-47-0	1	1	1	Benzonitrile {phenyl cyanide}	C_6H_5-CN	11.2
1141.		1	0	0	Benzonitrile, C_2-alkyl- {two isomers detected}		11.2
1142.		1	0	0	Benzonitrile, C_3-alkyl- {five isomers detected}		11.2
1143.	6136-68-1	1	0	0	Benzonitrile, 3-acetyl-		3.13, 11.2
1144.	1885-29-6	1	0	0	Benzonitrile, 2-amino- {anthranilonitrile}		11.2, 12.2
1145.	36541-24-9	1	0	0	Benzonitrile, dimethyl-		11.2
1146.	5724-56-1	1	0	0	Benzonitrile, 2,3-dimethyl-		11.2
1147.	21789-36-6	1	0	0	Benzonitrile, 2,4-dimethyl-		11.2
1148.	13730-09-1	1	0	0	Benzonitrile, 2,5-dimethyl-		11.2
1149.	6575-13-9	1	0	0	Benzonitrile, 2,6-dimethyl-		11.2
1150.	22884-95-3	1	0	0	Benzonitrile, 3,4-dimethyl-		11.2
1151.	34136-59-9	1	0	0	Benzonitrile, 2-ethyl-		11.2
1152.	25550-22-5	1	0	0	Benzonitrile, methyl-		11.2
1153.	529-19-1	1	1	1	Benzonitrile, 2-methyl-		11.2
1154.	34136-57-7	1	0	0	Benzonitrile, 3-ethyl-		11.2
1155.	873-62-1	1	0	0	Benzonitrile, 3-hydroxy-		9.22, 11.2
1156.	620-22-4	1	0	0	Benzonitrile, 3-methyl-		11.2
1157.	3435-51-6	1	0	0	Benzonitrile, 4-ethenyl-		11.2
1158.	25309-65-3	1	0	0	Benzonitrile, 4-ethyl-		11.2
1159.	767-00-0	1	0	0	Benzonitrile, 4-hydroxy-		9.22, 11.2
1160.	104-85-8	1	0	0	Benzonitrile, 4-methyl-		11.2
1161.	60484-66-4	1	0	0	Benzonitrile, 4-propyl-		11.2
1162.	77417-06-2	1	0	0	Benzonitrile, trimethyl-		11.2
1163.	2571-52-0	1	0	0	Benzonitrile, 2,4,6-trimethyl-		11.2
1164.	189-55-9	1	0	0	Benzo[*rst*]pentaphene {dibenzo[*a,i*]pyrene}		1.20, 23.5

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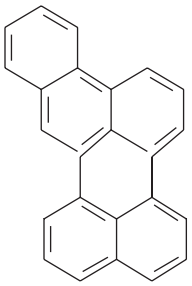
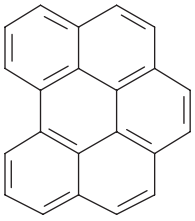
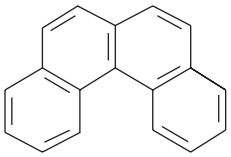
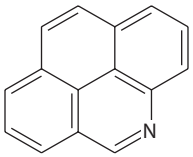
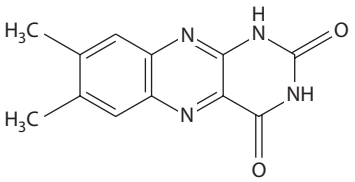
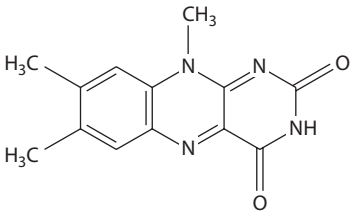
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1165.	11057-45-7	1	0	0	Benzoperylene		1.20
1166.	197-70-6	1	0	0	Benzo[*b*]perylene		1.20
1167.	191-24-2	1	1	1	Benzo[*ghi*]perylene		1.20
1168.	64760-22-1	1	0	0	Benzo[*ghi*]perylene, dimethyl- {at least three isomers in MSS}		1.20
1169.	41699-09-6	1	0	0	Benzo[*ghi*]perylene, methyl- {at least two isomers in MSS}		1.20
1170.	64760-23-2	1	0	0	Benzo[*ghi*]perylene, trimethyl- {at least two isomers in MSS}		1.20
1171.	65777-08-4	1	0	0	Benzophenanthrene		1.20
1172.	195-19-7	1	0	0	Benzo[*c*]phenanthrene		1.20
1173.	78328-47-9	1	0	0	Benzo[*c*]phenanthrene, methyl-		1.20
1174.	194-03-6	1	0	0	Benzo[*lmn*]phenanthridine {thebenidine}		17.21
1175.	4250-90-2	0	1	0	Benzo[*g*]pteridine-10(2*H*)-acetaldehyde, 3,4-dihydro-7, 8-dimethyl-2,4-dioxo-		3.12, 14.1, 17.23
1176.	1086-80-2	0	1	0	Benzo[*g*]pteridine-2,4(1*H*,3*H*)-dione, 7,8-dimethyl-		14.1, 17.23
1177.	1088-56-8	0	1	0	Benzo[*g*]pteridine-2,4(3*H*,10*H*)-dione, 7,8,10-trimethyl-		14.1, 17.23

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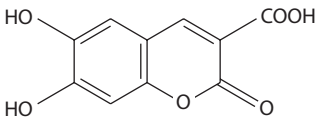
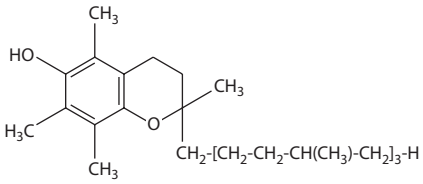
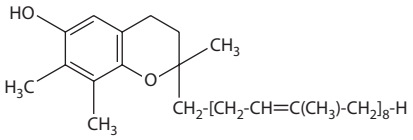
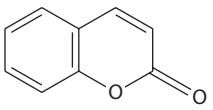
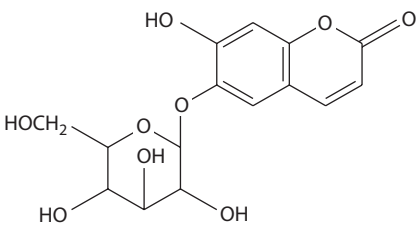
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1178.	99881-86-4	0	1	0	2*H*-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-		10.2
1179.		0	1	0	2*H*-1-Benzopyran-3-carboxylic acid, 6,7-dihydroxy-2-oxo-		4.3, 6.3, 9.22
1180.	19484-74-3	0	1	0	2*H*-1-Benzopyran-3-carboxylic acid, 7,8-dihydroxy-2-oxo-		4.3, 6.3, 9.22
1181.	124052-01-3	0	1	0	2*H*-1-Benzopyran-3,4-dione, 2-(3,4-dihydroxyphenyl)-2,5,7-trihydroxy-		2.5, 3.13, 9.22, 10.2
1182.	1406-66-2	1	1	1	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)- {tocopherol}		9.22, 10.2, 24.3, 26.9
1183.	59-02-9	1	1	1	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- {α-tocopherol}		0.4, 9.22, 10.2, 24.3, 25.29, 26.9
1184.	148-03-8	1	1	1	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- {β-tocopherol}		9.22, 10.2
1185.	7616-22-0	0	1	0	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-		9.22, 10.2
1186.	56084-94-7	0	1	0	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12,16,20,24,28,32-octamethyl-3,7,11,15,19,23,27,31-tritriacontaoctaenyl)- [3*E*,7*E*,11*E*,15*E*,19*E*,23,*E*,27*E*] {solanochromene, solanachromene}		9.22, 10.2
1187.	91-64-5	1	1	1	2*H*-1-Benzopyran-2-one {coumarin}		6.3, 26.9
1188.	26093-31-2	0	1	0	2*H*-Benzopyran-2-one, 7-amino-4-methyl-		6.3, 12.2
1189.	74712-71-3	0	1	0	2*H*-1-Benzopyran-2-one, 7-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-6-methoxy-		2.5, 6.3, 8.3
1190.	119-84-6	1	1	1	2*H*-1-Benzopyran-2-one, 3,4-dihydro- {dihydrocoumarin}		6.3
1191.	305-01-1	1	1	1	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}		6.3, 9.22, 26.9
1192.	60091-00-1	0	1	0	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-		2.5, 6.3, 8.3, 10.2
1193.	531-75-9	1	1	1	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin}		2.5, 6.3, 8.3, 9.22, 10.2

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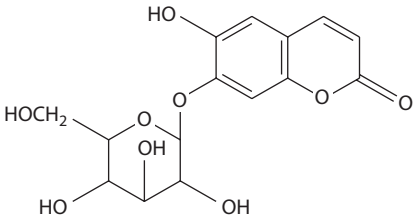
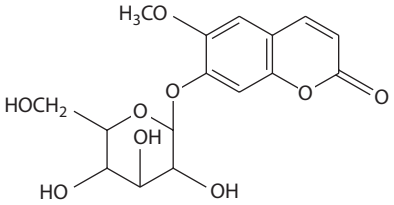
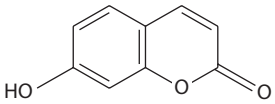
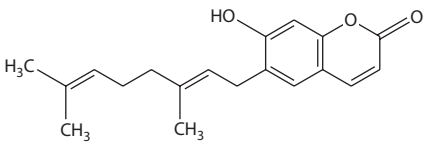
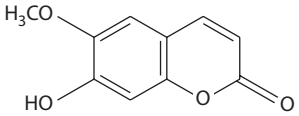
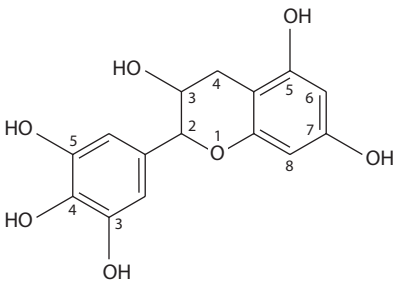
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1194.	531-58-8	0	1	0	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin}		2.5, 6.3, 9.22, 8.3, 10.2, 21.3
1195.	531-44-2	0	1	0	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-methoxy- {scopolin}		2.5, 6.3, 8.3, 10.2
1196.	93-35-6	0	1	0	2*H*-1-Benzopyran-2-one, 7-hydroxy-		6.3, 9.22
1197.	148-83-4	0	1	0	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-(3,7-dimethyl-2,6-octadienyl)- {ostruthin}		6.3, 9.22
1198.	92-61-5	1	1	1	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin}		0.4, 6.3, 9.22, 10.2, 21.3
1199.	90-33-5	0	1	0	2*H*-1-Benzopyran-2-one,7-hydroxy-4-methyl-		6.3, 9.22
1200.	531-59-9	0	1	0	2*H*-1-Benzopyran-2-one, 7-methoxy-		6.3, 10.2
1201.		0	1	0	2*H*-1-Benzopyran-2-one, 8-methoxy-		6.3, 10.2
1202.	71050-53-8	0	1	0	2*H*-1-Benzopyran-2-one, 6-methoxy-7-(β-*D*-xylofuranosyloxy)-		2.5, 6.3, 8.3, 10.2
1203.	18309-73-4	0	1	0	2*H*-1-Benzopyran-2-one, 6-methoxy-7-[(6-*O*-β-*D*-xylopyranosyl-β-*D*-glucopyranosyl)oxy]-		2.5, 6.3, 8.3, 10.2
1204.	2445-82-1	1	0	0	2*H*-1-Benzopyran-2-one, 3-methyl-		6.3
1205.	92-48-8	1	0	0	2*H*-1-Benzopyran-2-one, 6-methyl- {6-methylcoumarin}		6.3
1206.	66-76-2	1	0	0	2*H*-1-Benzopyran-2-one, 3,3′-methylenebis[4-hydroxy- {dicumarol}	Dicumarol not detected in MSS from coumarin-treated tobacco.	6.3, 9.22
1207.	4430-31-3	0	1	0	2*H*-1-Benzopyran-2-one, octahydro-		6.3
1208.	970-73-0	0	1	0	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*E*)-		2.5, 9.22, 10.2

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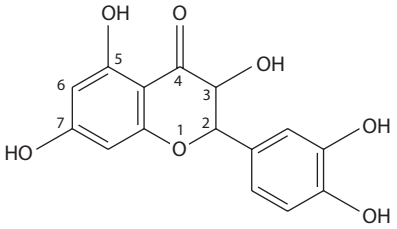
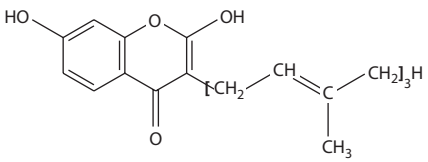
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1209.	970-74-1	0	1	0	2*H*-1-Benzopyran-3,5,7-triol,3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*Z*)-		2.5, 9.22, 10.2
1210.	17912-87-7	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricitrin}		2.5, 8.3, 9.22, 10.2
1211.	124052-00-2	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,3,5,7-tetrahydroxy-		2.5, 3.13, 9.22, 10.2
1212.	21637-25-2	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}		0.4, 2.5, 3.13, 8.3, 9.22, 10.2, 21.3
1213.	117-39-5	1	1	1	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin, 3,3a,4a,5,7-pentahydroxyflavone}		0.4, 2.5, 3.13, 9.22, 10.2, 25.29, 26.9
1214.	7215-44-3 20188-84-5	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl) oxy]-5,7-dihydroxy- {quercetin 3,3′-diglucoside}		2.5, 3.13, 8.3, 9.22, 10.2
1215.	1486-70-0	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-methoxy-		3.13, 9.22, 10.2
1216.	2068-02-2	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5-hydroxy-3,7-dimethoxy-		3.13, 9.22, 10.2
1217.	491-50-9	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}		2.5, 3.13, 8.3, 9.22, 10.2
1218.	124051-99-6	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-[[2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,6-dihydroxy-3-oxo-4-benzofuranyl]oxy]-2,3-dihydro-3,5-dihydroxy-		2.5, 3.13, 9.22, 10.2
1219.	480-41-1	0	1	0	4*H*-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)- {naringenin}		3.13, 9.22, 10.2
1220.	643-57-2	0	1	0	4*H*-1-Benzopyran-4-one, 2,7-dihydroxy-3-(3,7,11-trimethyldodeca-2,6,10-trienyl)- {ammoresinol}		3.13, 9.22, 10.2

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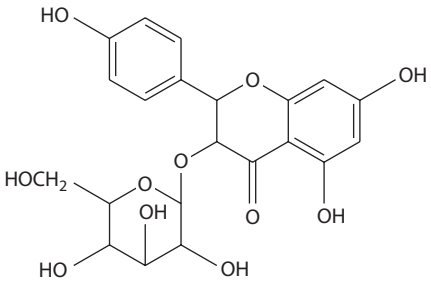
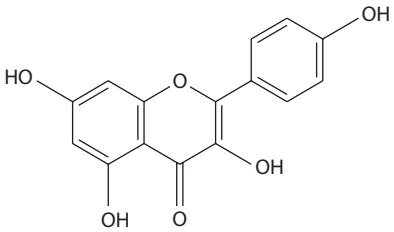
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1221.		0	1	0	4*H*-1-Benzopyran-4-one, 5, 7-dihydroxy-3-methyl-2-(3,4-dihydroxyphenyl)-{3a,4a,5,7-tetrahydroxy-3-methylflavone}		2.5, 3.13, 9.22, 10.2
1222.		0	1	0	4*H*-1-Benzopyran-4-one, 5, 7-dihydroxy-3-methyl-2-(3-methyl-4-hydroxyphenyl)-{4a,5,7-trihydroxy-3, 3a-dimethylflavone}		2.5, 3.13, 9.22, 10.2
1223.		0	1	0	4*H*-1-Benzopyran-4-one, 3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)-{3a,4a,5-trihydroxy-3, 5-dimethylflavone}		2.5, 3.13, 9.22, 10.2
1224.	480-10-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)-{kaempferol glucoside, 3,4a,5,7-tetrahydroxyflavone glucoside}		0.4, 2.5, 3.13, 8.3, 9.22, 10.2
1225.	520-18-3	1	1	1	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(4-hydroxyphenyl)-{kaempferol, 3,4a,5,7-tetrahydroxyflavone}		2.5, 3.13, 9.22, 10.2, 26.9
1226.	55136-76-0	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1227.	142235-82-3	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1228.	19895-95-5	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1229.	522-12-3	1	1	1	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-{quercetrin}		2.5, 3.13, 8.3, 9.22, 10.2

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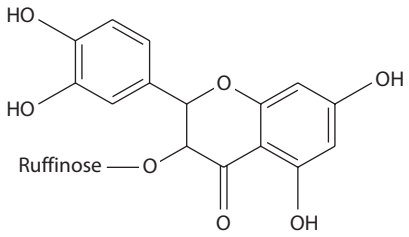
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1230.	55696-57-6	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→ 6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-		2.5, 3.13, 8.3, 9.22, 10.2
1231.	55804-74-5	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1→6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1232.	153-18-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-{rutin}		0.4, 2.5, 3.13, 8.3, 9.22, 10.2, 21.3, 25.29
1233.	17650-84-9	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1234.	30311-61-6	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-{rutin-7-glucoside}		2.5, 3.13, 8.3, 9.22, 10.2
1235.	34336-18-0	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1236.	29859-91-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1237.	27554-19-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1238.	58934-57-9	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-		2.5, 3.13, 8.3, 9.22, 10.2
1239.	828-82-0	1	0	0	4*H*-1-Benzopyran-4-one, 3-ethyl-		3.13, 10.2
1240.	520-34-3	0	1	0	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(3-hydroxy-4 methoxyphenyl)- {diosmetin}		3.13, 9.22, 10.2
1241.	4382-17-6	0	1	0	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-methoxy-		3.13, 9.22, 10.2

(*continued*)

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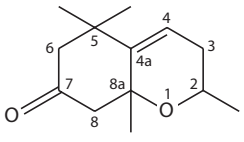
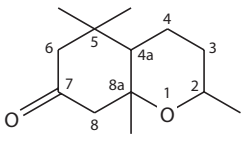
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1242.		0	1	0	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxyflavone, 3-glucoside}		2.5, 3.13, 8.3, 9.22, 10.2
1243.		1	0	0	4*H*-1-Benzopyran-4-one, hydroxy-		3.13, 9.22, 10.2
1244.	38445-24-8	1	0	0	4*H*-1-Benzopyran-4-one, 6-hydroxy-		3.13, 9.22, 10.2
1245.		0	1	0	4*H*-1-Benzopyran-4-one, 7-(β-*D*-rhamnoglucopyranosyloxy)-3,5-dimethyl-5-hydroxy-2-(3,4-dihydroxyphenyl)- {3a,4a,5-trihydroxy-3,5-dimethylflavone, 7-rhamnoglucoside}		2.5, 3.13, 8.3, 9.22, 10.2
1246.		0	1	0	4*H*-1-Benzopyran-4-one, 3-(β-*D*-rhamnoglucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {4a,5,7-trihydroxy-flavone, 3-rhamnoglucoside}		2.5, 3.13, 8.3, 9.22, 10.2
1247.	10236-47-2	0	1	0	4*H*-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}		2.5, 3.13, 8.3, 9.22, 10.2
1248.	57523-93-0	0	1	0	4*H*-1-Benzopyran-4-one, octahydro-2,5,5,7a-tetramethyl-		3.13, 10.2
1249.		0	1	0	4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,5′,7-pentahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2.5, 3.13, 8.3, 9.22, 10.2
1250.		0	1	0	4*H*-1-Benzopyran-4-one, 2-phenyl-, 3′,4′,5,7-tetrahydroxy-3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-		2.5, 3.13, 8.3, 9.22, 10.2
1251.	529-44-2	0	1	0	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(3,4,5- trihydroxyphenyl)- {myricetin}		2.5, 3.13, 9.22, 10.2
1252.		0	1	0	5*H*-1-Benzopyran-7-one, 2,3,6,7,8, 8a-hexahydro-2,5,5,8a-tetramethyl-		3.13, 10.2
1253.		0	1	0	7*H*-1-Benzopyran-7-one, 2,4a,5,6,8, 8a-hexahydro-2,5,5,8a-tetramethyl-		3.13, 10.2
1254.	20194-67-6	1	1	1	7*H*-1-Benzopyran-7-one, 2,3, 5,6,8,8a-hexahydro-2,5,5,8a-tetramethyl- {1,5,5,9-tetramethyl-10-oxabicyclo [4.4.0]dec-6-en-3-one}		3.13, 10.2
1255.	52811-22-0	1	1	1	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-5,5,8a-trimethyl-		3.13, 10.2
1256.	5835-18-7	1	1	1	7*H*-1-Benzopyran-7-one, octahydro-2,5,5,8a-tetramethyl- {7-chromanone, hexahydro-2,5,5,8a-tetramethyl-}		3.13, 10.2

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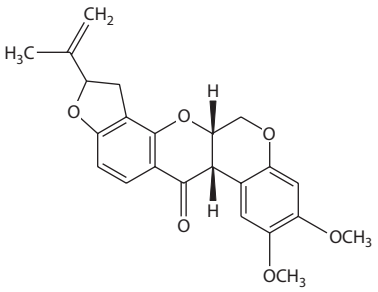
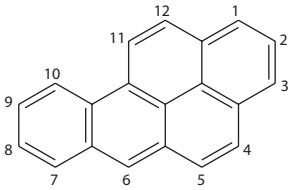
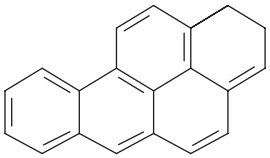
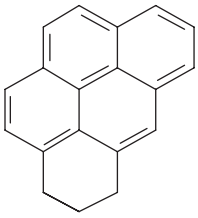
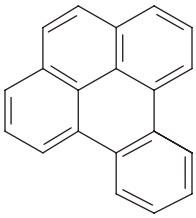
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1257.	83-79-4	0	1	0	Benzopyrano[3,4-*b*]furo[2,3-*h*][1] benzopyran-6(6a*H*)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-,[2R-(2α,6aα,12aα)]- {Rotenone®}		3.13, 10.2, 21.3
1258.	73467-76-2	1	0	0	Benzopyrene		1.20
1259.	65357-69-9	1	0	0	Benzopyrene, methyl-		1.20
1260.	50-32-8	1	1	1	Benzo[*a*]pyrene {B[*a*]P}		0.4, 1.20, 23.5
1261.		1	1	1	7,10-Benzo[*a*]pyrene-^{14}C {benzo[*a*]pyrene-7,10-^{14}C}		1.20, 25.29
1262.		1	0	0	Benzo[*a*]pyrene, alkyl-		1.20
1263.		1	0	0	Benzo[*a*]pyrene, dihydro-		1.20
1264.	110081-38-4	1	0	0	Benzo[*a*]pyrene, 3,4-dihydro-		1.20
1265.	17573-23-8	1	0	0	Benzo[*a*]pyrene, 7,8-dihydro-		1.20
1266.	25167-90-2	1	0	0	Benzo[*a*]pyrene, dimethyl- {at least two isomers in MSS}		1.20
1267.		1	0	0	Benzo[*a*]pyrene, ethyl-		1.20
1268.	25167-89-9	1	0	0	Benzo[*a*]pyrene, methyl- {at least two isomers in MSS}		1.20
1269.	69453-35-6	1	0	0	Benzo[*a*]pyrene diol		9.22
1270.	63455-19-6	1	0	0	Benzo[*a*]pyrenol		9.22
1271.	37574-48-4	1	0	0	Benzo[*a*]pyren-4-ol		9.22
1272.	20928-82-9	1	0	0	Benzo[*a*]pyren-6-yloxy		9.22
1273.	7130-15-6	1	0	0	3*H*-Benzo[*cd*]pyrene, 4,5-dihydro-		1.20
1274.	192-97-2	1	1	1	Benzo[*e*]pyrene {B[*e*]P}		1.20, 26.9

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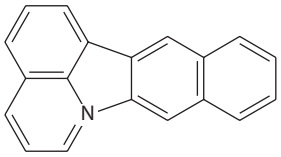
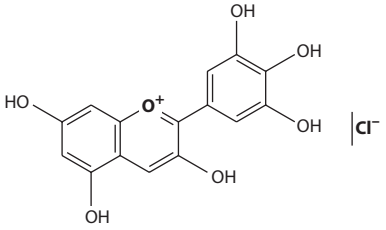
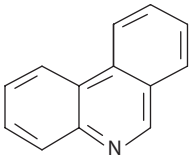
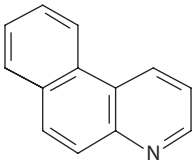
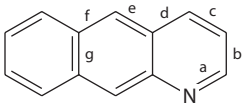
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1275.	41699-06-3	1	0	0	Benzo[*e*]pyrene, dimethyl- {at least two isomers in MSS}		1.20
1276.	41699-04-1	1	0	0	Benzo[*e*]pyrene, methyl- {at least two isomers in MSS}		1.20
1277.	64760-21-0	1	0	0	Benzo[*e*]pyrene, trimethyl-		1.20
1278.	30907-88-1	0	1	0	6*H*-Benzo[*c*]pyrido[3,2,1-*jk*]carbazole		17.21
1279.	528-58-5	0	1	0	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride		9.22, 10.2, 18.4
1280.	22688-80-8	0	1	0	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride		2.5, 8.3, 9.22, 10.2, 18.4
1281.	528-53-0	0	1	0	1-Benzopyrylium, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-, chloride		9.22, 10.2, 18.4
1282.	18719-76-1	0	1	0	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-, chloride		2.5, 8.3, 9.22, 10.2, 18.4
1283.	33978-17-5	0	1	0	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride		2.5, 8.3, 9.22, 10.2, 18.4
1284.	39327-16-7	1	0	0	Benzoquinoline		17.21
1285.		1	0	0	Benzoquinoline, dimethyl-		17.21
1286.	88813-63-2	1	0	0	Benzoquinoline, methyl-		17.21
1287.		1	0	0	Benzoquinoline, tetramethyl-		17.21
1288.		1	0	0	Benzoquinoline, trimethyl-		17.21
1289.	229-87-8	1	1	1	Benzo[*c*]quinoline {phenanthridine, 9-azaphenanthrene}		17.21
1290.	85-02-9	1	0	0	Benzo[*f*]quinoline {1-azaphenanthrene}		17.21
1291.	260-36-6	1	0	0	Benzo[*g*]quinoline		17.21

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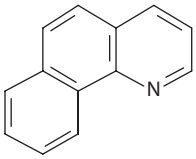
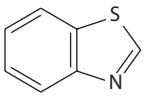
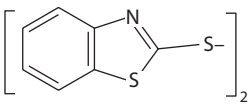
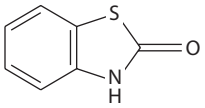
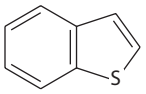
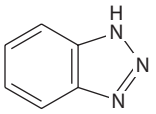
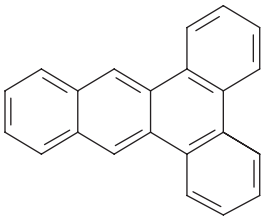
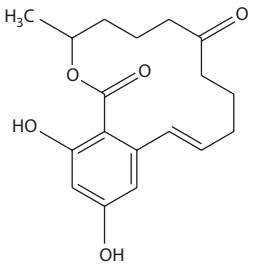
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1292.	230-27-3	1	0	0	Benzo[*h*]quinoline {4-azaphenanthrene}		17.21
1293.	63042-66-0	1	0	0	Benzo[*h*]quinoline, 2,3,4-trimethyl-		17.21
1294.		1	0	0	*o*-Benzosemiquinone radical		27.1
1295.	3225-29-4	1	0	0	*p*-Benzosemiquinone radical		27.1
1296.	95-16-9	1	1	1	Benzothiazole {benzosulfonazole}		18.1
1297.	120-78-5	0	1	0	Benzothiazole, 2,2′-dithiobis- {Thiofide®}		18.1, 21.3
1298.	615-22-5	0	1	0	Benzothiazole, 2-methylthio-		18.1
1299.	934-34-9	0	1	0	2(3*H*)-Benzothiazolone		18.1
1300.	1128-67-2	1	0	0	2(3*H*)-Benzothiazolone, 3-methyl-, hydrazone		18.1
1301.	95-15-8	1	0	0	Benzo[*b*]thiophene		18.1
1302.		1	0	0	Benzo[*b*]thiophene, C_2-alkyl-		18.1
1303.		1	0	0	Benzo[*b*]thiophene, C_3-alkyl-		18.1
1304.	31393-23-4	1	0	0	Benzo[*b*]thiophene, methyl- {four isomers reported}		18.1
1305.	14315-11-8	1	0	0	Benzo[*b*]thiophene, 4-methyl-		18.1
1306.	95-14-7	1	0	0	1*H*-Benzotriazole {1,2,3-triaza-1*H*-indene}		17.21
1307.	215-58-7	1	0	0	Benzo[*b*]triphenylene {dibenz[*a*,*c*]anthracene}		1.20, 26.9
1308.	64760-20-9	1	0	0	Benzo[*b*]triphenylene, methyl-		1.20
1309.	17924-92-4	0	1	0	1*H*-2-Benzoxacyclotetradecin-1,7(8*H*)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, [S-(*E*)]-		3.13, 5.3, 9.22

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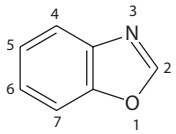
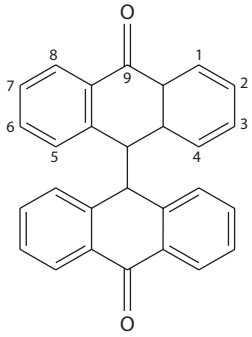
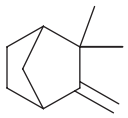
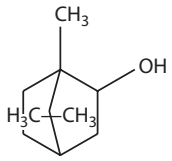
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1310.	273-53-0	1	0	0	Benzoxazole {1-oxa-3-azaindene}		17.15
1311.		1	0	0	Benzoxazole, C_2-alkyl-		17.15
1312.	72692-90-1	1	0	0	Benzoxazole, 2,4-dimethyl-		17.15
1313.	5676-58-4	1	0	0	Benzoxazole, 2,5-dimethyl-		17.15
1314.	72692-91-2	1	0	0	Benzoxazole, 4,6-dimethyl-		17.15
1315.	78210-58-9	1	0	0	Benzoxazole, 5,7-dimethyl-		17.15
1316.	78210-57-8	1	0	0	Benzoxazole, 7-ethyl-		17.15
1317.	95-21-6	1	0	0	Benzoxazole, 2-methyl-		17.15
1318.	27548-56-7	0	1	0	3-Benzoxepin-7-methanol, 5a,6,7,8,9,9a-hexahydro-α,α,5,9a-tetramethyl-, (5aα,7α,9aα)-(–)-		2.5, 10.2
1319.	7440-41-7	1	1	1	Beryllium	Be	20.5, 23.5
1320.	7787-47-5	0	1	0	Beryllium chloride		18.4, 20.6
1321.	434-85-5	1	0	0	[9,9′-Bianthracene]-10,10′(9*H*,9′*H*)-dione {bianthrone, dianthraquinone}		3.13, 9.24
1322.	121-46-0	0	1	0	Bicyclo[2.2.1]hepta-2,5-diene {norbornadiene}		1.12
1323.	79-92-5	1	1	1	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- {camphene}		1.12, 24.3, 25.29
1324.	8001-35-2	0	1	0	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated {Toxaphene®}		0.4, 18.4, 21.3
1325.	8001-50-1	0	1	0	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated + bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, polychlorinated {Strobane®, Dichloricide®}		18.4, 21.3
1326.	124-76-5	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *exo*- {isoborneol}		2.5
1327.	509-11-5	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7-dimethyl-, (exo,anti)-		2.5
1328.	464-45-9 507-70-0	1	1	1	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, endo- {borneol}		0.4, 2.5, 24.3, 25.29

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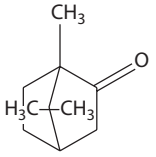
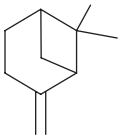
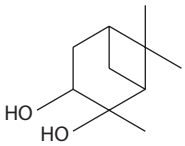
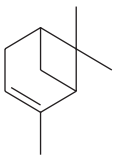
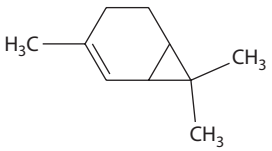
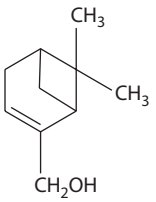
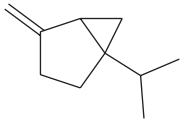
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1329.	125-12-2	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate {isobornyl acetate}		5.3
1330.	2756-56-1	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, propanoate, exo-		5.3
1331.	1195-79-5	0	1	0	Bicyclo[2.2.1]heptan-2-one,1,3,3-trimethyl-		3.13
1332.	4695-62-9	0	1	0	Bicyclo[2,2,1]heptan-2-one, 1,3,3-trimethyl- {*d*-fenchone}		3.13
1333.	76-22-2	0	1	0	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- {camphor}		3.13, 24.3
1334.	498-66-8	1	0	0	Bicyclo[2.2.1]hept-2-ene {norbornene}		1.12
1335.		1	0	0	Bicyclo[2.2.1]hept-2-ene, 5-acetyl- {ethanone, 1-bicyclo[2.2.1] hept-5-en-2-yl-}		3.13
1336.		1	0	0	Bicyclo[2.2.1]hept-2-ene, 5-ethyl-		1.12
1337.	127-91-3 18172-67-3	1	1	1	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- {β-pinene}		1.12, 24.3, 25.29
1338.	22422-34-0	0	1	0	Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl- {2,3-pinanediol}		2.5
1339.	80-56-8 7785-26-4	1	1	1	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- {α-pinene}		1.12, 24.3, 25.29
1340.	4889-83-2	0	1	0	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-		1.12
1341.	498-15-7 13466-78-9	0	1	0	Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- {(+)-3-carene}		1.12
1342.	4497-92-1	0	1	0	Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-, (1R, 6R)- {(+)-2-carene}		1.12
1343.	515-00-4	0	1	0	Bicyclo[3.1.1]hept-2-ene- 2-methanol, 6,6-dimethyl-		2.5
1344.	3387-41-5	0	1	0	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- {sabinene}		1.12

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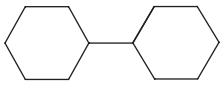
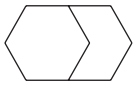
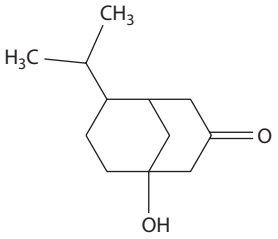
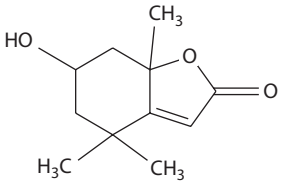
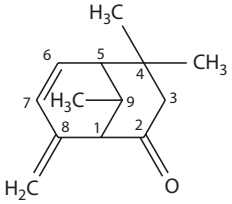
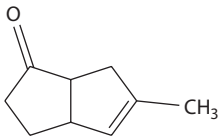
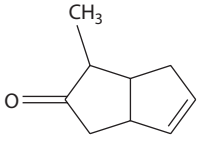
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1345.	471-16-9	0	1	0	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, [1S-(1α,3β,5α)]- {sabinol}		2.5
1346.	2867-05-2	0	1	0	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)- {3-thujene}		1.12
1347.	3917-48-4	0	1	0	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-, (1R)-		1.12
1348.	19250-17-0	0	1	0	Bicyclo[3.1.1]hept-2-ene-2-carboxylic acid, 6,6-dimethyl-		4.3
1349.	92-51-3	1	1	1	1,1′-Bicyclohexyl {cyclohexylcyclohexane}		1.12
1350.	280-65-9	1	0	0	Bicyclo[3.3.1]nonane		1.12
1351.	124749-69-5	1	0	0	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy-6-(1-methylethyl)-, endo-		2.5, 3.13
1352.	123695-64-7	1	0	0	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy-6-(1-methylethyl)-, exo-		2.5, 3.13
1353.	61927-07-9	1	0	0	Bicyclo[4,3,0]non-6-en-8-one, 3-hydroxy-9-oxo-1,5,5-trimethyl-		6.3
1354.	61185-25-9	0	1	0	Bicyclo[3.3.1]non-6-en-2-one, 4,4,9-trimethyl-8-methylene-, anti-		3.13
1355.		0	1	0	Bicyclo[3.3.1]non-6-en-2-one, 4,9,9-trimethyl-8-methylene-		3.13
1356.		0	1	0	Bicyclo[3.3.0]oct-2-en-6-one, 3-methyl-		3.13
1357.		0	1	0	Bicyclo[3.3.0]oct-2-en-7-one, 6-methyl-		3.13

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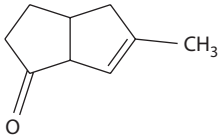
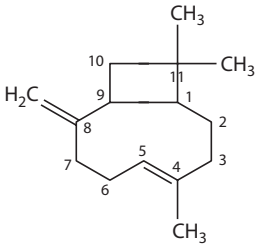
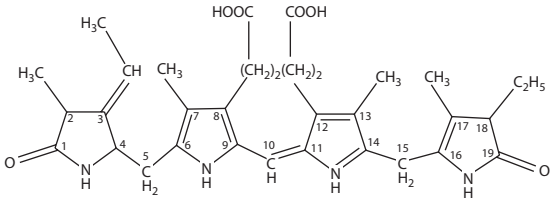
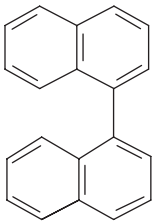
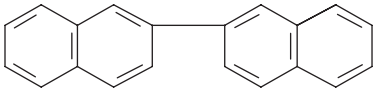
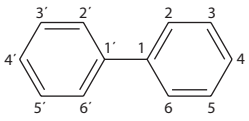
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1358.		0	1	0	Bicyclo[3.3.0]oct-2-en-8-one, 3-methyl-		3.13
1359.	87-44-5	0	1	0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- {β-caryophyllene}		1.12, 24.3, 25.29
1360.	32214-91-8	0	1	0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, acetate {β-caryophyllene acetate}		5.3
1361.	102488-10-8	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-		10.2
1362.	53093-94-0	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-, (*Z*)-(±)-		10.2
1363.	53093-95-1	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-, (*E*)-(±)-		10.2
1364.	53093-96-2	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethyl)-, (*Z*)-(±)-		10.2
1365.	53093-97-3	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethyl)-, (*E*)-(±)-		10.2
1366.	20298-86-6	0	1	0	21*H*-Biline-8,12-dipropanoic acid, 18-ethyl-3-ethylidene-1,2,3,19,22,24-hexahydro-2,7,13,17-tetramethyl-1,19-dioxo-, (2R,3*E*)-		4.3, 17.5, 17.13
1367.	604-53-5	1	0	0	1,1′-Binaphthalene		1.20
1368.	71265-39-9	1	0	0	1,1′-Binaphthalene, dimethyl-		1.20
1369.	71277-81-1	1	0	0	1,1′-Binaphthalene, ethyl-		1.20
1370.	59615-45-5	1	0	0	1,1′-Binaphthalene, methyl-		1.20
1371.	4325-74-0	1	0	0	1,2′-Binaphthalene		1.20
1372.	612-78-2	1	0	0	2,2′-Binaphthalene		1.20
1373.	71294-43-4	1	0	0	2,2′-Binaphthalene, dimethyl-		1.20
1374.	71277-82-2	1	0	0	2,2′-Binaphthalene, ethyl-		1.20
1375.	41637-91-6	1	0	0	2,2′-Binaphthalene, methyl-		1.20
1376.	92-52-4	1	1	1	1,1′-Biphenyl {diphenyl}		1.13

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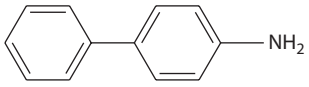
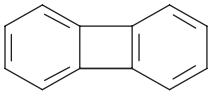
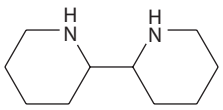
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1377.	2051-60-7	1	0	0	1,1′-Biphenyl, 2-chloro-		18.4
1378.	2051-24-3	1	1	1	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5, 5′,6,6′-decachloro- {1,1′-biphenyl, decachloro-}		18.4
1379.	92-87-5	1	0	0	1,1′-Biphenyl, 4,4′-diamino- {benzidine}		12.2
1380.	2050-67-1	1	0	0	1,1′-Biphenyl, 3,3′-dichloro-		18.4
1381.	2050-68-2	1	0	0	1,1′-Biphenyl, 4,4′-dichloro-		18.4
1382.	61141-66-0	0	1	0	1,1′-Biphenyl, 3,4-diethyl-		1.13
1383.	1133-63-7	1	0	0	1,1′-Biphenyl, 2,3-dihydroxy-		9.22
1384.	7383-90-6	0	1	0	1,1′-Biphenyl, 3,4′-dimethyl-		1.13
1385.	613-33-2	1	0	0	1,1′-Biphenyl, 4,4′-dimethyl-		1.13
1386.	28013-11-8	1	1	1	1,1′-Biphenyl, ar,ar′-dimethyl-		1.13
1387.	40529-66-6	1	0	0	1,1′-Biphenyl, ethyl-		1.13
1388.	1812-51-7	1	0	0	1,1′-Biphenyl, 2-ethyl-		1.13
1389.	71277-83-3	1	0	0	1,1′-Biphenyl, ethylmethyl-		1.13
1390.	52712-05-7	1	0	0	1,1′-Biphenyl, 2,2′,3,4,5,5′,6,-heptachloro-		18.4
1391.	38411-22-2	1	0	0	1,1′-Biphenyl, 2,2′,3,3′,6,6′-hexachloro-		18.4
1392.	28652-72-4	1	1	1	1,1′-Biphenyl, methyl-		1.13
1393.	643-58-3	1	0	0	1,1′-Biphenyl, 2-methyl-		1.13
1394.	643-93-6	1	0	0	1,1′-Biphenyl, 3-methyl-		1.13
1395.	644-08-6	1	0	0	1,1′-Biphenyl, 4-methyl-		1.13
1396.	92-93-3	1	0	0	1,1′-Biphenyl, 4-nitro-		16.1
1397.	40186-72-9	1	0	0	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6-nonachloro-		18.4
1398.	35694-08-7	1	0	0	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′-octachloro-		18.4
1399.	74472-39-2	1	0	0	1,1′-Biphenyl, 2,3′,4,5′,6-pentachloro-		18.4
1400.	71294-42-3	1	0	0	1,1′-Biphenyl, propyl-		1.13
1401.	2437-79-8	1	0	0	1,1′-Biphenyl, 2,2′,4,4′-tetrachloro-		18.4
1402.	37680-65-2	1	0	0	1,1′-Biphenyl, 2,2′,5-trichloro-		18.4
1403.	30581-97-6	1	0	0	1,1′-Biphenyl, trimethyl- {three isomers detected}		1.12
1404.	64850-01-7	1	0	0	[1,1′-Biphenyl]amine, *N*-methyl-		12.2
1405.	90-41-5	1	0	0	[1,1′-Biphenyl]-2-amine		12.2
1406.	2243-47-2	1	0	0	[1,1′-Biphenyl]-3-amine		12.2, 23.5
1407.	92-67-1	1	0	0	[1,1′-Biphenyl]-4-amine {4-aminobiphenyl}		12.2, 23.5
1408.	1322-20-9	1	0	0	[1,1′-Biphenyl]-ol		9.22
1409.	90-43-7	1	1	1	[1,1′-Biphenyl]-2-ol		9.22
1410.	92-69-3	1	0	0	[1,1′-Biphenyl]-4-ol		9.22
1411.	259-79-0	1	0	0	Biphenylene		1.20
1412.	531-67-9	0	1	0	2,2′-Bipiperidine		17.11
1413.	37275-48-2	1	0	0	Bipyridine		17.11
1414.	78310-61-9	1	0	0	Bipyridine, dimethyl- {two isomers detected}		17.11
1415.		1	0	0	Bipyridine, diphenyl-		17.11
1416.	64859-48-9	1	0	0	Bipyridine, ethyl-		17.11

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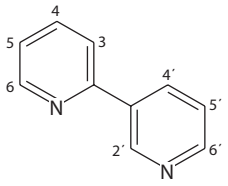
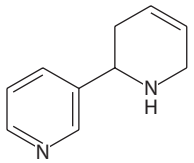
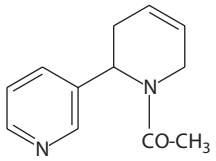
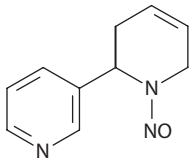
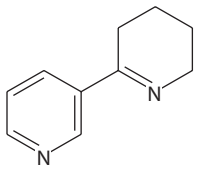
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1417.	64859-47-8	1	0	0	Bipyridine, methyl- {four isomers in all}		17.11
1418.	78310-62-0	1	0	0	Bipyridine, phenyl-		17.11
1419.	366-18-7	1	1	1	2,2′-Bipyridine {nicotine}		0.4, 17.11
1420.		1	0	0	2,2′-Bipyridine, amino-		12.2, 17.11
1421.	78210-73-8	1	0	0	2,2′-Bipyridine, 4,5-dimethyl-		17.11
1422.	56100-19-7	1	0	0	2,2′-Bipyridine, 4-methyl-		17.11
1423.	581-50-0	1	1	1	2,3′-Bipyridine {isonicoteine}		0.4, 17.11
1424.		1	0	0	2,3′-Bipyridine, dimethyl-		17.11
1425.		1	0	0	2,3′-Bipyridine, methyl-		17.11
1426.	2743-90-0	0	1	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (±)-		17.11
1427.	126454-22-6	1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (R)- {*d*-anatabine}		17.11
1428.	581-49-7	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (S)- {*l*-anatabine}		0.4, 17.11
1429.		1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-ethyl-		17.11
1430.		1	0	0	2,3′-Bipyridine,1,2,3,6-tetrahydro-methyl-		17.11
1431.	61892-64-6	1	1	1	2,3′-Bipyridine, 1-acetyl-1,2,3,6-tetrahydro-, (S)- {*N*′-acetylanatabine}		17.11
1432.	5953-51-5	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-methyl-, (S)-		0.4, 17.11
1433.	96552-71-5	1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxohexyl)-, (S)- {*N*′-hexanoylanatabine}		13.1, 17.11
1434.	96552-72-6	1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxooctyl)-, (S)- {*N*′-octanoylanatabine}		13.1, 17.11
1435.	71267-22-6 71608-13-4	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-nitroso-, (S)- {NAT}		15.8, 17.11, 23.5
1436.	3471-05-4	0	1	0	2,3′-Bipyridine, 3,4,5,6-tetrahydro- {anabaseine}		17.11

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1437.	61892-98-6	1	0	0	2,3′-Bipyridine, 1-ethyl-1,2,3,6-tetrahydro-, (S)-		17.11
1438.	26636-59-9	1	0	0	2,3′-Bipyridine, 2′(or 3)-methyl-		17.11
1439.	78210-76-1	1	0	0	2,3′-Bipyridine, 3-ethyl-		17.11
1440.	78210-75-0	1	0	0	2,3′-Bipyridine, 4-(2-butenyl)-		17.11
1441.	38840-05-0	1	1	1	2,3′-Bipyridine, 4-methyl-		17.11
1442.	78210-74-9	1	0	0	2,3′-Bipyridine, 4-(2-propenyl)-		17.11
1443.		1	0	0	2,3′-Bipyridine, 4-propyl-		17.11
1444.	20410-87-1	0	1	0	2,3′-Bipyridine, 5-(1-methyl-2-piperidinyl)-, (+)- {anabasamine}		17.11
1445.	78210-79-4	1	0	0	2,3′-Bipyridine, 5-(1-propenyl)-		17.11
1446.	78210-81-8	1	0	0	2,3′-Bipyridine, 5-ethenyl-		17.11
1447.	34671-89-1	1	0	0	2,3′-Bipyridine, 5-ethyl-		17.11
1448.	26844-80-4	1	1	1	2,3′-Bipyridine, 5-methyl-		17.11
1449.	78210-80-7	1	0	0	2,3′-Bipyridine, 5-propyl-		17.11
1450.	78210-77-2	1	0	0	2,3′-Bipyridine, 6-ethyl-		17.11
1451.		1	0	0	2,3′-Bipyridine, 6-hydroxy-3,4,5,6-tetrahydro-		2.5, 17.11
1452.	78210-78-3	1	0	0	2,3′-Bipyridine, 6-methyl-		17.11
1453.	61892-65-7	1	1	1	[2,3′-Bipyridine]-1(2*H*)-carboxaldehyde, 3,6-dihydro-, (S)- {*N*′-formylanatabine}		3.12, 13.1, 17.11
1454.	96552-70-4	1	0	0	[2,3′-Bipyridine]-1(2*H*)-carboxylic acid, 3,6-dihydro-, methyl ester, (S)-		5.3, 17.11
1455.	70898-21-4	1	0	0	[2,3′-Bipyridin]-6′(1′*H*)-one, 3,4,5,6-tetrahydro-		3.13, 17.11, 17.13
1456.	581-47-5	1	1	1	2,4′-Bipyridine		17.11
1457.	581-46-4	1	1	1	3,3′-Bipyridine		17.11
1458.	38840-06-1	0	1	0	3,3′-Bipyridine, 4-methyl-		17.11
1459.	78210-82-9	1	0	0	3,3′-Bipyridine, 5-methyl-		17.11
1460.	78210-83-0	1	0	0	3,3′-Bipyridine, 6-methyl-		17.11
1461.	553-26-4	1	1	1	4,4′-Bipyridine		17.11
1462.	7440-69-9	1	1	1	Bismuth	Bi	0.4, 20.5
1463.	14331-79-4	1	1	1	Bismuth, isotope of mass 210	^{210}Bi	20.5
1464.		0	1	0	Bismuth, isotope of mass 216	^{216}Bi	20.5
1465.	7440-42-8	1	1	1	Boron	B	0.4, 20.5
1466.	24959-67-9	1	1	1	Bromide	Br^{-1}	18.4, 20.5
1467.	7726-95-6	1	1	1	Bromine	Br_2	18.4, 19.5, 20.5
1468.	14686-69-2	1	1	1	Bromine, isotope of mass 82	$^{82}Br_2$	18.4, 20.5
1469.		0	1	0	*Burkholderia*		22.2
1470.	25339-57-5	1	0	0	Butadiene		1.11
1471.		1	0	0	Butadiene radical		27.1
1472.	590-19-2	1	0	0	1,2-Butadiene	$H_2C{=}C{=}CH\text{-}CH_3$	1.11
1473.	106-99-0	1	0	0	1,3-Butadiene	$H_2C{=}CH\text{-}CH{=}CH_2$	1.11, 23.5, 25.29
1474.	513-81-5	1	0	0	1,3-Butadiene, 2,3-dimethyl-	$H_2C{=}C(CH_3)\text{-}C(CH_3){=}CH_2$	1.11
1475.	78-79-5	1	1	1	1,3-Butadiene, 2-methyl- {isoprene}	$H_2C{=}C(CH_3)\text{-}CH{=}CH_2$	1.11, 23.5, 25.29
1476.		1	0	0	1,3-Butadiene, 2-methyl- radical {isoprene radical}		27.1
1477.		1	0	0	1,3-Butadiene, 1,2,4-trialkyl-1,3-Butadiene, 2-(4′,8′,12′-trimethyltridecyl)-	$R\text{-}CH{=}C(R_1)\text{-}CH{=}CH\text{-}R_2$ See 1-hexadecene, 3-methylene-7,11,15-trimethyl-	1.11
1478.	460-12-8	1	0	0	1,3-Butadiyne	$HC{\equiv}C\text{–}C{\equiv}CH$	1.11
1479.	123-72-8	1	1	1	Butanal {butyraldehyde}	$H_3C\text{-}(CH_2)_2\text{-}CH{=}O$	0.4, 3.12, 23.5

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1480.	4390-05-0	0	1	0	Butanal, 4-amino-	H_2N-$(CH_2)_3$-CH═O	3.12, 12.2
1481.	34764-22-2	1	0	0	Butanal, 3,4-dihydroxy-	$HOCH_2$-CHOH-CH_2-CH═O	2.5, 3.12
1482.	2109-98-0	1	0	0	Butanal, 2,3-dimethyl-		3.12
1483.	97-96-1	1	1	1	Butanal, 2-ethyl- {diethylacetaldehyde}	$(C_2H_5)_2$═CH-CH═O	0.4, 3.12
1484.	107-89-1	1	0	0	Butanal, 3-hydroxy- {aldol}	H_3C-CHOH-CH_2-CH═O	2.5, 3.12
1485.		0	1	0	Butanal, 3-hydroxy-2-oxo- {methylreductone}	H_3C-CHOH-CO-CH═O	2.5, 3.12, 3.13
1486.	25714-71-0	1	0	0	Butanal, 4-hydroxy-	HO-$(CH_2)_3$-CH═O	2.5, 3.12
1487.		1	0	0	Butanal, 4-(2-hydroxyethoxy)-	HO-CH_2CH_2-O-$(CH_2)_3$-CH═O	2.5, 3.12, 10.2
1488.	96-17-3	1	1	1	Butanal, 2-methyl- {2-methylbutyraldehyde}	H_3C-CH_2-$CH(CH_3)$-CH═O	3.12, 24.3, 25.29
1489.	590-86-3	1	1	1	Butanal, 3-methyl- {3-methylbutyraldehyde, isovaleraldehyde}	$(H_3C)_2$═CH-CH_2-CH═O	3.12, 24.3, 25.29
1490.	7729-27-3	0	1	0	Butanal, 4-(methylamino)-	H_3C-NH-$(CH_2)_3$-CH═O	3.12, 12.2
1491.	40654-82-8	0	1	0	Butanal, 2-methyl-4-phenyl-	C_5H_6-$(CH_2)_2$-$CH(CH_3)$-CH═O	3.12
1492.	4417-81-6	1	0	0	Butanal, 2-oxo- {ethylglyoxal}	H_3C-CH_2-CO-CH═O	3.12, 3.13
1493.	1758-51-6	0	1	0	Butanal, 2,3,4-trihydroxy-, (R*,R*)- {erythrose}	$HOCH_2$-$(CHOH)_2$-CH═O	2.5, 3.12, 8.3
1494.	541-35-5	1	0	0	Butanamide	H_3C-$(CH_2)_2$-CO-NH_2	13.1
1495.	66309-91-9	1	0	0	Butanamide, 2,3-dimethyl-	$(H_3C)_2$═CH-$CH(CH_3)$-CO-NH_2	13.1
1496.	1113-57-1	1	0	0	Butanamide, 2-methyl-	H_3C-CH_2-$CH(CH_3)$-CO-NH_2	13.1
1497.	61892-66-8	1	0	0	Butanamide, 3-cyano-3-methyl-	$(H_3C)_2$═C(CN)-CH_2-CO-NH_2	11.2, 13.1
1498.	541-46-8	1	0	0	Butanamide, 3-methyl-	$(H_3C)_2$═CH-CH_2-CO-NH_2	13.1
1499.	53897-27-1	1	0	0	Butanamide, 4-cyano-	NC-$(CH_2)_3$-CO-NH_2	11.2, 13.1
1500.	109-73-9	1	1	1	1-Butanamine	H_3C-$(CH_2)_3$-NH_2	12.2
1501.	71277-84-4	1	0	0	1-Butanamine, methyl-		12.2
1502.	96-15-1	1	1	1	1-Butanamine, 2-methyl-	H_3C-CH_2-$CH(CH_3)$-CH_2-NH_2	12.2
1503.	107-85-7	1	1	1	1-Butanamine, 3-methyl-	$(H_3C)_2$═CH-$(CH_2)_2$-NH_2	0.4, 12.2
1504.	78579-58-5	1	1	1	1-Butanamine, 3-methyl-*N*-propyl-	$(H_3C)_2$═CH-$(CH_2)_2$-NH-$(CH_2)_2$-CH_3	12.2
1505.	111-92-2	1	1	1	1-Butanamine, *N*-butyl-	$[H_3C$-$(CH_2)_3]_2$═NH	12.2
1506.	924-16-3	1	1	1	1-Butanamine, *N*-butyl-*N*-nitroso- {NDBA}	$[H_3C$-$(CH_2)_3]_2$═N-NO	12.2, 15.8, 23.5
1507.	110-68-9	1	1	1	1-Butanamine, *N*-methyl-	H_3C-$(CH_2)_3$-NH-CH_3	12.2
1508.	7068-83-9	1	0	0	1-Butanamine, *N*-methyl-*N*-nitroso-	H_3C-$(CH_2)_3$-N(NO)-CH_3	12.2, 15.8
1509.	39099-23-5	1	0	0	1-Butanamine, *N*-(1-methylethyl)-	H_3C-$(CH_2)_3$-NH-CH═$(CH_3)_2$	12.2
1510.	56375-33-8	1	0	0	1-Butanamine, *N*-nitroso-	H_3C-$(CH_2)_3$-NH-NO	12.2, 15.8
1511.	20810-06-4	1	1	1	1-Butanamine, *N*-(2-methylpropyl)-	H_3C-$(CH_2)_3$-NH-CH_2-CH═$(CH_3)_2$	12.2
1512.	20193-21-9	1	1	1	1-Butanamine, *N*-propyl-	H_3C-$(CH_2)_3$-NH-$(CH_2)_2$-CH_3	12.2
1513.	4104-44-3	0	1	0	1-Butanamine, *N*,3-dimethyl-	$(H_3C)_2$═CH-$(CH_2)_2$-NH-CH_3	12.2
1514.	13952-84-6	1	1	1	2-Butanamine	H_3C-CH_2-$CH(NH_2)$-CH_3	12.2
1515.	7713-69-1	1	1	1	2-Butanamine, *N*-methyl-	H_3C-CH_2-$CH(NH$-$CH_3)$-CH_3	12.2
1516.	626-23-3	0	1	0	2-Butanamine, *N*-(1-methylpropyl)-		12.2
1517.	106-97-8	1	0	0	Butane	H_3C-$(CH_2)_2$-CH_3	1.10
1518.	75-83-2	1	0	0	Butane, 2,2-dimethyl-	$(H_3C)_3$≡C-CH_2-CH_3	1.10
1519.	78-78-4 102056-77-9	1	1	1	Butane, 2-methyl- {methylbutane}	$(H_3C)_2$═CH-CH_2-CH_3	1.10
1520.	628-29-5	1	0	0	Butane, 1-(methylthio)- {butyl methyl sulfide}	H_3C-S-$(CH_2)_3$-CH_3	18.1
1521.	627-05-4	1	0	0	Butane, 1-nitro-	H_3C-$(CH_2)_2$-CH_2-NO_2	16.1
1522.	600-24-8	1	0	0	Butane, 2-nitro-	H_3C-CH_2-$CH(NO_2)$-CH_3	16.1
1523.	1613-46-3	1	0	0	Butane, 1-(propylthio)-	H_3C-$(CH_2)_2$-S-$(CH_2)_3$-CH_3	18.1

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1524.	544-40-1	1	0	0	Butane, 1,1′-thiobis- {dibutyl sulfide}	$H_3C\text{-}(CH_2)_3\text{-}S\text{-}(CH_2)_3\text{-}CH_3$	18.1
1525.	638-37-9	1	0	0	Butanedial {succinaldehyde}	$O{=}CH\text{-}(CH_2)_2\text{-}CH{=}O$	3.12
1526.	110-14-5	1	0	0	Butanediamide {succinamide}	$H_2N\text{-}CO\text{-}(CH_2)_2\text{-}CO\text{-}NH_2$	13.1
1527.	16748-73-5	0	1	0	Butanediamide, 2-amino-, (S)- {asparagine amide}	$H_2N\text{-}CO\text{-}CH_2\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$	12.2, 13.1
1528.	110-60-1	0	1	0	1,4-Butanediamine {putrescine}	$H_2N\text{-}(CH_2)_4\text{-}NH_2$	12.2
1529.	70185-59-0	0	1	0	1,4-Butanediamine, *N*-[3-(amino)-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy- {*p*-coumaroylspermidine}		12.2, 13.1
1530.	124-20-9	0	1	0	1,4-Butanediamine, *N*-(3-aminopropyl)- {spermidine}	$H_2N\text{-}(CH_2)_4\text{-}NH\text{-}(CH_2)_3\text{-}NH_2$	12.2
1531.	71-44-3	0	1	0	1,4-Butanediamine, *N,N′*-bis (3-aminopropyl)- {spermine}	$H_2N\text{-}(CH_2)_3\text{-}NH\text{-}(CH_2)_4\text{-}NH\text{-}(CH_2)_3\text{-}NH_2$	12.2
1532.	15657-58-6	0	1	0	1,4-Butanediamine, 2-methyl-	$H_2N\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\text{-}NH_2$	12.2
1533.	14475-60-6	0	1	0	1,4-Butanediamine, *N*-methyl-	$H_2N\text{-}(CH_2)_4\text{-}NH\text{-}CH_3$	12.2
1534.		0	1	0	1,4-Butanediamine, 3-phenylpropenoyl- {cinnamoylputrescine}		5.3, 12.2
1535.	110-61-2	1	0	0	Butanedinitrile {succinonitrile}	$NC\text{-}(CH_2)_2\text{-}CN$	11.2
1536.	16411-13-5	0	1	0	Butanedinitrile, 2,3-dimethyl-	$NC\text{-}CH(CH_3)\text{-}CH(CH_3)\text{-}CN$	11.2
1537.		1	1	1	Butanedioate, hydroxy- {malate}		2.5, 20.6
1538.	110-15-6	1	1	1	Butanedioic acid {succinic acid}	$HOOC\text{-}(CH_2)_2\text{-}COOH$	0.4, 4.3
1539.	121-75-5	1	1	1	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester {Malathion®}	$(H_3CO)_2{=}P{=}S$ | S | $HC\text{-}COO\text{-}C_2H_5$ | $H_2C\text{-}COO\text{-}C_2H_5$	5.3, 10.2, 18.1, 21.3
1540.	106-65-0	1	1	1	Butanedioic acid, dimethyl ester {dimethyl succinate}	$H_3C\text{-}OOC\text{-}(CH_2)_2\text{-}COO\text{-}CH$	5.3, 24.3
1541.	6915-15-7	1	1	1	Butanedioic acid, hydroxy- {malic acid}	$HOOC\text{-}CHOH\text{-}CH_2\text{-}COOH$	0.4, 2.5, 4.3, 24.3, 25.29
1542.		1	1	1	Butanedioic acid, hydroxy-, labeled with ^{14}C {malic acid-^{14}C}		2.5, 4.3, 25.29
1543.	16426-50-9	0	1	0	Butanedioic acid, hydroxy-, calcium salt		0.4, 2.5, 20.6
1544.	1587-15-1	1	0	0	Butanedioic acid, hydroxy-, dimethyl ester {dimethyl malate, malic acid dimethyl ester}	$H_3C\text{-}OOC\text{-}CHOH\text{-}CH_2\text{-}COO\text{-}CH_3$	2.5, 5.3
1545.	585-09-1	0	1	0	Butanedioic acid, hydroxy-, dipotassium salt	$KOOC\text{-}CHOH\text{-}CH_2\text{-}COOK$	0.4, 2.5, 20.6
1546.	676-46-0	0	1	0	Butanedioic acid, hydroxy-, disodium salt	$NaOOC\text{-}CHOH\text{-}CH_2\text{-}COONa$	2.5, 20.6
1547.	869-06-7	0	1	0	Butanedioic acid, hydroxy-, magnesium salt		0.4, 2.5, 20.6
1548.	71608-04-3	1	0	0	Butanedioic acid, (hydroxymethylene)-		2.5, 4.3
1549.	498-21-5	1	0	0	Butanedioic acid, methyl-	$HOOC\text{-}CH(CH_3)\text{-}CH_2\text{-}COOH$	4.3
1550.	636-60-2	1	0	0	Butanedioic acid, methyl-, (±)-		4.3
1551.	97-65-4	1	1	1	Butanedioic acid, methylene- {itaconic acid}	$HOOC\text{-}C(=CH_2)\text{-}CH_2\text{-}COOH$	4.3
1552.	2338-45-6	0	1	0	Butanedioic acid, (1-methylethyl)-		4.3
1553.	3878-55-5	1	1	1	Butanedioic acid, monomethyl ester	$HOOC\text{-}(CH_2)_2\text{-}COO\text{-}CH_3$	4.3, 5.3
1554.	328-42-7	0	1	0	Butanedioic acid, oxo- {oxalacetic acid}	$HOOC\text{-}CO\text{-}CH_2\text{-}COOH$	3.13, 4.3

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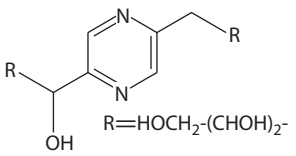
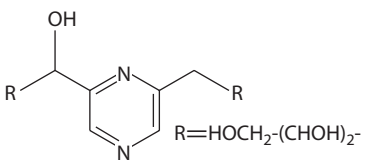
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1555.	3237-44-3	0	1	0	Butanedioic acid, 2-hydroxy-2-(1-methylethyl)-		2.5, 4.3
1556.	18734-79-7	0	1	0	Butanedioic acid, 2-methyl-3-phenyl-		4.3
1557.	35392-77-9	0	1	0	Butanedioicacid, 2,3-diethyl-,(R*,R*)-(±)- {succinic acid, 2,3-diethyl-}	$HOOC\text{-}CH(C_2H_5)\text{-}CH(C_2H_5)\text{-}COOH$	4.3
1558.	526-83-0	1	1	1	Butanedioic acid, 2,3-dihydroxy- {tartaric acid}	$HOOC\text{-}CHOH\text{-}CHOH\text{-}COOH$	2.5, 4.3, 24.3
1559.	147-71-7	0	1	0	Butanedioic acid, 2,3-dihydroxy- {*d*-tartaric acid}		2.5, 4.3
1560.	87-69-4	0	1	0	Butanedioic acid, 2,3-dihydroxy- {*l*-tartaric acid}		2.5, 4.3, 25.29
1561.	133-37-9	0	1	0	Butanedioic acid, 2,3-dihydroxy- {*dl*-tartaric acid}		2.5, 4.3
1562.	147-73-9	0	1	0	Butanedioic acid, 2,3-dihydroxy- {meso-tartaric acid}		2.5, 4.3
1563.	921-53-9	0	1	0	Butanedioic acid, 2,3-dihydroxy- [R-(R*,R*)]-, dipotassium salt		2.5, 20.6
1564.	13545-04-5	0	1	0	Butanedioic acid, 2,3-dimethyl- {succinic acid, 2,3-dimethyl-}	$HOOC\text{-}CH(CH_3)\text{-}CH(CH_3)\text{-}COOH$	4.3
1565.	52642-07-6	1	0	0	Butanediol, monoacetate		2.5, 5.3
1566.	107-88-0	1	1	1	1,3-Butanediol {1,3-butylene glycol}	$H_3C\text{-}CHOH\text{-}CH_2\text{-}CH_2OH$	2.5, 24.3, 25.29
1567.	110-63-4	0	1	0	1,4-Butanediol {tetramethylene glycol}	$HOCH_2\text{-}(CH_2)_2\text{-}CH_2OH$	2.5, 25.29
1568.	513-85-9	1	1	1	2,3-Butanediol	$H_3C\text{-}CHOH\text{-}CHOH\text{-}CH_3$	2.5
1569.	6982-25-8	1	0	0	*DL*-2,3-Butanediol		2.5
1570.	5341-95-7	1	0	0	2,3-Butanediol, (R*,S*)-		2.5
1571.	1438-90-0	1	0	0	1,2-Butanedione, 1-(2-furanyl)-		3.13, 10.2
1572.	431-03-8 29350-67-2	1	1	1	2,3-Butanedione {diacetyl, biacetyl}	$H_3C\text{-}CO\text{-}CO\text{-}CH_3$	0.4, 3.13, 24.3, 25.29
1573.	109-74-0	1	0	0	Butanenitrile	$H_3C\text{-}(CH_2)_2\text{-}CN$	11.2
1574.	13989-82-7	1	0	0	Butanenitrile, 4-(dimethylamino)-	$(H_3C)_2{=}N\text{-}(CH_2)_3\text{-}CN$	11.2, 12.2
1575.	4476-02-2	1	0	0	Butanenitrile, 2-hydroxy-	$H_3C\text{-}CH_2\text{-}CHOH\text{-}CN$	2.5, 11.2
1576.	15344-34-0	1	0	0	Butanenitrile, 2-hydroxy-3-methyl-	$(H_3C)_2{=}CH\text{-}CHOH\text{-}CN$	2.5, 11.2
1577.	18936-17-9 25570-03-0	1	0	0	Butanenitrile, 2-methyl-	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CN$	11.2
1578.	625-28-5	1	1	1	Butanenitrile, 3-methyl-	$(H_3C)_2{=}CH\text{-}CH_2\text{-}CN$	11.2
1579.	149-32-6	1	1	1	1,2,3,4-Butanetetrol, (R*,S*)- {erythritol}	$HOCH_2\text{-}(CHOH)_2\text{-}CH_2OH$	2.5, 8.3
1580.	68510-02-1	0	1	0	1,2,3,4-Butanetetrol, 1-[5-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,5-deoxyfructosazine}		2.5, 8.3, 17.7
1581.	68510-03-2	0	1	0	1,2,3,4-Butanetetrol, 1-[6-(2,3,4-trihydroxybutyl) pyrazinyl]- {2,6-deoxyfructosazine}		2.5, 8.3, 17.7
1582.	2431-51-1	1	0	0	Butanethioic acid, *S*-methyl ester		5.3, 18.1
1583.	109-79-5	1	0	0	1-Butanethiol {butyl mercaptan}	$H_3C\text{-}(CH_2)_3\text{-}SH$	18.1
1584.	541-31-1	1	0	0	1-Butanethiol, 3-methyl-	$(H_3C)_2{=}CH\text{-}(CH_2)_2\text{-}SH$	18.1
1585.	513-53-1	1	0	0	2-Butanethiol	$H_3C\text{-}CH_2\text{-}CH(SH)\text{-}CH_3$	18.1
1586.	4435-50-1	1	0	0	1,2,3-Butanetriol {1-methylglycerol}	$H_3C\text{-}CHOH\text{-}CHOH\text{-}CH_2OH$	2.5

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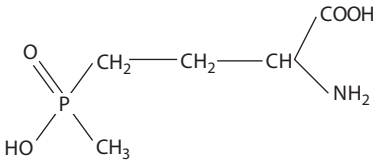
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1587.	3068-00-6	0	1	0	1,2,4-Butanetriol	$H_2COH\text{-}CHOH\text{-}CH_2\text{-}CH_2OH$	2.5
1588.		1	1	1	Butanimine	$H_3C\text{-}(CH_2)_2\text{-}CH{=}NH$	12.2
1589.	107-92-6	1	1	1	Butanoic acid {butyric acid}	$H_3C\text{-}(CH_2)_2\text{-}COOH$	0.4, 4.3, 24.3, 25.29
1590.	109-21-7	0	1	0	Butanoic acid, butyl ester	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}(CH_2)_3\text{-}CH_3$	5.3
1591.	10094-34-5	0	1	0	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester		5.3
1592.	106-29-6	0	1	0	Butanoic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl butyrate}		5.3
1593.	105-54-4	1	1	1	Butanoic acid, ethyl ester {ethyl butyrate}	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}C_2H_5$	5.3, 24.3, 25.29
1594.	26912-31-2	0	1	0	Butanoic acid, hexenyl ester	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}(CH_2)_{4-n}\text{-}CH{=}CH\text{-}(CH_2)_n\text{-}H$	5.3
1595.	623-42-7	0	1	0	Butanoic acid, methyl ester	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}CH_3$	5.3
1596.	539-90-2	0	1	0	Butanoic acid, 2-methylpropyl ester		5.3
1597.	540-18-1	0	1	0	Butanoic acid, pentyl ester	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}(CH_2)_4\text{-}CH_3$	5.3
1598.		1	0	0	Butanoic acid, phenyl ester	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}C_6H_5$	5.3
1599.	103-52-6	0	1	0	Butanoic acid, phenylethyl ester		5.3
1600.	103-37-7	1	1	1	Butanoic acid, phenylmethyl ester {benzyl butyrate}	$H_3C\text{-}(CH_2)_2\text{-}COO\text{-}CH_2\text{-}C_6H_5$	5.3, 24.3, 25.29
1601.	80-60-4	1	1	1	Butanoic acid, 2-amino-	$H_3C\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 12.2, 25.29
1602.	7004-04-8	1	1	1	Butanoic acid, 2-amino-3-hydroxy-	$H_3C\text{-}CHOH\text{-}CH(NH_2)\text{-}COOH$	2.5, 4.3, 4.10, 12.2
1603.	1927-25-9	0	1	0	Butanoic acid, 2-amino-4-hydroxy-		2.5, 4.3, 4.10, 12.2
1604.	51276-47-2 53369-07-6	0	1	0	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®}		4.3, 12.2, 21.3
1605.	454-41-1	0	1	0	Butanoic acid, 2-amino-4-(methylsulfinyl)-		4.3, 4.10, 12.2, 18.1
1606.	1118-85-0 3226-65-1	0	1	0	Butanoic acid, 2-amino-4-(methylsulfonyl)- {methionine sulfone, methionine S-oxide}	$H_3C\text{-}SO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 12.2, 18.1, 25.29
1607.	2338-03-6	0	1	0	Butanoic acid, 2-amino-4-oxo-, (S)-	$O{=}CH\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	3.12, 4.3, 4.10, 12.2
1608.	7492-70-8	0	1	0	Butanoic acid, 2-butoxy-1-methyl-2-oxoethyl ester {butyl butyryl lactate}		5.3
1609.	597-04-6	0	1	0	Butanoic acid, 2,2-dimethyl-3-oxo-		3.13, 4.3
1610.	14287-61-7	0	1	0	Butanoic acid, 2,3-dimethyl-	$(H_3C)_2{=}CH\text{-}CH(CH_3)\text{-}COOH$	4.3
1611.	141-16-2	0	1	0	Butanoic acid, 3,7-dimethyl-6-octenyl ester {citronellyl butyrate}		5.3
1612.	88-09-5	1	1	1	Butanoic acid, 2-ethyl- {diethylacetic acid}	$(H_3C\text{-}CH_2)_2{=}CH\text{-}COOH$	4.3
1613.	565-70-8	1	1	1	Butanoic acid, 2-hydroxy-	$H_3C\text{-}CH_2\text{-}CHOH\text{-}COOH$	2.5, 4.3
1614.	3739-30-8	0	1	0	Butanoic acid, 2-hydroxy-2-methyl-	$H_3C\text{-}CH_2\text{-}C(CH_3)(OH)\text{-}COOH$	2.5, 4.3
1615.	4026-18-0	1	1	1	Butanoic acid, 2-hydroxy-3-methyl-	$H_3C\text{-}CH(CH_3)\text{-}CHOH\text{-}COOH$	2.5, 4.3
1616.	116-53-0	1	1	1	Butanoic acid, 2-methyl- {2-methylbutyric acid}	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}COOH$	4.3, 24.3, 25.29
1617.	7452-79-1	0	1	0	Butanoic acid, 2-methyl-, ethyl ester	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}COO\text{-}CH_2\text{-}CH_3$	5.3, 24.3, 25.29
1618.	10032-15-2	0	1	0	Butanoic acid, 2-methyl-, hexyl ester	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}COO\text{-}(CH_2)_5\text{-}CH_3$	5.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1619.	868-57-5	0	1	0	Butanoic acid, 2-methyl-, methyl ester	H_3C-CH_2-CH(CH_3)-COO-CH_3	5.3
1620.	2445-78-5	0	1	0	Butanoic acid, 2-methyl-, 2-methylbutyl ester		5.3
1621.		0	1	0	Butanoic acid, 2-methyl-, 3-methylbutyl ester		5.3
1622.		0	1	0	Butanoic acid, 2-methyl-, 2-methylpropyl ester		5.3
1623.		0	1	0	Butanoic acid, 2-methyl-, 2-phenylethyl ester		5.3
1624.	600-18-0	1	1	1	Butanoic acid, 2-oxo-	H_3C-CH_2-CO-COOH	3.13, 4.3
1625.	78986-08-0	0	1	0	Butanoic acid, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-2-cyclohexen-1-yl ester		3.13, 5.3
1626.	2835-82-7	0	1	0	Butanoic acid, 3-amino-	H_3C-CH(NH_2)-CH_2-COOH	4.3, 4.10, 12.2
1627.	1070-83-3	0	1	0	Butanoic acid, 3,3-dimethyl-	$(H_3C)_3$≡C-CH_2-COOH	4.3
1628.	300-85-6	1	0	0	Butanoic acid, 3-hydroxy-	H_3C-CHOH-CH_2-COOH	2.5, 4.3
1629.	625-08-1	1	1	1	Butanoic acid, 3-hydroxy-3-methyl-	H_3C-C(CH_3)(OH)-CH_2-COOH	2.5, 4.3
1630.	503-74-2	1	1	1	Butanoic acid, 3-methyl- {isovaleric acid}	$(H_3C)_2$═CH-CH_2-COOH	0.4, 4.3, 24.3, 25.29
1631.	109-19-3	0	1	0	Butanoic acid, 3-methyl-, butyl ester		5.3
1632.	1009-20-6	0	1	0	Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadieny-1-yl ester		5.3
1633.	76-50-6	0	1	0	Butanoic acid, 3-methyl-, 1,7,7-trimethylbicyclo-[2.2.1]hept-2-yl ester, endo- {bornyl isovalerate}		5.3, 24.3
1634.	2445-77-4	0	1	0	Butanoic acid, 3-methyl-, 2-methylbutyl ester		5.3
1635.	78-35-3	0	1	0	Butanoic acid, 3-methyl-, 3, 7-dimethyl-1,6-octadien-6-yl ester {linalyl isobutyrate}		5.3
1636.	16409-46-4	0	1	0	Butanoic acid, 3-methyl-, 5-methyl-2-(1-methylethyl)-cyclohexanyl ester {menthyl isovalerate}		5.3
1637.	55066-56-3	1	1	1	Butanoic acid, 3-methyl-, 4-methylphenyl ester		5.3
1638.	589-59-3	0	1	0	Butanoic acid, 3-methyl-, 2-methylpropyl ester		5.3
1639.	140-26-1	1	1	1	Butanoic acid, 3-methyl-, 2-phenylethyl ester {phenethyl isovalerate}		5.3, 24.3, 25.29
1640.	108-64-5	1	1	1	Butanoic acid, 3-methyl-, ethyl ester {ethyl isovalerate}	$(H_3C)_2$═CH-CH_2-COO-C_2H_5	5.3, 24.3, 25.29
1641.	556-24-1	0	1	0	Butanoic acid, 3-methyl-, methyl ester {methyl isovalerate}	$(H_3C)_2$═CH-CH_2-COO-CH_3	5.3, 24.3, 25.29
1642.	659-70-1	1	1	1	Butanoic acid, 3-methyl-, 3-methylbutyl ester {isoamyl isovalerate}		5.3, 24.3, 25.29
1643.		1	0	0	Butanoic acid, 3-methyl-, 4-oxopentyl ester		3.13, 5.3
1644.	103-38-8	0	1	0	Butanoic acid, 3-methyl-, phenylmethyl ester {benzyl isovalerate}		5.3, 24.3, 25.29
1645.	140-27-2	1	1	1	Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester		5.3, 24.3, 25.29
1646.	106-27-4	0	1	0	Butanoic acid, 3-methylbutyl ester		5.3

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	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1647.	541-50-4	0	1	0	Butanoic acid, 3-oxo- {acetoacetic acid}	H_3C-CO-CH_2-COOH	3.13, 4.3
1648.	141-97-9	0	1	0	Butanoic acid, 3-oxo-, ethyl ester		3.13, 5.3
1649.	105-45-3	0	1	0	Butanoic acid, 3-oxo-, methyl ester {methyl acetoacetate}		3.13, 5.3
1650.	56-12-2	1	1	1	Butanoic acid, 4-amino-	H_2N-$(CH_2)_3$-COOH	0.4, 4.3, 4.10, 12.2
1651.	61445-55-4 133201-39-5	1	1	1	Butanoic acid, 4-(methylnitrosoamino)- = butanoic acid, 4-[(nitrosomethyl) amino]- {NMBA}	H_3C-N(NO)-$(CH_2)_3$-COOH	4.3, 4.10, 12.2, 15.8, 25.29
1652.	67557-56-6	1	0	0	Butanoic acid, 4-(methylnitrosoamino)-, methyl ester	H_3C-N(NO)-$(CH_2)_3$-$COOCH_3$	5.3, 12.2, 15.8
1653.	583-92-6	0	1	0	Butanoic acid, 4-(methylthio)-2-oxo-	H_3C-S-$(CH_2)_2$-CO-COOH	3.13, 4.3, 18.1
1654.	54344-76-2	0	1	0	Butanoic acid, 4-(2,6,6-trimethylcyclohexen-1-yl)-		4.3
1655.	462-10-2	0	1	0	Butanoic acid, 4,4′-dithiobis [2-amino- {homocystine}	[S-$(CH_2)_2$-CH(NH_2)-COOH]$_2$	4.3, 4.10, 12.2, 18.1
1656.	71-36-3	1	1	1	1-Butanol {*n*-butyl alcohol}	H_3C-$(CH_2)_2$-CH_2OH	2.5, 24.3, 25.29, 26.9
1657.	20281-85-0	0	1	0	1-Butanol, 2,3-dimethyl-		2.5
1658.		0	1	0	1-Butanol, 2-ethoxy-		2.5, 10.2
1659.	97-95-0	1	1	1	1-Butanol, 2-ethyl-		2.5
1660.	91599-03-0	0	1	0	1-Butanol, 4-[(7-β-*D*-glucopyranosyl-7*H*-purin-6-yl)amino]-2-methyl-		2.5, 10.2
1661.	137-32-6	1	1	1	1-Butanol, 2-methyl-		2.5
1662.	23599-75-9	1	1	1	1-Butanol, 2-methyl-4-(1*H*-purin-6-ylamino)- {dihydrozeatin}		2.5, 12.2
1663.	123-51-3	1	1	1	1-Butanol, 3-methyl- {isoamyl alcohol}		2.5
1664.	94-46-2	1	1	1	1-Butanol, 3-methyl-, benzoate {isoamyl benzoate}		5.3
1665.	78-92-2 15892-23-6	1	1	1	2-Butanol {*sec*-butyl alcohol}	H_3C-CH_2-CHOH-CH_3	2.5
1666.	6291-17-4	1	0	0	2-Butanol, 3-amino-2-methyl-		2.5, 12.2
1667.	155728-85-1	0	1	0	2-Butanol, 1-(4-bromophenoxy)-3-[(phenylmethyl)amino]-, (R*,R*)-		2.5, 12.2, 18.4
1668.	75-85-4	1	0	0	2-Butanol, 2-methyl-		2.5
1669.	598-75-4	1	0	0	2-Butanol, 3-methyl-		2.5
1670.	3293-47-8	0	1	0	2-Butanol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-		2.5
1671.	35734-62-4	1	0	0	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-		2.5, 3.13
1672.	51769-21-2	0	1	0	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (±)-		2.5, 3.13
1673.	495-40-9	1	0	0	1-Butanone, 1-phenyl-	H_3C-$(CH_2)_2$-CO-C_6H_5	3.13
1674.	61892-81-7	1	0	0	1-Butanone, 1-pyrazinyl-		3.13, 17.7
1675.	1701-70-8	1	1	1	1-Butanone, 1-(3-pyridinyl)- {propyl pyridyl ketone}		3.13, 17.7
1676.	28384-26-1	0	1	0	1-Butanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-		3.13
1677.		1	0	0	1-Butanone, 1-(methyl-2-pyridinyl)-		3.13, 17.7
1678.	22971-32-0	1	0	0	1-Butanone, 1-(2-pyridinyl)-		3.13, 17.7
1679.		1	0	0	1-Butanone, 1-(3-methyl-2-pyridinyl)-		3.13, 17.7
1680.		1	0	0	1-Butanone, 1-(4-methyl-2-pyridinyl)-		3.13, 17.7
1681.	78210-70-5	1	0	0	1-Butanone, 2-methyl-1-(3-pyridinyl)-		3.13, 17.7

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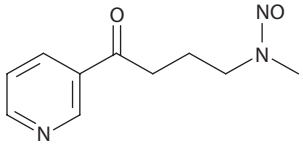
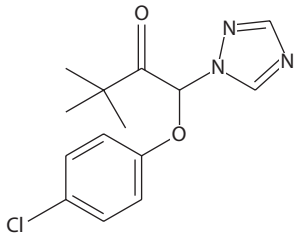
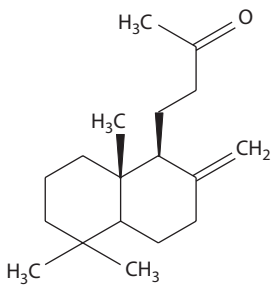
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1682.	68697-66-5	0	1	0	1-Butanone, 3-(methylthio)-1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-		3.13, 18.1
1683.		0	1	0	1-Butanone, 3-(methylthio)-1-(2,6,6-trimethylcyclohexenyl)-		3.13, 18.1
1684.	71278-11-0	1	1	1	1-Butanone, 4-amino-1-(3-pyridinyl)- {poikiline}		0.4, 3.13, 12.2, 17.7
1685.	59578-62-0	1	1	1	1-Butanone, 4-hydroxy-1-(3-pyridinyl)-		2.5, 3.13, 17.7
1686.		0	1	0	1-Butanone, 4-(methylamino)-1-(2.6-dihydroxy-3-pyridinyl)-		2.5, 3.13, 12.2, 17.7
1687.		0	1	0	1-Butanone, 4-(methylamino)-1-(6-hydroxy-pyridinyl)-		2.5, 3.13, 12.2, 17.7
1688.	2055-23-4	0	1	0	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)- {pseudooxynicotine}		0.4, 3.13, 12.2, 17.7
1689.	26165-82-0 64091-91-4 110053-55-9 121268-99-3	1	1	1	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK} {1-Butanone, 4-[(nitrosomethyl) amino]-1-(3-pyridinyl)-}		3.13, 12.2, 15.8, 17.7, 23.5
1690.	76014-82-9	0	1	0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-, *N*-oxide		3.13, 12.2, 15.8, 17.7
1691.	78-93-3	1	1	1	2-Butanone {methyl ethyl ketone}	H_3C-CO-CH_2-CH_3	3.13, 23.5, 24.3
1692.	1575-57-1	1	1	1	2-Butanone, 1-(acetyloxy)-	H_3C-CH_2-CO-CH_2-OOC-CH_3	3.13, 5.3
1693.	43121-43-3	0	1	0	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl) {Triadimefon®}		3.13, 10.2, 17.4, 18.4, 21.3
1694.	5077-67-8	1	1	1	2-Butanone, 1-hydroxy-	H_3C-CH_2-CO-CH_2OH	2.5, 3.13
1695.	1007-32-5	1	0	0	2-Butanone, 1-phenyl-	C_6H_5-CH_2-CO-CH_2-CH_3	3.13
1696.	75-97-8	1	0	0	2-Butanone, 3,3-dimethyl-	H_3C-CO-C≡$(CH_3)_3$	3.13
1697.	38895-88-4	1	0	0	2-Butanone, 3,3-dimethyl-4-hydroxy-	H_3C-CO-C═$(CH_3)_2$-CH_2OH	2.5, 3.13
1698.	57011-15-1	1	0	0	2-Butanone, 3,4-dihydroxy-	H_3C-CO-CHOH-CH_2OH	2.5, 3.13
1699.	513-86-0	1	1	1	2-Butanone, 3-hydroxy- {acetoin}	H_3C-CO-CHOH-CH_3	2.5, 3.13, 24.3, 25.29
1700.	563-80-4	1	1	1	2-Butanone, 3-methyl-	H_3C-CO-CH═$(CH_3)_2$	3.13
1701.	53872-97-2	1	0	0	2-Butanone, 3-methyl-1-(3-pyridinyl)-		3.13, 17.7
1702.	10150-87-5	1	0	0	2-Butanone, 4-(acetyloxy)-	H_3C-CO-CH_2-CH_2-OOC-CH_3	3.13, 5.3
1703.	10266-75-8	0	1	0	2-Butanone, 4-(decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl)-, [1S-(1α,4aβ,8aα)]-		3.13
1704.	699-17-2	1	1	1	2-Butanone, 4-(2-furanyl)-		3.13, 10.2

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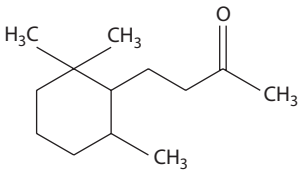
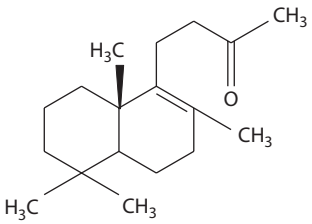
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1705.	590-90-9	1	1	1	2-Butanone, 4-hydroxy-	$H_3C\text{-}CO\text{-}CH_2\text{-}CH_2OH$	2.5, 3.13
1706.	1823-90-1	1	0	0	2-Butanone, 4-hydroxy-3,3-dimethyl-	$H_3C\text{-}CO\text{-}C(CH_3)_2\text{-}CH_2OH$	2.5, 3.13
1707.	104-20-1	0	1	0	2-Butanone, 4-(4-methoxyphenyl)-		3.13, 10.2
1708.	34047-39-7	1	1	1	2-Butanone, 4-(methylthio)-		3.13, 18.1
1709.	2550-26-7	1	0	0	2-Butanone, 4-phenyl-	$H_3C\text{-}CO\text{-}(CH_2)_2\text{-}C_6H_5$	3.13
1710.	50767-77-6	0	1	0	2-Butanone, 4-(2-ethenyl-2, 6,6-trimethylcyclohexyl)-		3.13
1711.	133007-80-4	0	1	0	2-Butanone, 4-(6-ethenyl-2, 2,6-trimethylcyclohexyl)-		3.13
1712.	6138-85-8	0	1	0	2-Butanone,4-(2,2,6-trimethylcyclohexyl)- {tetrahydroionone}		3.13
1713.	60761-23-1	0	1	0	2-Butanone, 4-(2,2,6-trimethylcyclohexyl)-, *cis*- {*cis*-tetrahydroionone}		3.13
1714.	58720-40-4	0	1	0	2-Butanone, 4-(2,3,6-trimethylphenyl)-		3.13
1715.	20483-36-7	0	1	0	2-Butanone, 4-(2,6,6-trimethyl-1, 3-cyclohexadien-1-yl)-		3.13
1716.	14506-65-1	0	1	0	2-Butanone, 4-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, (4aS-*trans*)-		3.13
1717.	158815-72-6	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1, 2-dioxin-3-yl]-, (*E*)-		2.5, 3.13, 10.2
1718.	158815-73-7	0	1	0	2-Butanone,4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)-		2.5, 3.13, 10.2
1719.	160115-51-5	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)- (+)-		2.5, 3.13, 10.2
1720.	160115-52-6	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)-(-)-		2.5, 3.13, 10.2
1721.		0	1	0	2-Butanone, 4-[5,6-dihydro-3-methyl-6-(1-methylethyl)-pyran-2yl]-		3.13, 10.2
1722.	5471-51-2	1	1	1	2-Butanone, 4-(4-hydroxyphenyl)- {4-(*p*-hydroxyphenyl)-2-butanone}		3.13, 9.22, 24.3, 25.29
1723.	13679-56-6	1	1	1	2-Butanone, 4-(5-methyl-2-furanyl)-		3.13, 10.2
1724.		0	1	0	2-Butanone, 4-(2-methyl-5-(1-methylethyl)-2-furanyl)-		3.13, 10.2
1725.		0	1	0	2-Butanone, 4-(2-methyl-6-(1-methylethyl)-2-tetrahydropyranyl)-		3.13, 10.2
1726.		0	1	0	2-Butanone, 4-[5,6-dihydro-3-methyl-6-(1-methylethyl)-pyran-2-yl]-		3.13, 10.2

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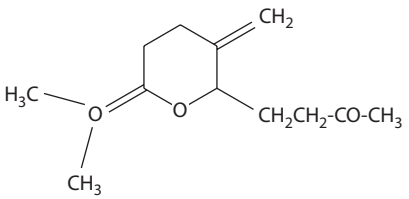
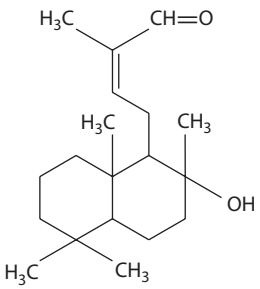
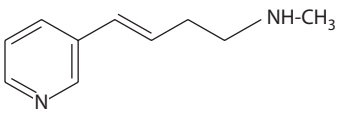
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1727.		0	1	0	2-Butanone, 4-(4,5-dihydro-3-methylene-6-dimethylmethylene-2-pyranyl)-		3.13, 10.2
1728.	52690-42-3	0	1	0	2-Butanone, 4-[2,2,6-trimethyl-6-(methylethylene)cyclohexyl]-		3.13
1729.	4170-30-3	1	1	1	2-Butenal {crotonaldehyde}	H_3C-CH═CH-CH═O	3.12, 23.5
1730.	1115-11-3	1	1	1	2-Butenal, 2-methyl-	H_3C-CH═C(CH_3)-CH═O	3.12
1731.	107-86-8	1	0	0	2-Butenal, 3-methyl- {senecialdehyde}	H_3C-C(CH_3)═CH-CH═O	3.12
1732.	83841-47-8	0	1	0	2-Butenal, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-2-methyl-, [1R-[1α(*E*),2β,4aβ,8aα]]-		2.5, 3.12
1733.	7319-38-2	1	0	0	3-Butenal	H_2C═CH-CH_2-CH═O	3.12
1734.	123-73-9	1	1	1	2-Butenal (*E*)		3.12
1735.	15798-64-8	1	0	0	2-Butenal (*Z*)		3.12
1736.	497-03-0	1	0	0	2-Butenal, 2-methyl-, (*E*)- {tiglic aldehyde}		3.12
1737.	625-37-6 23350-58-5	1	0	0	2-Butenamide, (*E*)- {*trans*-crotonamide}	H_3C-CH═CH-CO-NH_2	13.1
1738.	31110-30-2	1	0	0	2-Butenamide, (*Z*)-		13.1
1739.	1187-41-3 72693-06-2	1	0	0	2-Butenamide, *N*,2-dimethyl-		13.1
1740.	23350-60-9	1	0	0	2-Butenamide, *N*-ethyl-		13.1
1741.	6923-22-4	0	1	0	2-Butenamide, 3-hydroxy-*N*-methyl-, dimethylphosphate, (*Z*)- {Monocrotophos®}		2.5, 13.1, 21.3
1742.	32793-37-6	1	0	0	2-Butenamide, 2-methyl-		13.1
1743.	28446-58-4	1	0	0	3-Butenamide	H_2C═CH-CH_2-CO-NH_2	13.1
1744.	18938-03-9	1	0	0	3-Butenamide, 3-methyl-		13.1
1745.	82806-40-4	1	1	1	Butenamine		12.2
1746.	692-31-9	1	0	0	2-Buten-1-amine, *N*,*N*-dimethyl-	H_3C-CH═CH-CH_2-N═(CH_3)$_2$	12.2
1747.	2524-49-4	1	0	0	3-Buten-1-amine	H_2C═CH-CH_2-CH_2-NH_2	12.2
1748.	20173-36-8	1	0	0	3-Buten-1-amine, *N*,*N*-dimethyl-4-(3-pyridinyl)-		12.2, 17.7
1749.	538-79-4	1	1	1	3-Buten-1-amine, *N*-methyl-4-(3-pyridinyl)- {metanicotine}		0.4, 12.2, 17.7
1750.		1	0	0	1-Buten-1-aminocarbonyl- (1*E*)- {[(1*E*)-1-but-1-en-1-yl]aminocarbonyl-}	CH_3CH_2-CH═CH-NH-C═O	27.1
1751.	25167-67-3	1	0	0	Butene		1.11
1752.		1	0	0	Butene, dimethyl-		1.11

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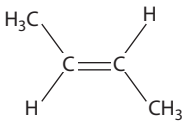
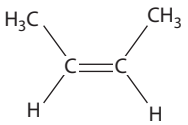
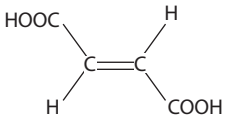
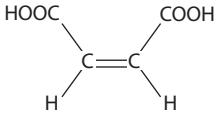
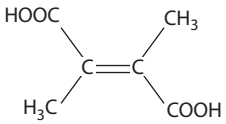
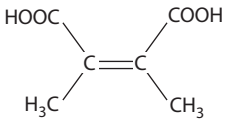
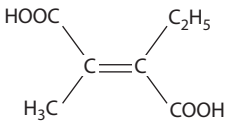
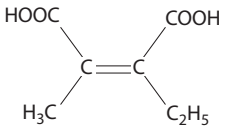
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1753.		1	0	0	Butene, methyl-		1.11
1754.	26760-64-5	1	0	0	Butene, 2-methyl-		1.11
1755.	106-98-9 9003-28-5	1	0	0	1-Butene	$H_2C{=}CH\text{-}CH_2\text{-}CH_3$	1.11
1756.	563-78-0	1	1	1	1-Butene, 2,3-dimethyl-	$H_2C{=}C(CH_3)\text{-}CH{=}(CH_3)_2$	1.11
1757.	558-37-2	1	0	0	1-Butene, 3,3-dimethyl-	$H_2C{=}CH\text{-}C{\equiv}(CH_3)_3$	1.11
1758.	563-46-2	1	0	0	1-Butene, 2-methyl-	$H_2C{=}C(CH_3)\text{-}CH_2\text{-}CH_3$	1.11
1759.	563-45-1	1	0	0	1-Butene, 3-methyl-	$H_2C{=}CH\text{-}CH{=}(CH_3)_2$	1.11
1760.	107-01-7	1	0	0	2-Butene	$H_3C\text{-}CH{=}CH\text{-}CH_3$	1.11
1761.	624-64-6	1	0	0	2-Butene, (*E*)		1.11
1762.	590-18-1	1	0	0	2-Butene, (*Z*)-		1.11
1763.	563-79-1	1	0	0	2-Butene, 2,3-dimethyl-	$(H_3C)_2{=}C{=}C{=}(CH_3)_2$	1.11
1764.	513-35-9	1	1	1	2-Butene, 2-methyl-	$(H_3C)_2{=}C{=}CH\text{-}CH_3$	1.11
1765.	6915-18-0	0	1	0	2-Butenedioic acid	$HOOC\text{-}CH{=}CH\text{-}COOH$	4.3
1766.	110-17-8	1	1	1	2-Butenedioic acid (*E*)- {fumaric acid}		0.4, 4.3, 25.29
1767.	110-16-7	1	1	1	2-Butenedioic acid (*Z*)- {maleic acid}		4.3
1768.	623-91-6	0	1	0	2-Butenedioic acid (*E*)-, diethyl ester {diethyl fumarate}		5.3
1769.	141-05-9	1	0	0	2-Butenedioic acid (*Z*)-, diethyl ester {diethyl maleate}		5.3
1770.	21788-49-8	0	1	0	2-Butenedioic acid, 2,3-dimethyl-, (*E*)-		4.3
1771.	488-21-1	0	1	0	2-Butenedioic acid, 2,3-dimethyl-, (*Z*)-		4.3
1772.	624-48-6	1	0	0	2-Butenedioic acid (*Z*)-, dimethyl ester		5.3
1773.	28098-80-8	0	1	0	2-Butenedioic acid, 2-ethyl-3-methyl-, (*E*)-		4.3
1774.	41654-09-5	0	1	0	2-Butenedioic acid, 2-ethyl-3-methyl-, (*Z*)-		4.3

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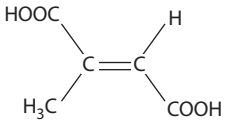
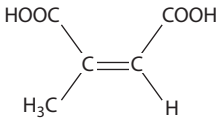
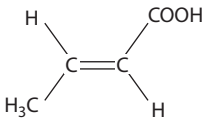
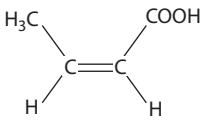
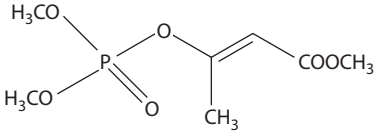
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
1775.	498-24-8	1	0	0	2-Butenedioic acid, 2-methyl-, (*E*)- {mesaconic acid}		4.3
1776.	498-23-7	1	1	1	2-Butenedioic acid, 2-methyl-, (*Z*)- {citraconic acid}		4.3
1777.	4151-35-3	1	0	0	2-Butenedioic acid (*E*)-, dipotassium salt		20.6
1778.	17013-01-3	1	0	0	2-Butenedioic acid (*E*)-, disodium salt		20.6
1779.	497-06-3	1	0	0	3-Butene-1,2-diol	$HOCH_2$-CHOH-CH=CH_2	2.5
1780.	4786-20-3	1	0	0	2-Butenenitrile {crotononitrile}	H_3C-CH=CH-CN	11.2
1781.	1190-76-7	1	0	0	2-Butenenitrile [*cis* or *trans*]		11.2
1782.	4786-24-7	1	0	0	2-Butenenitrile, 3-methyl-		11.2
1783.	109-75-1	1	0	0	3-Butenenitrile {allyl cyanide}	H_2C=CH-CH_2-CN	11.2
1784.	4786-19-0	1	0	0	3-Butenenitrile, 3-methyl-		11.2
1785.	3724-65-0	1	1	1	2-Butenoic acid {crotonic acid}	H_3C-CH=CH-COOH	4.3
1786.	107-93-7	1	1	1	2-Butenoic acid, (*E*)- {*trans*-crotonic acid}		4.3
1787.	503-64-0	1	0	0	2-Butenoic acid, (*Z*)- {*cis*-crotonic acid}		4.3
1788.	10544-63-5	0	1	0	2-Butenoic acid (*E*)-, ethyl ester {ethyl crotonate}		5.3
1789.	18707-60-3	0	1	0	2-Butenoic acid, methyl ester {methyl crotonate}	H_3C-CH=CH-COO-CH_3	5.3
1790.	13201-46-2	1	1	1	2-Butenoic acid, 2-methyl-, (*Z*)- {angelic acid}		4.3, 24.3
1791.	80-59-1	1	1	1	2-Butenoic acid, 2-methyl-, (*E*)- {tiglic acid}		4.3, 24.3, 25.29
1792.	37526-88-8	0	1	0	2-Butenoic acid, 2-methyl-, phenylmethyl ester {benzyl tiglate}		5.3
1793.	39300-45-3	0	1	0	2-Butenoic acid, 2-(1-methylheptyl)-4,6-dinitrophenyl ester {Dinocap®}		5.3, 16.1, 21.3
1794.	7786-34-7	0	1	0	2-Butenoic acid, 3[(dimethoxyphosphinyl)oxy]-, methyl ester {Mevinphos®, Phosdrin®}		5.3, 10.2, 21.3
1795.	541-47-9	1	1	1	2-Butenoic acid, 3-methyl-		4.3, 24.3
1796.	32040-41-8	0	1	0	2-Butenoic acid, 4-(formylamino)-4-oxo-, (Z)-	O=CH-NH-CO-CH=CH-COOH	4.3, 13.1
1797.	625-38-7	1	0	0	3-Butenoic acid	H_2C=CH-CH_2-COOH	4.3
1798.	1617-31-8	1	1	1	3-Butenoic acid, 3-methyl-		4.3
1799.	2243-53-0	1	1	1	3-Butenoic acid, 4-phenyl- {styrylacetic acid}		4.3
1800.	43000-45-9	1	1	1	1-Buten-1-ol, 3-methyl-		2.5
1801.	4675-87-0	0	1	0	2-Buten-1-ol, 2-methyl-		2.5

(*continued*)

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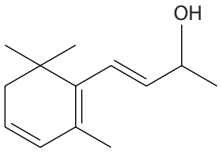
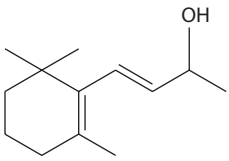
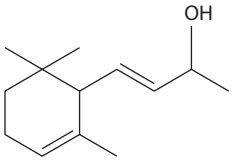
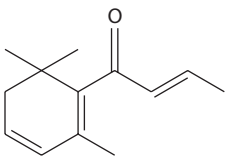
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1802.	556-82-1	0	1	0	2-Buten-1-ol, 3-methyl-		2.5
1803.	1637-39-4	0	1	0	2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylamino)-, (*E*)-		2.5, 12.2
1804.		0	1	0	2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylaminoribosyl)-		2.5, 8.3, 12.2
1805.	29736-33-2	0	1	0	2-Buten-1-ol, 2-methyl-4-[[2-(methylthio)-1*H*-purin-6-yl]amino]-, (*E*)-		2.5, 12.2, 18.1
1806.	72074-11-4	0	1	0	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2-yl)-, [2S-[2α(*E*),3aα,5aβ,9aα,9bβ]]-		2.5, 10.2
1807.	87584-34-7	0	1	0	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2-yl)-, [2R-[2α(*E*),3aβ,5aα,9aβ,9bα]]-		2.5, 10.2
1808.	627-27-0	1	0	0	3-Buten-1-ol	$H_2C{=}CH\text{-}CH_2\text{-}CH_2OH$	2.5
1809.	115-18-4	1	0	0	3-Buten-2-ol, 2-methyl-	$H_2C{=}CH\text{-}CHOH{=}(CH_3)_2$	2.5
1810.	1504-55-8	0	1	0	3-Buten-2-ol, 4-phenyl-	$C_6H_5\text{-}CH{=}CH\text{-}CHOH\text{-}CH_3$	2.5
1811.	13215-89-9	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-		2.5
1812.	33759-63-6	1	1	1	3-Buten-2-ol, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-{3-hydroxy-β-ionol}		2.5
1813.	27185-80-4	0	1	0	3-Buten-2-ol, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-{4-hydroxy-β-ionol}		2.5
1814.	27008-60-2 22029-76-1	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-{β-ionol}		2.5
1815.	472-80-0	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3*E*)-{β-ionol, (*E*)}		2.5
1816.	472-78-6	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-{α-ionol}		2.5
1817.	79925-80-7	0	1	0	3-Buten-2-ol, 4-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)-		2.5
1818.	54345-38-9	0	1	0	2-Buten-1-one, 1-(2,3,6-trimethylphenyl)-, (*E*)-		3.13
1819.	23726-93-4 23696-85-7	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)-{β-damascenone}		3.13, 24.3, 25.29

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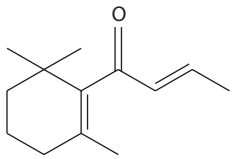
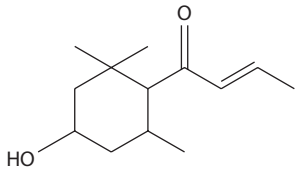
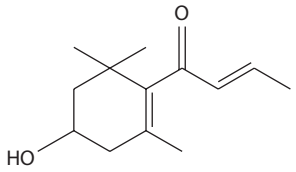
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1820.		0	1	0	2-Buten-1-one, 1-(2,6,6-trimethyl-1, 3-cyclohexadien-1-yl)- {β-damascenone isomer}		3.13
1821.	80111-68-8 23770-92-3 35044-68-9	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)- {damascone}		3.13, 24.3
1822.	23726-91-2	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-		3.13
1823.	23726-92-3 85949-43-5	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)- {β-damascone}		3.13
1824.	43052-87-5	0	1	0	2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-damascone}		3.13
1825.	102488-09-5	1	1	1	2-Buten-1-one, 1-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {3-hydroxy-β-damascone}		2.5, 3.13
1826.	80508-24-3	1	0	0	2-Buten-1-one, 1-(3-pyridinyl)-		3.13, 17.7
1827.	53398-17-7	0	1	0	2-Buten-1-one, 1-(4-hydroxy-2,6, 6-trimethycyclohexanyl)- {4-hydroxydihydro-β-damascone}		2.5, 3.13
1828.	56915-02-7	1	1	1	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-damascone}		2.5, 3.13
1829.	35734-61-3	1	1	1	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-		2.5, 3.13
1830.	160550-79-8	0	1	0	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, [R-(*E*)]-		2.5, 3.13
1831.	87562-12-7	0	1	0	2-Buten-1-one, 1-[3-(formyloxy)-2,6, 6-trimethyl-1-cyclohexen-1-yl]-, (*E*)-		3.13, 5.3
1832.	62512-25-8	0	1	0	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-		2.5, 3.13, 8.3, 10.2
1833.	160550-77-6	0	1	0	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-		2.5, 3.13, 8.3, 10.2
1834.	495-45-4	0	1	0	2-Buten-1-one, 1,3-diphenyl-		3.13
1835.	78-94-4	1	1	1	3-Buten-2-one {methyl vinyl ketone}	$H_2C{=}CH\text{-}CO\text{-}CH_3$	3.13
1836.	814-78-8	1	0	0	3-Buten-2-one, 3-methyl-	$H_2C{=}C(CH_3)\text{-}CO\text{-}CH_3$	3.13
1837.	127-51-5	0	1	0	3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-isomethylionone}		3.13
1838.	73892-47-4	0	1	0	3-Buten-2-one, 4-[3-(acetyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-,[R-(*E*)]-		3.13, 5.3

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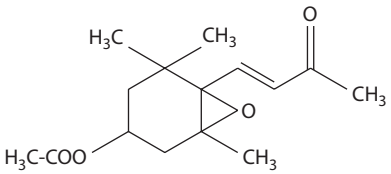
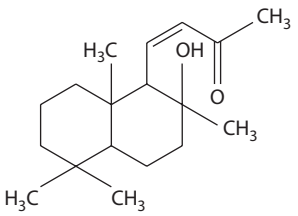
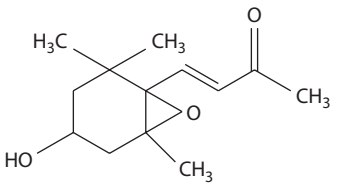
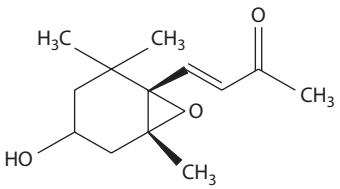
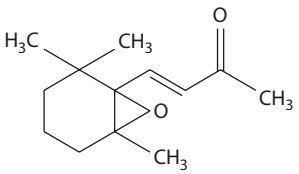
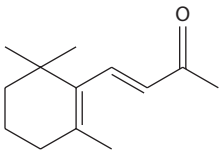
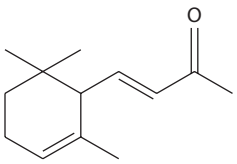
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1839.	50281-40-8	0	1	0	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0] hept-1-yl]-, [1R-[1α(*E*),4β,6α]]-		3.13, 5.3, 10.2
1840.	50281-41-9	0	1	0	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0] hept-1-yl]-, [1S-[1α(*E*),4α,6α]]-		3.13, 5.3, 10.2
1841.	52811-61-7	1	0	0	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-		2.5, 3.13
1842.	42569-64-2	0	1	0	3-Buten-2-one, 4-(decahydro-2-hydroxy-2, 5,5,8a-tetramethyl-1-naphthalenyl)-, [1R-[1α(*E*),2β,4aβ,8aα]]-		2.5, 3.13
1843.	54656-80-3	0	1	0	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1α(*E*),2α,4aβ,8aα]-(±)-		2.5, 3.13
1844.	36340-49-5	0	1	0	3-Buten-2-one, 4-(1,2-epoxy-2,6,6-trimethylcyclohexyl)-, (*E*)-		3.13, 10.2
1845.	623-15-4	1	1	1	3-Buten-2-one, 4-(2-furanyl)-		3.13, 10.2, 24.3
1846.	81540-27-4	1	1	1	3-Buten-2-one, 4-(2-furanyl)-3-methyl-		3.13, 10.2
1847.	15356-75-9	0	1	0	3-Buten-2-one, 4(1-hydroxy-2,2-dimethyl-6-methylenecyclohexyl)-		2.5, 3.13
1848.	15356-76-0	0	1	0	3-Buten-2-one, 4-(1-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)-		2.5, 3.13
1849.	15401-34-0	0	1	0	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-		2.5, 3.13
1850.	14398-34-6	0	1	0	3-Buten-2-one,4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-		2.5, 3.13
1851.	61892-82-8	1	0	0	3-Buten-2-one, 4-(4-hydroxy-1-cyclohexen-1-yl)-		2.5, 3.13
1852.	31253-95-9	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)		2.5, 3.13
1853.	50281-42-0	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1S-[1α(*E*),4α,6α]]-		2.5, 3.13, 10.2
1854.	61116-99-2	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1R-[1α(*E*),4β,6α]]-		2.5, 3.13, 10.2

(continued)

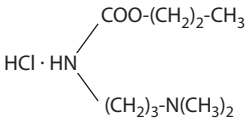
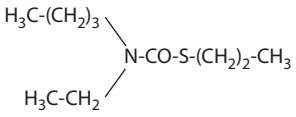
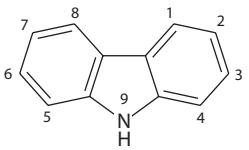
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1855.	72491-46-4	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-ionone}		2.5, 3.13
1856.	38963-41-6	1	0	0	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)- {4-hydroxy-α-i}		2.5, 3.13
1857.	23120-57-2	1	0	0	3-Buten-2-one, 4-(5-methyl-2-furanyl)-		3.13, 10.2
1858.	66434-99-9	0	1	0	3-Buten-2-one, 4-(5-methyl-2-furanyl)-,(*E*)-		3.13, 10.2
1859.	98910-85-1	0	1	0	3-Buten-2-one, 4-(4-oxo-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-oxo-β-ionone}		3.13
1860.	122-57-6	1	1	1	3-Buten-2-one, 4-phenyl-	C_6H_5-CH═CH-CO-CH_3	3.13, 24.3, 25.29
1861.	2433-57-0	1	0	0	3-Buten-2-one, 4-(1*H*-pyrrol-2-yl)-, (*E*)-		3.13, 17.4
1862.	79-69-6	0	1	0	3-Buten-2-one, 4-(2,5,6,6-tetramethyl-2-cyclohexen-1-yl)- {α-irone}		3.13
1863.	23267-57-4	0	1	0	3-Buten-2-one, 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-		3.13, 10.2
1864.	56681-06-2	0	1	0	3-Buten-2-one, 4-(2,3,6-trimethylphenyl)-		3.13
1865.	1203-08-3	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- {dehydro-β-ionone}		3.13
1866.	14398-35-7	0	1	0	3-Buten-2-one, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)-		3.13
1867.	14901-07-6	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- {β-ionone}		3.13, 24.3, 25.29
1868.	79-77-6	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)-		3.13
1869.	127-41-3 8013-90-9 6901-97-9	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- {α-ionone}		3.13, 24.3, 25.29
1870.	689-97-4	1	0	0	1-Buten-3-yne	H_2C═CH-C≡CH	1.11
1871.	19062-98-7	1	0	0	Butoxyl radical	$CH_3(CH_2)_3O$	27.1
1872.		1	0	0	*tert*-Butoxyl radical		27.1
1873.	1119-19-3	1	0	0	2-Butynal	H_3C-C≡C-CH═O	3.12
1874.		1	0	0	Butyne	H-$(CH_2)_n$-C≡C-$(CH_2)_{(2-n)}$-H	1.11
1875.	107-00-6	1	0	0	1-Butyne	H_3C-CH_2-C ≡CH	1.11
1876.	503-17-3	1	1	1	2-Butyne	H_3C-C≡C-CH_3	1.11
1877.	7440-43-9	1	1	1	Cadmium	Cd	0.4, 20.5, 23.5
1878.	7440-70-2	1	1	1	Calcium	Ca	0.4, 20.5
1879.	1305-78-8	0	1	0	Calcium hydroxide	$Ca(OH)_2$	20.6
1880.	14127-61-8	0	1	0	Calcium, ion	Ca^{+2}	20.5

(*continued*)

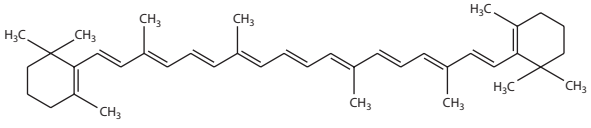
(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1881.	10043-52-4	0	1	0	Calcium chloride	$CaCl_2$	18.4, 20.6
1882.	1305-78-8	0	1	0	Calcium oxide	CaO	20.6
1883.	15124-81-9	0	1	0	Calcium, isotope of mass 49		20.5
1884.	9064-51-1 54724-00-4	0	1	0	Callose {1,3-β-*D*-glucan}		2.5, 8.3
1885.		0	1	0	*Campylobacter*		22.2
1886.	101-21-3	0	1	0	Carbamic acid, 3-chlorophenyl-, (1-methylethyl) ester {Chloropropham®}		5.3, 18.4, 21.3
1887.	23103-98-2	0	1	0	Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester {Pirimicarb®}		5.3, 13.1, 21.3, 17.7, 21.3
1888.	25606-41-1	0	1	0	Carbamic acid, 3-(dimethylamino)propyl-, propyl ester, hydrochloride {Propamocarb hydrochloride®}		5.3, 13.1, 18.4, 21.3
1889.	51-79-6	1	1	1	Carbamic acid, ethyl ester {urethane}	$H_2N\text{-}COO\text{-}C_2H_5$	5.3, 13.1, 23.5
1890.	598-55-0	0	1	0	Carbamic acid, methyl ester	$H_2N\text{-}COO\text{-}CH_3$	5.3, 13.1
1891.	137-42-8	0	1	0	Carbamic acid, *N*-methyldithio-, monosodium salt {Metham-sodium®}		18.1, 20.6, 21.3
1892.	594-07-0	0	1	0	Carbamodithioic acid	$H_2N\text{-}CSSH$	4.3, 18.1
1893.	9006-42-2	0	1	0	Carbamodithioic acid, 1,2-ethylene(bis-, polymer with ammonia complex of zinc ethylenebis-dithiocarbamate {Metiram®}		18.1, 20.6, 21.3
1894.	1114-71-2	0	1	0	Carbamothioic acid, butylethyl-, *S*-propyl ester {Tillam®, Pebulate®}		5.3, 13.1, 18.1, 21.3
1895.	759-94-4	0	1	0	Carbamothioic acid, dipropyl-, *S*-ethyl ester {EPTC®}		5.3, 13.1, 18.1, 21.3
1896.	1929-77-7	0	1	0	Carbamothioic acid, dipropyl-, *S*-propyl ester {Vernolate®}		5.3, 13.1, 18.1, 21.3
1897.	2303-17-5	0	1	0	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester {Triallate®}		5.3, 13.1, 18.1, 18.4, 21.3
1898.	9012-49-1	0	1	0	Carbamoyltransferase, aspartate		22.2
1899.		1	0	0	Carbazole		17.21
1900.	86-74-8	1	0	0	9*H*-Carbazole {9-azafluorene, dibenzo[*b,d*]pyrrole}		17.21, 25.29
1901.		1	0	0	9*H*-Carbazole, alkyl-		17.21
1902.		1	0	0	9*H*-Carbazole, 9-alkyl-		17.21
1903.	4539-51-9	1	0	0	9*H*-Carbazole, 2-amino-		12.2
1904.		1	0	0	9*H*-Carbazole, 2-aminoethyl-		12.2
1905.	30642-38-7	1	0	0	9*H*-Carbazole, dimethyl-		17.21
1906.	14171-85-8	1	0	0	9*H*-Carbazole, 1,9-dimethyl-		17.21
1907.	24075-47-6	1	0	0	9*H*-Carbazole, 2,9-dimethyl-		17.21
1908.	24075-48-7	1	0	0	9*H*-Carbazole, 3,9-dimethyl-		17.21
1909.	24075-49-8	1	0	0	9*H*-Carbazole, 4,9-dimethyl-		17.21
1910.	71277-85-5	1	0	0	9*H*-Carbazole, ethyl-		17.21

(continued)

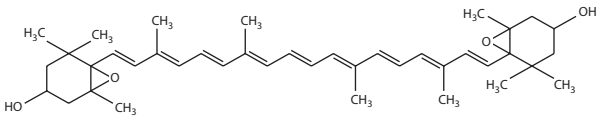
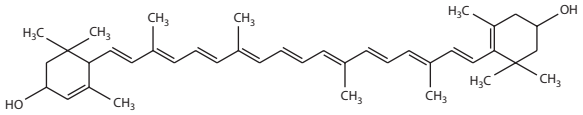
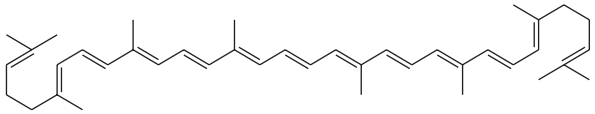
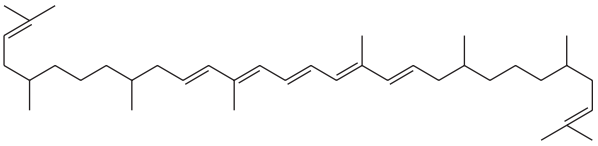
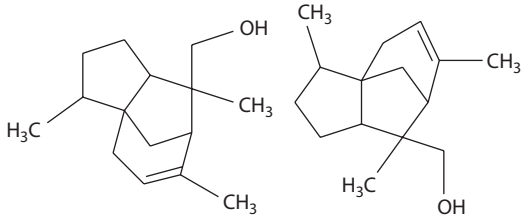
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1911.	86-28-2	1	0	0	9*H*-Carbazole, 9-ethyl-		17.21
1912.	27323-29-1	1	0	0	9*H*-Carbazole, methyl-		17.21
1913.	6510-65-2	1	0	0	9*H*-Carbazole, 1-methyl-		17.21
1914.	3652-91-3	1	0	0	9*H*-Carbazole, 2-methyl-		17.21
1915.	4630-20-0	1	0	0	9*H*-Carbazole, 3-methyl-		17.21
1916.	3770-48-7	1	0	0	9*H*-Carbazole, 4-methyl-		17.21
1917.	1484-12-4	1	0	0	9*H*-Carbazole, 9-methyl-		17.21
1918.	64844-53-7	1	0	0	9*H*-Carbazole, tetramethyl-		17.21
1919.	64844-51-5	1	0	0	9*H*-Carbazole, trimethyl-		17.21
1920.	7440-44-0	1	1	1	Carbon	C	0.4, 20.5
1921.	14762-75-5	1	0	0	Carbon, isotope of mass 14	^{14}C	20.5
1922.	124-38-9	1	1	1	Carbon dioxide	CO_2	0.4, 19.5, 21.3, 24.3
1923.	51-90-1	1	0	0	Carbon-^{14}C dioxide	$^{14}CO_2$	19.5
1924.	75-15-0	1	1	1	Carbon disulfide	CS_2	0.4, 18.1, 19.5, 21.3, 26.9
1925.	630-08-0	1	0	0	Carbon monoxide	CO	0.4, 19.5, 23.5
1926.	7665-54-5	1	0	0	Carbon-^{14}C monoxide	^{14}CO	19.5
1927.	463-58-1	1	0	0	Carbon oxide sulfide (COS) {carbonyl sulfide}	COS	18.1, 19.5
1928.	75-44-5	0	1	0	Carbon oxychloride {phosgene}	$COCl_2$	19.5, 18.4, 21.3
1929.	2944-05-0	1	0	0	Carbon sulfide	CS	18.1, 19.5
1930.	56-23-5	1	1	1	Carbon tetrachloride	CCl_4	18.4, 21.3
1931.	463-79-6	0	1	0	Carbonic acid	H_2CO_3	0.4, 20.6
1932.	10361-29-2	1	0	0	Carbonic acid, ammonium salt	$(NH_4)_2CO_3$	0.4, 20.6
1933.	471-34-1	1	0	0	Carbonic acid, calcium salt	$CaCO_3$	20.6
1934.	13717-00-5	0	1	0	Carbonic acid, magnesium salt	$MgCO_3$	0.4, 20.6
1935.	584-08-7	0	1	0	Carbonic acid, dipotassium salt	K_2CO_3	0.4, 20.6
1936.	497-19-8	0	1	0	Carbonic acid, disodium salt {sodium carbonate}	Na_2CO_3	20.6
1937.	1066-33-7	1	1	1	Carbonic acid, monoammonium salt {ammonium hydrogen carbonate}	$(NH_4)HCO_3$	20.6
1938.	298-14-6	0	1	0	Carbonic acid, monopotassium salt	$KHCO_3$	20.6
1939.	144-55-8	0	1	0	Carbonic acid, monosodium salt	$NaHCO_3$	20.6
1940.	9031-55-4	0	1	0	Carboxylase		22.2
1941.	9067-77-0	0	1	0	Carboxylase, phosphoenolpyruvate (phosphate)		22.2
1942.	37341-54-1	0	1	0	Carboxylase, phosphopyruvate		22.2
1943.	131201-61-1	0	1	0	Carboxylase, ribulose diphosphate (*Nicotiana sylvestris* clone NySS4 small subunit precursor reduced)		22.2
1944.	9031-98-5	0	1	0	Carboxypeptidase		22.2
1945.		0	1	0	Carotene		1.12
1946.	7235-40-7	1	1	1	β,β-Carotene {β-carotene, all-*trans*}		0.4, 1.12, 24.3, 24.3, 25.29, 26.9
1947.	6811-73-0	0	1	0	β,β-Carotene, 13-*cis*-		1.12
1948.	68295-84-1	0	1	0	β,β-Carotene, *neo*		1.12
1949.	14660-91-4	0	1	0	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S,9′-*cis*)- {neoxanthin}		2.5, 10.2

(*continued*)

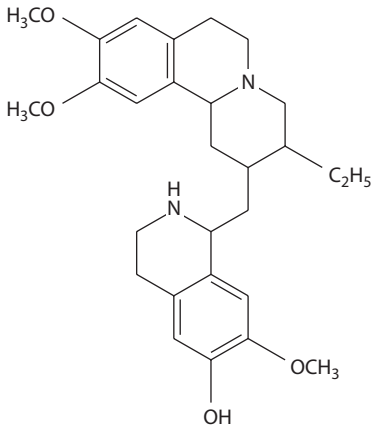
(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1950.	30743-41-0	0	1	0	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S)-		2.5, 10.2
1951.	29472-68-2	0	1	0	β,β-Carotene-3,3′-diol {zeaxanthin}		2.5
1952.	144-68-3	0	1	0	β,β-Carotene-3,3′-diol, (3R,3′R)- {zeaxanthin}		2.5
1953.	126-29-4	0	1	0	β,β-Carotene-3,3′-diol,5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S)- {violaxanthin}		2.5, 10.2
1954.	26927-07-1	0	1	0	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S,9-*cis*)-		2.5, 10.2
1955.	68831-78-7	0	1	0	β,β-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,9-*cis*)-		2.5, 10.2
1956.	472-70-8	0	1	0	β,β-Caroten-3-ol, (3R)- {cryptoxanthin}		2.5
1957.	7488-99-5	0	1	0	β,ε-Carotene, (6′R)- {α-carotene}		1.12
1958.	17539-43-4	0	1	0	β,ε-Carotene-3,3′-diol,5,6-epoxy-5,6-dihydro-		2.5, 10.2
1959.	28368-08-3	0	1	0	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,6′R)-		2.5, 10.2
1960.	512-29-8	0	1	0	β,ε-Carotene-3,3′-diol, 5,8-epoxy-5,8-dihydro-, (3S,3′R,5R,6′R,8R)- {flavoxanthin}		2.5, 10.2
1961.	127-40-2	0	1	0	β,ε-Carotene-3,3′-diol, (3R,3′R,6′R)- {xanthophyll, lutein}		0.4, 2.5
1962.	502-65-8	1	1	1	ψ,ψ-Carotene {lycopene}		1.11
1963.	540-04-5	0	1	0	ψ,ψ-Carotene, 7,7′,8,8′,11,11′,12,12′-octahydro- {phytoene}		1.11
1964.	540-05-6 27664-65-9	0	1	0	ψ,ψ-Carotene, 7,7′,8,8′,11,12-hexahydro- {phytofluene}		1.11
1965.	9001-05-2	0	1	0	Catalase		0.4, 22.2
1966.	28231-03-0	0	1	0	Cedrenol		2.5
1967.	528-50-7	0	1	0	Cellobiose		2.5, 8.3, 10.2
1968.	9012-54-8	0	1	0	Cellulase		0.4, 22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1969.	9004-34-6	1	1	1	Cellulose		0.4, 2.5, 8.3, 10.2, 24.3, 25.29
1970.		0	1	0	Cellulose, labeled with ^{14}C {cellulose-^{14}C}		2.5, 8.3, 10.2, 25.29
1971.	9000-11-7	0	1	0	Cellulose, carboxymethyl ether		2.5, 8.3, 10.2
1972.	9004-57-3	0	1	0	Cellulose, ethyl ether		2.5, 8.3, 10.2
1973.	9004-67-5	0	1	0	Cellulose, methyl ether		2.5, 8.3, 10.2
1974.	483-17-0	0	1	0	Cephalin		0.4, 9.22, 10.2
1975.	7440-45-1	1	1	1	Cerium	Ce	0.4, 20.5
1976.	14762-78-8	0	1	0	Cerium, isotope of mass 144	^{144}Ce	20.5
1977.	7440-46-2	1	1	1	Cesium	Cs	0.4, 20.5
1978.	13967-70-9	1	1	1	Cesium, isotope of mass 134	^{134}Cs	20.5
1979.	10045-97-3	1	1	1	Cesium, isotope of mass 137	^{137}Cs	20.5
1980.	9001-06-3	0	1	0	Chitinase		22.2
1981.	131554-01-3	0	1	0	Chitinase (*Nicotiana tabacum* samsun isoenzyme reduced)		22.2
1982.	148348-37-2	0	1	0	Chitinase (*Nicotiana tabacum* xanthi clone pBSCL226 isoenzyme III precursor reduced)		22.2
1983.	152619-17-5	0	1	0	Chitinase (tobacco basic isoenzyme III precursor reduced)		22.2
1984.	128285-05-2	0	1	0	Chitinase (tobacco clone lambda CHN17 basic isoenzyme precursor reduced)		22.2
1985.	128285-06-3	0	1	0	Chitinase (tobacco clone lambda CHN17 basic isoenzyme reduced)		22.2
1986.	159520-75-9	0	1	0	Chitinase (tobacco clone 59 gene chi-V precursor reduced)		22.2
1987.	16887-00-6	1	1	1	Chloride	Cl^{-1}	0.4, 18.4, 20.5
1988.	7782-50-5	1	1	1	Chlorine	Cl_2	18.4, 19.5, 20.5
1989.	14158-34-0	0	1	0	Chlorine, isotope of mass 38	$^{38}Cl_2$	18.4, 20.5
1990.		0	1	0	*Chloroflexi*, *Chloroflexi*		22.2
1991.		0	1	0	*Chlorogloeopsis*		22.2
1992.	9025-96-1	0	1	0	Chlorophyllase		22.2
1993.	42617-16-3	0	1	0	Chlorophyll a {also listed under magnesium}		5.3, 17.5, 20.6
1994.	519-62-0	0	1	0	Chlorophyll b {also listed under magnesium}		0.4, 5.3, 17.5, 20.6
1995.	1406-65-1	0	1	0	Chlorophylls a + b		0.4, 5.3, 17.5, 20.6
1996.	14897-06-4	0	1	0	Chlorophyllide		17.5, 20.6

(*continued*)

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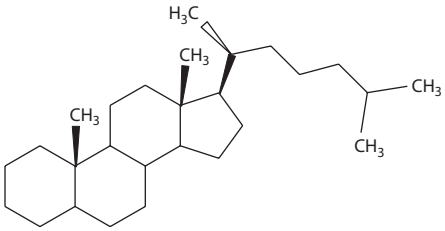
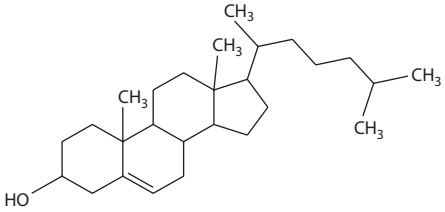
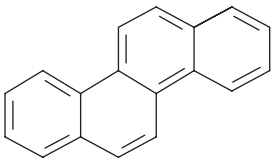
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
1997.	15611-43-5 11006-34-1	0	1	0	Chlorophyllin		17.5, 20.6
1998.	119973-28-3	1	0	0	Chol-3-ene, 23-methyl-, (5α)-		1.12, 2.7
1999.	747-90-0	1	0	0	Cholesta-3,5-diene		1.12, 2.7
2000.		1	0	0	Cholesta-3,5-diene, 24-ethyl-		1.12, 2.7
2001.	481-21-0	0	1	0	Cholestane, (5α)- {coprostane}		1.12, 2.7
2002.	80-97-7	0	1	0	Cholestan-3-ol (3β) {dihydrocholesterol}		2.5, 2.7
2003.		1	0	0	Cholesta-3,5,22-triene, 24-methyl-		1.12, 2.7
2004.	96443-01-5	1	0	0	Cholest-4-en-3-ol, 4-methyl- (3α)		2.5, 2.7
2005.	57-88-5	1	1	1	Cholest-5-en-3-ol (3β)- {cholesterol}		0.4, 2.5, 2.7, 25.29, 26.9
2006.	2645-22-4	0	1	0	Cholest-5-en-3-ol (3β)-, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {cholesteryl linolenate}		2.7, 5.3, 25.29
2007.	303-43-5	0	1	0	Cholest-5-en-3-ol (3β)-, 9-octadecenoate, [3β(*Z*),22*E*]- {cholesteryl oleate}		2.7, 5.3, 25.29
2008.	35602-69-8	0	1	0	Cholest-5-en-3-ol (3β)-, octadecanoate, (3β,22*E*)- {cholesteryl stearate}		2.7, 5.3, 25.29
2009.	474-77-1	0	1	0	Cholest-5-en-3-ol, (3α)- {epicholesterol}		2.5, 2.7
2010.	604-35-3	1	0	0	Cholest-5-en-3-ol (3β)-, acetate {cholesteryl acetate}		2.5, 2.7, 5.3
2011.	1253-88-9	0	1	0	Cholest-5-en-3-ol, 4,4-dimethyl-, (3β)-		2.5, 2.7
2012.	6036-58-4	0	1	0	Cholest-7-en-3-ol, (3β)-		2.5, 2.7
2013.	481-25-4	0	1	0	Cholest-7-en-3-ol, 4-methyl-,(3β,4α,5α)-		2.5, 2.7
2014.	6062-47-1	0	1	0	Cholest-8-en-3-ol, 14-methyl-, (3β,5α)-		2.5, 2.7
2015.	5241-24-7	0	1	0	Cholest-8-en-3-ol, 4,4-dimethyl-,(3β,5α)-		2.5, 2.7
2016.	5241-22-5	0	1	0	Cholest-8-en-3-ol, 4-methyl-,(3β,4α,5α)-		2.5, 2.7
2017.	100017-41-2	0	1	0	Cholest-9(11)-en-3-ol, 14-methyl-,(3β,5α)-		2.5, 2.7
2018.	7440-47-3	1	1	1	Chromium	Cr	0.4, 20.5, 23.5
2019.	14392-02-0	1	1	1	Chromium, isotope of mass 51	^{51}Cr	20.5
2020.	16055-83-1	1	0	0	Chromium ion (3+)		20.6
2021.	***18540-29-9***	1	0	0	Chromium ion (6+)		20.6
2022.	218-01-9	1	1	1	Chrysene {1,2-benzophenanthrene}		1.20, 23.5

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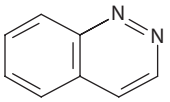
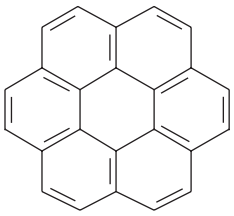
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2023.		1	0	0	Chrysene, alkyl-		1.20
2024.	2642-98-0	1	0	0	Chrysene, 6-amino- {6-chysenamine}		12.2
2025.	41637-92-7	1	0	0	Chrysene, dimethyl- {at least three isomers in MSS}		1.20
2026.	71277-86-6	1	0	0	Chrysene, ethyl-		1.20
2027.	71277-87-7	1	0	0	Chrysene, ethylmethyl-		1.20
2028.	41637-90-5	1	0	0	Chrysene, methyl-		1.20
2029.	3351-28-8	1	1	1	Chrysene, 1-methyl-		1.20
2030.	3351-32-4	1	0	0	Chrysene, 2-methyl-		1.20
2031.	3351-31-3	1	1	1	Chrysene, 3-methyl-		1.20
2032.	3351-30-2	1	1	1	Chrysene, 4-methyl-		1.20
2033.	3697-24-3	1	1	1	Chrysene, 5-methyl-		1.20, 23.5
2034.	1705-85-7	1	1	1	Chrysene, 6-methyl-		1.20
2035.	7496-02-8	1	0	0	Chrysene, 6-nitro-		16.1
2036.	71277-88-8	1	0	0	Chrysene, pentamethyl-		1.20
2037.	71277-89-9	1	0	0	Chrysene, propyl-		1.20
2038.	71277-90-2	1	0	0	Chrysene, tetramethyl-		1.20
2039.	60826-77-9	1	0	0	Chrysene, trimethyl-		1.20
2040.	253-66-7	1	0	0	Cinnoline {1,2-diazanaphthalene}		17.21
2041.	63863-33-2	1	0	0	Cinnoline, dihydro-		17.21
2042.	14722-38-4	1	0	0	Cinnoline, 4-methyl-		17.21
2043.	9001-12-1	0	1	0	*Clostridium*		22.2
2044.	7440-48-4	1	1	1	Cobalt	Co	0.4, 20.5, 23.5
2045.	10198-40-0	1	1	1	Cobalt, isotope of mass 60	^{60}Co	20.5
2046.	10210-68-1	1	0	0	Cobalt carbonyl	$Co_2(CO)_8$	20.6
2047.	1332-82-7	0	1	0	Cobalt chloride		18.4, 20.6
2048.	85-61-0	0	1	0	Coenzyme A		22.2
2049.	604-98-8	0	1	0	Coenzyme A, S-(hydrogen butanedioate)		22.2
2050.		0	1	0	*Comamonas testosteroni*		22.2
2051.	7440-50-8	1	1	1	Copper	Cu	0.4, 20.5, 21.3
2052.		0	1	0	Copper, ion	Cu^{+2}	20.5
2053.	7447-39 4	0	1	0	Copper chloride (cupric chloride)	$CuCl_2$	18.4, 20.6
2054.	1317-39-1	0	1	0	Copper oxide		20.6, 21.3
2055.	1332-40-7 1332-65-6	0	1	0	Copper oxychloride {RAME}		20.6, 18.4, 21.3
2056.	8012-69-9	0	1	0	Copper oxychloride sulfate	$Cu_2Cl(OH)_3 + Cu_4(OH)_6(SO_4)$	20.6, 18.4, 21.3
2057.	1333-22-8	0	1	0	Copper oxysulfate	$Cu_4(OH)_6(SO_4)$	20.6, 18.4
2058.	191-07-1	1	1	1	Coronene		1.20
2059.	64760-15-2	1	0	0	Coronene, dimethyl-		1.20
2060.	13119-86-3	1	0	0	Coronene, methyl-		1.20
2061.		0	1	0	*Corynebacterium xerosis*		22.2
2062.	115742-70-6	0	1	0	Cryptogein		22.2
2063.	156-62-7	0	1	0	Cyanamide, calcium salt	Ca═N-CN	11.2, 20.6, 21.3
2064.	1467-79-4	1	0	0	Cyanamide, dimethyl-	$(CH_3)_2$═N-CN	11.2

(*continued*)

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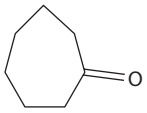
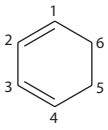
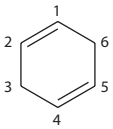
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2065.	590-28-3	0	1	0	Cyanic acid, potassium salt	$K\text{-}OCN^-$	20.6, 21.3
2066.	57-12-5	1	0	0	Cyanide ion	CN^{-1}	0.4, 11.2
2067.		1	0	0	Cyanide radical	CN	27.1
2068.		1	0	0	Cyanide radical {acrylonitrile radical}	C_3H_2N	27.1
2069.		1	0	0	Cyanide radical	C_3H_4N	27.1
2070.		0	1	0	*Cyanobacteria*, *Cyanobacteria*		22.2
2071.		0	1	0	*Cyanobacteria*, *Cyanophyceae*		22.2
2072.	94185-89-4	0	1	0	Cyclase, farnesyl pyrophosphate		22.2
2073.	60485-38-3	0	1	0	9,19-Cyclocholest-24-en-3-ol, 4, 14-dimethyl-, (3β,4α,5α)-		2.5, 2.7
2074.	34443-88-4	0	1	0	9,19-Cycloergost-24(28)-en-3-ol, 14-methyl-, (3β,5α)-		2.5, 2.7
2075.	469-39-6	0	1	0	9,19-Cycloergost-24(28)-en-3-ol, 4, 14-dimethyl-, (3β,4α,5α)-		2.5, 2.7
2076.	34347-58-5	0	1	0	9,19-Cycloergostan-3-ol, 14-methyl-, (3β,5α,9β)-		2.5, 2.7
2077.	59780-40-4	0	1	0	9,19-Cycloergostan-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-		2.5, 2.7
2078.	503-93-5	0	1	0	2,4-Cycloheptadien-1-one, 2,6,6-trimethyl- {eucarvone}		3.13
2079.	502-42-1	1	1	1	Cycloheptanone {suberone}		3.13
2080.	544-25-2	1	0	0	1,3,5-Cycloheptatriene {tropilidene}		1.12, 1.13
2081.	1121-66-0	1	0	0	2-Cyclohepten-1-one		3.13
2082.	29797-09-9	1	0	0	Cyclohexadiene		1.12
2083.	592-57-4	1	0	0	1,3-Cyclohexadiene		1.12
2084.	99-86-5	1	1	1	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- {α-terpinene}		1.12
2085.	99-83-2	1	1	1	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- {α-phellandrene}		1.12, 24.3, 25.29
2086.	4221-98-1	1	1	1	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)-, (R)- {α-phellandrene}		1.12, 24.3
2087.	116-26-7	0	1	0	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl- {safranal}		3.12
2088.	514-96-5	0	1	0	1,3-Cyclohexadiene, 1,2,6,6-tetramethyl-		1.12
2089.	628-41-1	1	0	0	1,4-Cyclohexadiene		1.12
2090.	4313-57-9	1	0	0	1,4-Cyclohexadiene, 1-methyl-		1.12
2091.	99-85-4	0	1	0	1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-		1.12

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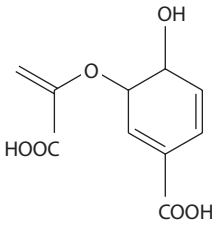
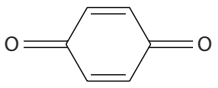
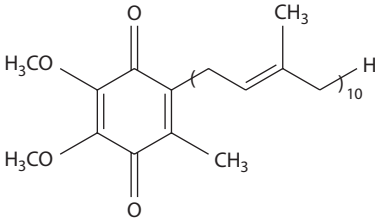
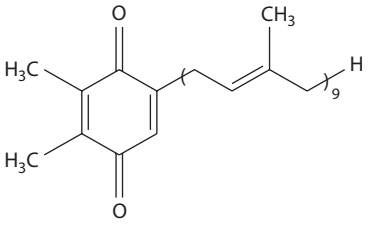
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2092.	617-12-9	0	1	0	1,5-Cyclohexadiene-1-carboxylic acid, 3-[(1-carboxyethenyl)oxy]-4-hydroxy-, (3R-*E*)- {chorismic acid}		2.5, 4.3, 10.2
2093.	78919-13-8	1	0	0	Cyclohexadienedione {quinone}		9.24
2094.	106-51-4	1	0	0	2,5-Cyclohexadiene-1,4-dione {*p*-benzoquinone}		9.24
2095.	106-34-3	1	0	0	2,5-Cyclohexadiene-1,4-dione, compd. with 1,4-benzenediol (1:1)		9.22, 9.24
2096.		1	0	0	2,5-Cyclohexadiene-1,4-dione,2,3-dihydro-		9.24
2097.		1	1	1	2,5-Cyclohexadiene-1,4-dione, 2,3-dihydro-2,2,6-trimethyl-		9.24
2098.	303-98-0	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-(3,7,11,15,19,23,27,31,35,39-decamethyl-2,6,10,14,18,22,26,30,34,38-tetracontadecenyl)-6-methyl- {ubiquinone-10}		9.24, 10.2
2099.	526-86-3	1	0	0	2,5-Cyclohexadiene-1,4-dione,2,3-dimethyl-		9.24
2100.	137-18-8	1	0	0	2,5-Cyclohexadiene-1,4-dione,2,5-dimethyl-		9.24
2101.		0	1	0	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-		9.24
2102.	527-61-7	1	0	0	2,5-Cyclohexadiene-1,4-dione,2,6-dimethyl-		9.24
2103.	4299-57-4	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethyl-5-(3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22, 26,30, 34-hexatriacontanonaenyl)-, (all-*E*)- {plastoquinone 9}		9.24
2104.	606-06-4	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2-(3,7-dimethyl-2,6-octadienyl)-5,6-dimethoxy-3-methyl-, (*E*)-		9.24, 10.2
2105.	2474-72-8	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2-hydroxy-		2.5, 9.24
2106.	3361-10-2	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15-tetramethylhexadecyl)-6-methyl-		2.5, 9.24
2107.	7559-04-8	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15-tetramethylhexadecyl)-3,5,6-trimethyl-, [3R-(3R*,7R*,11R*)]-		2.5, 9.24
2108.		1	0	0	2,5-Cyclohexadiene-1,4-dione, 2-methoxy-		9.24, 10.2
2109.	553-97-9	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2-methyl-		9.24
2110.	527-17-3	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl-		9.24
2111.	935-92-2	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,3,5-trimethyl-		9.24

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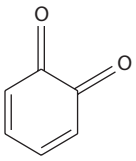
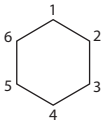
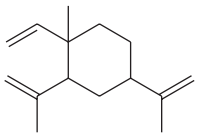
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2112.	583-63-1	1	1	1	3,5-Cyclohexadiene-1,2-dione {*o*-benzoquinone}		9.24
2113.	13487-30-4	0	1	0	2,4-Cyclohexadien-1-one, 2,6,6-trimethyl-		3.13
2114.		0	1	0	2,5-Cyclohexadien-1-one, 2,6-bis (1,1-dimethylethyl)-4-hydoxy-4-methyl-		2.5, 3.13
2115.	110-82-7	1	1	1	Cyclohexane		1.12
2116.	27195-67-1	1	1	1	Cyclohexane, dimethyl-		1.12
2117.	1678-91-7	1	0	0	Cyclohexane, ethyl-		1.12
2118.	30677-34-0	1	0	0	Cyclohexane, ethylmethyl-		1.12
2119.	108-87-2	1	0	0	Cyclohexane, methyl-		1.12
2120.	1678-92-8	1	0	0	Cyclohexane, propyl-		1.12
2121.	27013-35-0	1	0	0	Cyclohexane, methyl-(1-methylethenyl)-		1.12
2122.	933-40-4	1	0	0	Cyclohexane, 1.1-dimethoxy-		10.2
2123.	18349-16-1	1	0	0	Cyclohexane, 1.1-dimethoxy-3-methyl-		10.2
2124.	18349-20-7	1	0	0	Cyclohexane, 1.1-dimethoxy-4-methyl-		10.2
2125.	29887-60-3	0	1	0	Cyclohexane, 1,2-dimethoxy-, (*E*)		10.2
2126.	590-66-9	1	0	0	Cyclohexane, 1,1-dimethyl-		1.12
2127.	2207-01-4	1	0	0	Cyclohexane, 1,2-dimethyl-, (*Z*)		1.12
2128.	6876-23-9	1	0	0	Cyclohexane, 1,2-dimethyl-, (*E*)		1.12
2129.	591-21-9	1	0	0	Cyclohexane, 1,3-dimethyl-		1.12
2130.	624-29-3	1	0	0	Cyclohexane, 1,4-dimethyl-, (*Z*)		1.12
2131.	2207-04-7	1	0	0	Cyclohexane, 1,4-dimethyl-, (*E*)		1.12
2132.	33880-83-0	0	1	0	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis (1-methylethenyl)-, (1α,2β,4β)-		1.12
2133.	515-13-9	0	1	0	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-		1.12
2134.	62238-31-7	1	0	0	Cyclohexane, 1-ethyl-1,3-dimethyl-, (*Z*)-		1.12
2135.	62238-29-3	1	0	0	Cyclohexane, 1-ethyl-1,3-dimethyl-, (*E*)-		1.12
2136.	62238-30-6	1	0	0	Cyclohexane, 1-ethyl-1,4-dimethyl-, (*Z*)-		1.12
2137.	62238-32-8	1	0	0	Cyclohexane, 1-ethyl-1,4-dimethyl-, (*E*)-		1.12
2138.	62238-33-9	1	0	0	Cyclohexane, 1-ethyl-2-propyl-		1.12
2139.	608-73-1	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro-		0.4, 18.4, 21.3
2140.	319-84-6	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {alpha-HCH, HCH-alpha, α-Lindane®}		18.4, 21.3
2141.	319-85-7	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {β-Lindane®}		18.4, 21.3
2142.	58-89-9	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1α,2α,3β,4α,5α,6β)- {gamma-HCH, HCH-gamma; γ-Lindane®}		18.4, 21.3
2143.	319-86-8	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {δ-Lindane®}		18.4, 21.3
2144.	13828-34-7	1	0	0	Cyclohexane, 1-methyl-3-(1-methylethylidene)-		1.12
2145.	99-62-1	1	0	0	Cyclohexane,1-methyl-4-(1-methylethyl)- {*p*-menthane}		1.12
2146.	61142-00-5	1	0	0	Cyclohexane, 1,2,4,5-tetraethyl-		1.12

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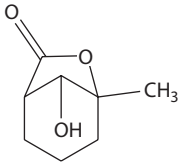
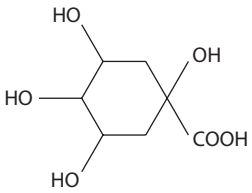
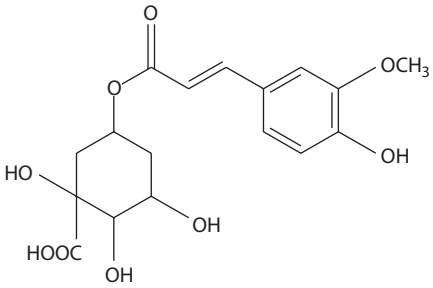
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2147.	3073-66-3	1	0	0	Cyclohexane, 1,1,3-trimethyl-		1.12
2148.	110053-64-0	1	0	0	1,3-Cyclohexanecarbolactone, 2-hydroxy-3-methyl-		2.5, 6.3
2149.	2043-61-0	0	1	0	Cyclohexanecarboxaldehyde		3.12
2150.	34214-77-2	1	1	1	Cyclohexanecarboxylic acid, 3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]trihydroxy-, (1α,3α,4α,5β)-		2.5, 4.3, 5.3, 10.22
2151.	534-61-2	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy- [1S-(1α,3β,4β,5α)]- {isochlorogenic acid}		2.5, 4.3, 5.3, 9.22
2152.	77-95-2 562-73-2	1	1	1	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy- {quinic acid}		0.4, 2.5, 4.3
2153.	36413-60-2	0	1	0	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, (1α,3α,4α,5β)-		2.5, 4.3
2154.	1899-29-2	0	1	0	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl] oxy]-, (1α,3α,4α,5β)- {3-*O*-feruloylquinic acid}		2.5, 4.3, 5.3, 9.22, 10.2
	27044-07-1				Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-		
2155.	1899-30-5	0	1	0	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]-, [1S-(1α,3α,4α,5β)]- {*p*-coumaroylquinic acid}		2.5, 4.3, 5.3, 9.22
2156.	2450-53-5	0	1	0	Cyclohexanecarboxylic acid, 3,5-bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4-dihydroxy-, [1R-(1α,3α,4α,5β)]- {isochlorogenic acid A}		2.5, 4.3, 5.3, 9.22
2157.	15016-60-1	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*Z*),4α,5α]]-		2.5, 4.3, 5.3, 9.22

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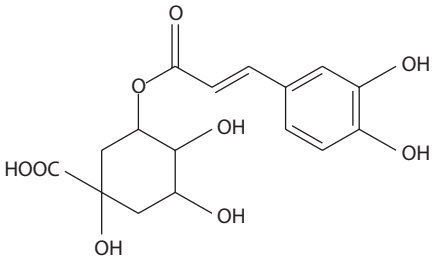
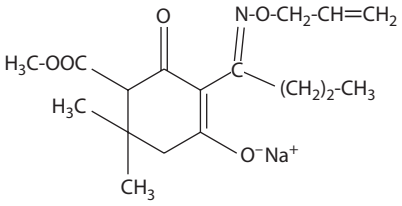
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2158.	15076-00-3	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*E*),4α,5α]]-		2.5, 4.3, 5.3, 9.22
2159.	327-97-9 93451-46-8	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- {chlorogenic acid, 3-*O*-caffeoylquinic acid}		0.4, 2.5, 4.3, 5.3, 9.22, 21.3, 25.29, 26.9
2160.	906-33-2	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-(1α,3α,4α,5β)]- {neochlorogenic acid, 5-*O*-caffeoylquinic acid} Also listed as cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-		2.5, 4.3, 5.3, 9.22, 10.2
2161.	55635-13-7	0	1	0	Cyclohexanecarboxylic acid, 2, 2-dimethyl-2,4-dioxo-3-(1-((2-propenyloxy) amino)butylidene)-, methyl ester, sodium salt {Alloxydim-sodium®}		3.13, 5.3, 20.6, 21.3
2162.	24321-18-4	0	1	0	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dioxo-1,5-cyclohexadien-1-yl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-		2.5, 4.3, 5.3
2163.	70898-22-5	0	1	0	Cyclohexanecarboxylic acid, 3- [[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-		2.5, 4.3, 5.3, 8.3, 9.22, 10.2
2164.	17608-52-5	0	1	0	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy- {4-*O*-caffeoylquinic acid}		2.5, 4.3, 5.3, 9.22
2165.		0	1	0	Cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-5-phenyl		2.5, 4.3, 5.3, 9.22
2166.	905-99-7	0	1	0	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-, (1α,3α,4α,5β)-		2.5, 4.3, 5.3, 9.22
2167.	931-17-9	0	1	0	1,2-Cyclohexanediol, (*E*)-		2.5
2168.	82612-14-4	0	1	0	1,2-Cyclohexanediol, 4-[1-(acetyloxy)-1-methylethyl]-1-methyl-, (1α,2β,4α)-(±)-		2.5, 5.3
2169.	6296-84-0	0	1	0	1,4-Cyclohexanediol, 1-methyl-		2.5

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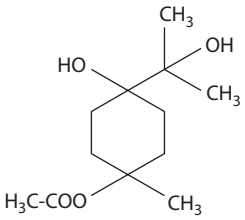
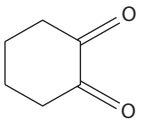
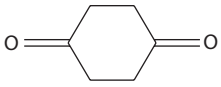
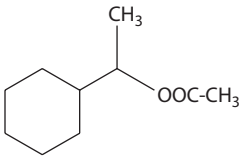
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2170.		0	1	0	1,4-Cyclohexanediol, 1-methyl- {isomer}		2.5
2171.	56859-02-0	0	1	0	1,2-Cyclohexanediol, 2-(3-hydroxy-1-butenyl)-1,3,3-trimethyl-		2.5
2172.	112019-00-8	0	1	0	1,2-Cyclohexanediol, 2-(3-hydroxy-1-butenyl)-1,3,3-trimethyl-, [1R-[1α,2α, 2(1E,3S*)]]-		2.5
2173.	38713-11-0	0	1	0	1,2-Cyclohexanediol, 1,3,3-trimethyl-		2.5
2174.	23832-27-1	0	1	0	1,2-Cyclohexanediol, 4-methyl-		2.5
2175.	556-48-9	0	1	0	1,4-Cyclohexanediol		2.5
2176.	88663-71-2	0	1	0	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*E*)-		2.5, 5.3
2177.	88663-72-3	0	1	0	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*Z*)-		2.5, 5.3
2178.	59632-88-1	0	1	0	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*Z*)-		2.5, 5.3
2179.	59632-87-0	0	1	0	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*E*)-		2.5, 5.3
2180.	54993-31-6	0	1	0	1,4-Cyclohexanediol, 2,2,6-trimethyl-		2.5
2181.	765-87-7	0	1	0	1,2-Cyclohexanedione		3.13
2182.	18310-19-5	1	0	0	1,2-Cyclohexanedione, 4-methyl-		3.13
2183.	3008-43-3	0	1	0	1,2-Cyclohexanedione, 6-methyl-		3.13
2184.	126-81-8	0	1	0	1,3-Cyclohexanedione, 5,5-dimethyl-		3.13
2185.	1919-64-8	0	1	0	1,3-Cyclohexanedione, 5,5-dimethyl-2-propyl-		3.13
2186.	1193-55-1	1	1	1	1,3-Cyclohexanedione, 2-methyl-		3.13
2187.	637-88-7	1	1	1	1,4-Cyclohexanedione		3.13
2188.	20547-99-3	1	1	1	1,4-Cyclohexanedione, 2,2,6-trimethyl- {4-ketodihydroisophorone}		3.13
2189.	13487-27-9	0	1	0	Cyclohexanemethanol, α-methyl-, acetate		5.3
2190.	639-99-6	0	1	0	Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)-, [1R-(1α,3α,4β)]-		2.5
2191.	80-53-5	1	0	0	Cyclohexanemethanol, 4-hydroxy-α,α,4-trimethyl- {*p*-menthane-1,8-diol}		2.5
2192.	2451-01-6	1	0	0	Cyclohexanemethanol, 4-hydroxy-α,α,4-trimethyl-, monohydrate, *cis*- {terpin hydrate}		2.5

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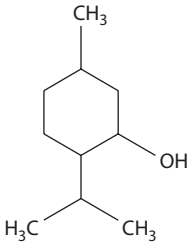
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2193.	104153-60-8	0	1	0	1,2,3-Cyclohexanetriol, 1-methyl-4-(1-methylethyl)-		2.5
2194.	108-93-0	1	0	0	Cyclohexanol		2.5
2195.	60759-94-6	0	1	0	Cyclohexanol, 1-(3-hydroxy-1-butenyl)-2,2-dimethyl-6-methylene-		2.5
2196.	586-81-2	0	1	0	Cyclohexanol, 1-methyl-4-(1-methylethylidene)-		2.5
2197.	10235-63-9	0	1	0	Cyclohexanol, 1-methyl-4-(1-methylethylidene)-, acetate		5.3
2198.	619-01-2	0	1	0	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-		2.5
2199.	22567-22-2	0	1	0	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, [1R-(1α,2α,5β)]-		2.5
2200.	51773-45-6	0	1	0	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, [1R-(1α,2α,5α)]-		2.5
2201.	88437-32-5	0	1	0	Cyclohexanol, 4-(2-hydroxy-1-methylethylidene)-1-methyl-, 1-acetate		5.3
2202.	89-79-2	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, [1R-(1α,2β,5α)]-		2.5
2203.	1490-04-6	1	1	1	Cyclohexanol, 5-methyl-2-(1-methylethyl)- {*DL*-menthol}		2.5
2204.	89-78-1	1	1	1	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {menthol}		0.4, 2.5, 24.3, 25.29
2205.		1	1	1	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-^{14}C(U), labeled with ^{14}C {^{14}C-menthol (U)}		2.5, 25.29
2206.	23283-97-8 490-99-3	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5β)- {isomenthol}		2.5
2207.	491-01-0	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {*D*-neomenthol}		2.5
2208.	2216-51-5	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, [1R-(1α,2β,5α)]-		2.5
2209.	89-48-5 16409-45-3	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate {menthyl acetate}		5.3
2210.	108-94-1	1	0	0	Cyclohexanone		3.13
2211.	2816-57-1	0	1	0	Cyclohexanone, 2,6-dimethyl-		3.13
2212.	71607-84-6	1	0	0	Cyclohexanone, ethenylmethyl-		3.13
2213.	50874-76-5	0	1	0	Cyclohexanone, trimethyl-		3.13
2214.	7500-42-7	0	1	0	Cyclohexanone, 2-hydroxy-2,6,6-trimethyl-		2.5, 3.13

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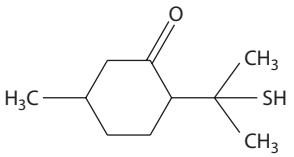
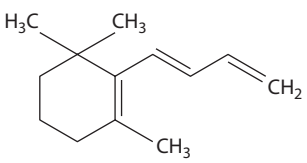
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2215.	38462-22-5	0	1	0	Cyclohexanone, 2-(1-mercapto-1-methylethyl)-5-methyl-		3.13, 18.1
2216.	583-60-8	0	1	0	Cyclohexanone, 2-methyl-		3.13
2217.	7764-50-3	1	0	0	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-		3.13
2218.	6909-25-7	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, (2S-*cis*)-		3.13
2219.	5948-04-9	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, *trans*-		3.13
2220.	491-07-6	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethyl)-, (*E*)- {*dl*-isomenthone}		3.13
2221.	499-70-7 59471-80-6	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethyl)- {carvomenthone}		3.13
2222.		0	1	0	Cyclohexanone, 2-(1-methylethyl)- {two isomers}		3.13
2223.	15189-14-7	0	1	0	Cyclohexanone, 2,2,5,5-tetramethyl-		3.13
2224.	2408-37-9	1	1	1	Cyclohexanone, 2,2,6-trimethyl- {2,6,6-trimethylcyclohexanone}		3.13, 24.3
2225.		0	1	0	Cyclohexanone, 2,4,4-trimethyl-3-(1-oxobutyl)-		3.13
2226.	591-24-2	1	0	0	Cyclohexanone, 3-methyl-		3.13
2227.	13368-65-5	1	0	0	Cyclohexanone, 3-methyl- (+)		3.13
2228.	133561-49-6	0	1	0	Cyclohexanone, 3,3,5-trimethyl-4-(3-oxobutyl)-		3.13
2229.	60026-21-3	0	1	0	Cyclohexanone, 3,3,5-trimethyl-4-(3-oxo-1-butenyl)-		3.13
2230.	123716-12-1	1	0	0	Cyclohexanone, 4-(1-methylethyl)-3-(2-oxopropyl)-		3.13
2231.	72491-45-3	0	1	0	Cyclohexanone, 4-(2-butenylidene)-3,3,5-trimethyl-		3.13
2232.	20548-02-1	1	1	1	Cyclohexanone, 4-hydroxy-2,2,6-trimethyl-		2.5, 3.13
2233.	20548-03-2	1	1	1	Cyclohexanone, 4-hydroxy-3,3,5-trimethyl-		2.5, 3.13
2234.	589-92-4	1	0	0	Cyclohexanone, 4-methyl-		3.13
2235.	529-00-0	0	1	0	Cyclohexanone, 5-methyl-2-(1-methylethenyl)- {isopulegone}		3.13
2236.	89-80-5 10458-16-7	1	1	1	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}		3.13, 24.3, 25.29
2237.	14073-97-3	1	0	0	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *(L)* {*L*-menthone}		3.13, 24.3
2238.	89-82-7	0	1	0	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)- {pulegone}		3.13
2239.	110-83-8	1	0	0	Cyclohexene		1.12
2240.	74423-06-6	0	1	0	Cyclohexene, 2-(1,3-butadienyl)-1,3,3-trimethyl-, (*E*)- {megastigmatriene}		1.12

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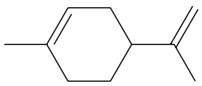
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2241.	2808-76-6	1	0	0	Cyclohexene, 1,3-dimethyl-		1.12
2242.	70688-47-0	1	0	0	Cyclohexene, 1,4-dimethyl-		1.12
2243.	1743-61-9	1	0	0	Cyclohexene, 1,4-dimethyl-4-ethenyl-		1.12
2244.	70941-91-2	0	1	0	Cyclohexene, 6-(3,7-dimethyl-1,3,5, 7-octatetraenyl)-1,5,5-trimethyl-, (*E,E,E*)-		1.12
2245.	495-62-5	0	1	0	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl- {bisabolene}		1.12
2246.	25168-07-4	0	1	0	Cyclohexene, ethenyl-		1.12
2247.		1	0	0	Cyclohexene, 3-ethenyl-1,3-di (4′,8′,12′-trimethyltridecyl)-		1.12
2248.	100-40-3	1	0	0	Cyclohexene, 4-ethenyl-		1.12
2249.	20307-84-0	0	1	0	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)- {δ-elemene}		1.12
2250.		1	0	0	Cyclohexene, 4-ethenyl-1,4-di (4′,8′,12′-trimethyltridecyl)-		1.12
2251.	1611-21-8	1	0	0	Cyclohexene, 5-ethenyl-1,5-dimethyl-		1.12
2252.	591-49-1	1	0	0	Cyclohexene, 1-methyl-		1.12
2253.		1	0	0	Cyclohexene, 3-(1-methylethyl)-		1.12
2254.	38738-60-2	1	0	0	Cyclohexene, 1-methyl-3-(1-methylethenyl)- {sylvestrene}		1.12
2255.	138-86-3	1	1	1	Cyclohexene, 1-methyl-4-(1-methylethenyl)- {limonene, *p*-mentha-1,8-diene}		1.12, 26.9
2256.	5989-27-5	1	0	0	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- {*d*-limonene}		1.12, 26.9
2257.	5989-54-8	1	0	0	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)- {*l*-limonene}		1.12
2258.	5502-88-5	1	1	1	Cyclohexene, 1-methyl-4-(1-methylethyl)-		1.12
2259.	586-62-9	0	1	0	Cyclohexene, 1-methyl-4-(1-methylethylidene)- {terpinolene}		1.12
2260.	1461-27-4	0	1	0	Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)- {sylvestrene}		1.12
2261.	591-48-0	1	0	0	Cyclohexene, 3-methyl-		1.12
2262.	591-47-9	1	0	0	Cyclohexene, 4-methyl-		1.12
2263.	14072-82-3	1	0	0	Cyclohexene, 4-(1-methylethyl)-		1.12
2264.	586-67-4	1	0	0	Cyclohexene, 4-methyl-1-(1-methylethenyl)- {3,8-menthadiene}		1.12
2265.	5256-65-5	1	0	0	Cyclohexene, 3-methyl-6-(1-methylethyl)-		1.12
2266.	13828-33-6	0	1	0	Cyclohexene, 5-methyl-1-(1-methylethyl)- {*m*-menthene}		1.12
2267.	23733-91-7	0	1	0	Cyclohexene, 3-methylene-4-(1-methylethenyl)-, (R)-		1.12
2268.		1	0	0	Cyclohexene, 3-(1″-methylene-5″,9″, 13″-trimethyltetradecyl)-1-(4′,8′,12′-trimethyltridecyl)-		1.12
2269.		1	0	0	Cyclohexene, 4-(1″-methylene-5″,9″, 13″-trimethyltetradecyl)-1-(4′,8′,12′-trimethyltridecyl)-		1.12
2270.	503-45-7	1	0	0	Cyclohexene, 3,3,5-trimethyl-		1.12
2271.	1321-16-0	1	0	0	Cyclohexenecarboxaldehyde		3.12
2272.	1192-88-7	1	0	0	1-Cyclohexene-1-carboxaldehyde		3.12

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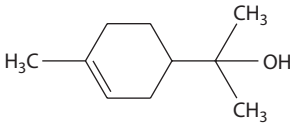
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2273.	18378-66-0	0	1	0	1-Cyclohexene-1-carboxaldehyde, 3-oxo-2,6,6-trimethyl-		3.12, 3.13
2274.	432-25-7 52844-21-0	1	1	1	1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- {β-cyclocitral}		3.12
2275.	471-90-9	0	1	0	1-Cyclohexene-1-carboxylic acid, 2,6,6-trimethyl- {cyclogeranic acid}		4.3
2276.	138-59-0	0	1	0	1-Cyclohexene-1-carboxylic acid, 3,4,5-trihydroxy-, [3R-(3α,4α,5β)]- {shikimic acid}		2.5, 4.3
2277.	6082-44-6	0	1	0	1-Cyclohexene-1-carboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-4,5-dihydroxy-,(3α,4α,5β)-		2.5, 4.3, 5.3, 9.22
2278.	38073-89-1	0	1	0	3-Cyclohexene-1-carboxylic acid, 6-(1-methylethyl)-, *cis*-		4.3
2279.	19894-91-8	0	1	0	1-Cyclohexene-1,4-dimethanol, α4,α4-dimethyl-, (S)-		2.5
2280.		1	1	1	2-Cyclohexene, 1-(2-oxopropyl)-3,5,5-trimethyl-		3.13
2281.	35692-98-9	0	1	0	2-Cyclohexene-1,4-dione, 2-hydroxy-3,5,5-trimethyl-		2.5, 3.13
2282.	38770-37-5	1	0	0	2-Cyclohexene-1,4-dione, 2,5,5-trimethyl-		3.13
2283.	1125-21-9	1	1	1	2-Cyclohexene-1,4-dione, 2,6,6-trimethyl- {4-ketoisophorone, 4-oxoisophorone}		3.13, 24.3
2284.	13835-30-8	0	1	0	3-Cyclohexene-1-ethanol, β,4-dimethyl- {8-menthen-2-ol}		2.5
2285.	472-65-1	0	1	0	1-Cyclohexene-1-ethanol, 2,6,6-trimethyl- {β-cyclohomogeraniol}		2.5
2286.	88663-73-4	0	1	0	1-Cyclohexene-1-methanol, 4-(acetyloxy)-α,α,4-trimethyl-		2.5, 5.3
2287.	472-20-8	0	1	0	1-Cyclohexene-1-methanol,2,6,6-trimethyl- {β-cyclogeraniol}		2.5
2288.	42370-41-2	0	1	0	3-Cyclohexene-1-methanol, 5-hydroxy-α,α,4-trimethyl-, *trans*-		2.5
2289.	498-71-5	0	1	0	3-Cyclohexene-1-methanol, 5-hydroxy-α,α,4-trimethyl-		2.5
2290.	8000-41-7	1	0	0	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {terpineol}		2.5
2291.	98-55-5	1	1	1	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {α-terpineol}		2.5, 24.3, 25.29
2292.	10482-56-1	1	1	1	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, (S)-		2.5
2293.	80-26-2	1	1	1	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate {α-terpinyl acetate}		5.3, 24.3, 25.29
2294.	822-67-3	1	1	1	2-Cyclohexen-1-ol		2.5
2295.	536-30-1	0	1	0	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethyl)-, (1S-*Z*)-		2.5
2296.	27185-80-4	0	1	0	2-Cyclohexen-1-ol, 3-(3-hydroxy-1-butenyl)-2,4,4-trimethyl-		2.5
2297.	470-99-5	0	1	0	2-Cyclohexen-1-ol, 3,5,5-trimethyl- {isophorol}		2.5

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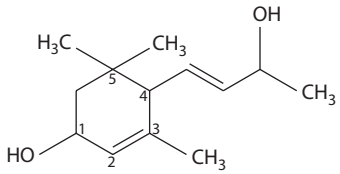
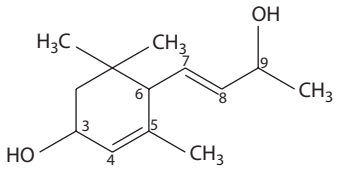
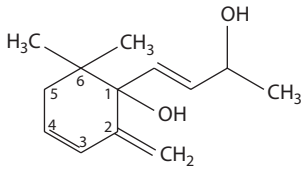
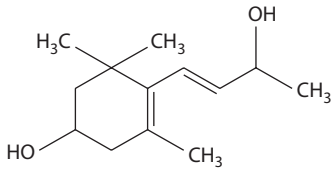
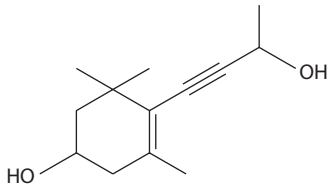
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2298.		0	1	0	2-Cyclohexen-1-ol, 3,5,5-trimethyl-4-methylene-		2.5
2299.	13215-90-2	0	1	0	2-Cyclohexen-1-ol, 4-(2-butenylidene)-3,5,5-trimethyl- {megastigmatrienol}		2.5
2300.	62660-03-1	0	1	0	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-	  Nomenclature by Enzell et al.	2.5
2301.	68831-80-1	0	1	0	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [1*S*-[1α,4α(1*E*,3S*)]]-		2.5
2302.	68831-81-2	0	1	0	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [1*S*-[1α,4α(1*E*,3R*)]]-		2.5
2303.	78830-91-8	0	1	0	3-Cyclohexen-1-ol, 1-(3-hydroxy-1-butenyl)-6,6-dimethyl-2-methylene-		2.5
2304.	33759-63-6	0	1	0	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-		2.5
2305.	121269-03-2	0	1	0	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, (*E*)-		2.5
2306.	31162-45-5 58023-72-6	1	1	1	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butynyl)-3,5,5-trimethyl-		2.5
2307.	562-74-3	1	1	1	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- {4-carvomenthol}		2.5, 24.3, 25.29
2308.	23811-18-9	0	1	0	3-Cyclohexen-1-ol, 3,5,5-trimethyl-, (±)-		2.5
2309.	930-68-7	1	1	1	2-Cyclohexen-1-one		3.13
2310.	74051-80-2	0	1	0	2-Cyclohexen-1-one, 2-[1-(ethoximino) butyl]-5-[2-(ethylthio)-propyl] -3hydroxy- {Sethoxydim®}		2.5, 3.13, 18.1, 21.3
2311.	10316-66-2	1	0	0	2-Cyclohexen-1-one, 2-hydroxy-		2.5, 3.13
2312.	3400-78-0	1	0	0	2-Cyclohexen-1-one, 2-hydroxy-3-methyl-		2.5, 3.13
2313.	490-03-9	0	1	0	2-Cyclohexen-1-one, 2-hydroxy-3-methyl-6-(1-methylethyl)- {diosphenol}		2.5, 3.13
2314.	55310-49-1	1	0	0	2-Cyclohexen-1-one, 2-hydroxy-3-propyl-		2.5, 3.13

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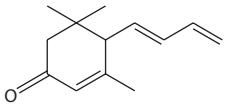
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2315.		1	0	0	2-Cyclohexen-1-one, 2-hydroxy-3,5,5-trimethyl-		2.5, 3.13
2316.	1121-18-2	1	0	0	2-Cyclohexen-1-one, 2-methyl-		3.13
2317.	99-49-0 6485-40-1	1	1	1	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*l*-carvone}		3.13, 24.3, 25.29
2318.	2244-16-8	1	1	1	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*d*-carvone}		3.13
2319.	43205-82-9	1	0	0	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)- {dihydrocarvone}		3.13
2320.		1	0	0	2-Cyclohexen-1-one, 2-propyl-3-methyl- {two isomers}		3.13
2321.		1	0	0	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(1,3-butadienyl)-		3.13
2322.	27185-77-9	0	1	0	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-		3.13
2323.	29790-29-2	0	1	0	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-, (1*E*)-		3.13
2324.	20013-73-4	0	1	0	2-Cyclohexen-1-one, 2,6,6-trimethyl-		3.13
2325.	5220-49-5	1	0	0	2-Cyclohexen-1-one, 3-amino-		3.13, 12.2
2326.	67401-25-6	0	1	0	2-Cyclohexen-1-one, 3-(2-butenyl)-2,4,4-trimethyl-, (*Z*)-		3.13
2327.	1193-18-6	1	0	0	2-Cyclohexen-1-one, 3-methyl-		3.13
2328.	89-81-6	1	1	1	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- {*D*-piperitone}		3.13, 24.3, 25.29
2329.		0	1	0	2-Cyclohexen-1-one, 3-methyl-2-(1,3-pentadienyl)-		3.13
2330.	78-59-1	1	1	1	2-Cyclohexen-1-one, 3,5,5-trimethyl- {isophorone}		3.13
2331.	133304-85-5	1	0	0	2-Cyclohexen-1-one, 3,4-dimethyl-2-hydroxy-		2.5, 3.13
2332.	2748-09-6	1	0	0	2-Cyclohexen-1-one, 3,5-dimethyl-2-hydroxy-		2.5, 3.13
2333.	2748-08-5	1	0	0	2-Cyclohexen-1-one, 3, 6-dimethyl-2-hydroxy-		2.5, 3.13
2334.	41577-83-7	1	0	0	2-Cyclohexen-1-one, 3-ethyl-2-hydroxy-		2.5, 3.13
2335.	51771-56-3	1	1	1	2-Cyclohexen-1-one, 3,5,5-trimethyl-2-(1-methylethenyl)-		3.13
2336.	53398-09-7	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(1-oxo-2-butenyl)-		3.13
2337.	60026-25-7	1	1	1	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(1-propenyl)-		3.13
2338.	20194-68-7	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-		3.13
2339.	79734-43-3	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-, (*E*)- {3-oxo-α-ionone}		3.13
2340.	33601-06-8	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-, (R)-(+)-		3.13
2341.	20548-00-9	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-methylene- {methyleneisophorone}		3.13
2342.		1	0	0	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-triethyl-		3.13
2343.	5896-02-6	1	1	1	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-trimethyl-		3.13

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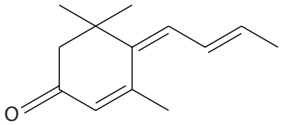
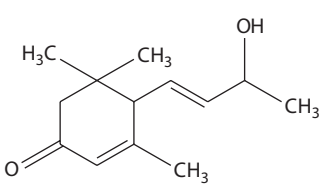
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2344.	38818-55-2	1	1	1	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-trimethyl-, (*E*)-		3.13
2345.	102488-06-2	0	1	0	2-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-, (*E*)		3.13
2346.	77761-55-8	0	1	0	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)-3,5,5-trimethyl-		2.5, 3.13
2347.	77842-24-1	0	1	0	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)-3,5,5-trimethyl- {isomer}		2.5, 3.13
2348.		1	0	0	2-Cyclohexen-1-one, 4-(2-butenyl)-3,5,5-trimethyl-		3.13
2349.	13215-88-8	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-		3.13, 24.3
2350.	5164-78-3	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*E,E*)- {megastigmatrienone} {*trans*-, *trans*-K_{1a}}		3.13, 24.3
2351.	5298-13-5	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*E,Z*)- {*trans*-,*cis*-K_{2a}}		3.13, 24.3
2352.	5492-79-5	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,E*)- {*cis*-, *trans*-K_{1b}}		3.13, 24.3
2353.	5164-79-4	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,Z*)- {*cis*-, *cis*-K_{2b}}		3.13, 24.3
2354.		1	1	1	2-Cyclohexen-1-one, 4-(3-butenylidene)-3,5,5-trimethyl-		3.13
2355.		0	1	0	2-Cyclohexen-1-one, 4-ethyl-		3.13
2356.	62512-22-5	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-		2.5, 3.13, 8.3, 10.2
2357.	77699-19-5	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-		2.5, 3.13, 8.3, 10.2
2358.	159813-37-3	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [4R-[4R*(1E,3S*)]]-		2.5, 3.13, 8.3, 10.2
2359.	54835-70-0	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-4-hydroxy-3,5,5-trimethyl-, [R-[R*,S*-(*E*)]]-		2.5, 3.13, 8.3, 10.2
2360.	62512-23-6	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy) butyl]-3,5,5-trimethyl-		2.5, 3.13, 8.3, 10.2
2361.	91048-13-4	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy) butylidene]-3,5,5-trimethyl-		2.5, 3.13, 8.3, 10.2
2362.	34318-21-3	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {4-keto-α-ionol}		2.5, 3.13

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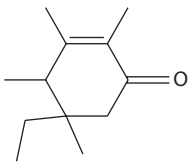
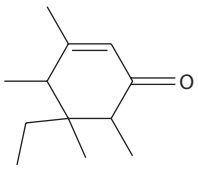
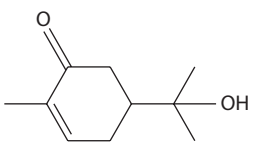
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2363.	52210-15-8	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-		2.5, 3.13
2364.	68759-08-0	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-,[S-[R*,S*-(*E*)]]-		2.5, 3.13
2365.		1	0	0	2-Cyclohexen-1-one, 4-hydroxy 4-(3-methyl-1, 3-dibutenyl)-3,5,5-trimethyl-		2.5, 3.13
2366.	7070-24-8	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-4-(3-oxo-1-butenyl)-3,5,5-trimethyl-		2.5, 3.13
2367.	60047-19-0	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl- {4-ketodihydro-α-ionol}		2.5, 3.13
2368.	36151-02-7	1	1	1	2-Cyclohexen-1-one,4-(3-hydroxybutyl)-3,5,5-trimethyl-, [R-(R*,R*)]-		2.5, 3.13
2369.	60026-24-6	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-		2.5, 3.13
2370.	102488-07-3	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-, (*E*)		2.5, 3.13
2371.	19620-37-2	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-2,6,6-trimethyl-		2.5, 3.13
2372.	14203-59-9	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-		2.5, 3.13
2373.	23526-45-6	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-(+) {Blumenol A}		2.5, 3.13
2374.	24427-77-8	1	0	0	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {vomifoliol}		2.5, 3.13
2375.	23069-00-3	1	1	1	2-Cyclohexen-1-one, 4-hydroxymethyl-3,5,5-trimethyl-		2.5, 3.13
2376.	500-02-7	0	1	0	2-Cyclohexen-1-one, 4-(1-methylethyl)-		3.13
2377.	51171-72-3	1	0	0	2-Cyclohexen-1-one, 4-phenyl-		3.13
2378.	1073-13-8	1	0	0	2-Cyclohexen-1-one, 4,4-dimethyl-		3.13
2379.	5715-25-3	0	1	0	2-Cyclohexen-1-one, 4,5-dimethyl-		3.13
2380.	56691-69-1	0	1	0	2-Cyclohexen-1-one, 5-[1-(acetyloxy)-1-methylethyl]-2-methyl-, (R)-		3.13, 5.3
2381.	17369-60-7	0	1	0	2-Cyclohexen-1-one, 5-ethyl-2,3,4,5-tetramethyl-		3.13
2382.		0	1	0	2-Cyclohexen-1-one, 5-ethyl-3,4,5,6-tetramethyl-		3.13
2383.	7712-46-1	0	1	0	2-Cyclohexen-1-one, 5-(1-hydroxy-1-methylethyl)-2-methyl-		2.5, 3.13

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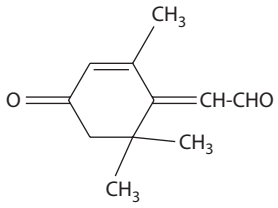
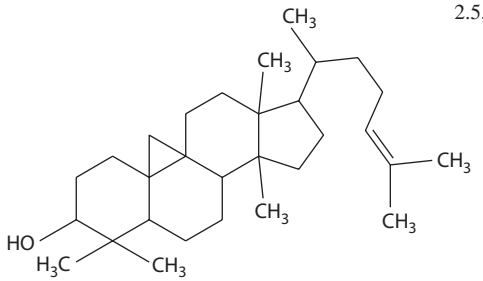
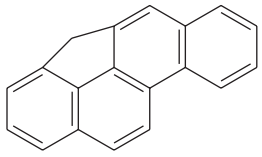
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2384.	499-74-1	1	0	0	2-Cyclohexen-1-one, 6-methyl-3-(1-methylethyl)-		3.13
2385.	4096-34-8	1	0	0	3-Cyclohexen-1-one		3.13
2386.		0	1	0	3-Cyclohexen-1-one,4-(1-butenyl)-3,5,5-trimethyl-		3.13
2387.	102488-08-4	0	1	0	3-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-, (*E*)		3.13
2388.	471-01-2	1	0	0	3-Cyclohexen-1-one, 3,5,5-trimethyl-		3.13
2389.	69874-67-5	1	0	0	5-Cyclohexen-1-one, 2-acetyl-3,5,5-trimethyl-		3.13
2390.	60026-16-6	0	1	0	Cyclohexenylideneacetaldehyde, 4-oxo-2,6,6-trimethyl-		3.12, 3.13
2391.	4657-58-3	0	1	0	9,19-Cyclolanostan-3-ol, (3β)-		2.5, 2.7
2392.	26955-76-0	0	1	0	9,19-Cyclolanostan-3-ol, 24,25-epoxy-, (3β)-		2.5, 2.7
2393.	1449-09-8	0	1	0	9,19-Cyclolanostan-3-ol, 24-methylene-, (3β)-		2.5, 2.7
2394.	469-38-5	1	0	0	9,19-Cyclolanost-24-en-3-ol, (3β)- {cycloartenol}		2.5, 2.7
							2.5, 2.7
2395.	25692-13-1	0	1	0	9,19-Cyclolanost-24-en-3-ol, 24-methyl-, (3β)-		2.5, 2.7
2396.	51088-90-5	0	1	0	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3β,24S)-		2.5, 2.7
2397.	511-61-5	0	1	0	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3β,24S)-		2.5, 2.7
2398.	124713-05-9	0	1	0	9,19-Cyclolanost-5-en-3-ol, 24-methylene-, (3β)-		2.5, 2.7
2399.	629-20-9	1	0	0	1,3,5,7-Cyclooctatetraene		1.12, 1.13
2400.	149331-19-1	0	1	0	Cyclononane, 1,1,4,4,7,7-hexamethyl-		1.12
2401.	98791-40-3	1	0	0	1*H*-Cyclopent[*d*]acenaphthylene, 2,7-dihydro-		1.20
2402.	219-86-3	1	0	0	7*H*-Cyclopent[*d*]acenaphthylene		1.20
2403.	202-98-2	1	0	0	4*H*-Cyclopenta[*def*]chrysene {4,5-methylenechrysene}		1.20

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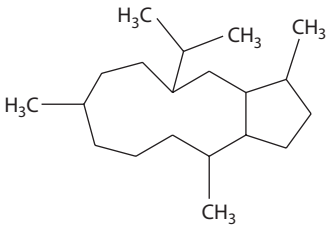
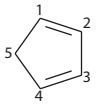
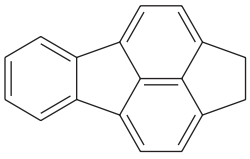
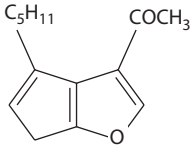
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2404.	126458-49-9	0	1	0	4*H*-Cyclopenta[3′,4′]cycloocta[1′,2′:1,5] cyclopent[1,2-*b*]oxiren-4-one, 1,2,2a,5,6,8,9, 10,10a,10b-decahydro-2,6,10a-trimethyl-8-(1-methylethyl)-, [2aS-(2aα,3aS*,6β,8β,10aβ,10bβ)]-		3.13
2405.	86154-08-7	0	1	0	4*H*-Cyclopenta[3′,4′]cycloocta[1′,2′:1,5] cyclopent[1,2-*b*]oxiren-4-one, 1,2,2a, 7,7a,8,9,10,10a,10b-decahydro-2a,6,10a-trimethyl-8-(1-methylethyl)-, (2aα,3aR*,7aβ,8β,10aβ,10bβ)-		3.13
2406.	142750-43-4	0	1	0	Cyclopentacycloundecene, tetradecahydro-1,4,8-trimethyl-11-(1-methylethyl)-		1.12
2407.	142750-40-1	0	1	0	4,10(1*H*,5*H*)-Cyclopentacycloundecenedione, 2,3,3a,6,7,11,12,12a-octahydro-1,3, 12-trihydroxy-3,8,12-trimethyl-5-(1-methylethyl)-, (1R*,3S*,3aR*,5S*,8Z, 12R*,12aR*)-(–)-		2.5, 3.13
2408.	541-91-3	0	1	0	Cyclopentadecanone, 3-methyl-		3.13
2409.	542-92-7	1	1	1	1,3-Cyclopentadiene {pyropentylene}		1.12
2410.	77208-25-4	1	0	0	1,3-Cyclopentadiene, dimethyl-		1.12
2411.	26519-92-6	1	0	0	1,3-Cyclopentadiene, ethyl-		1.12
2412.	26519-91-5	1	0	0	1,3-Cyclopentadiene, methyl-		1.12
2413.	33320-27-3	1	0	0	1,3-Cyclopentadiene-1-carboxaldehyde		3.12
2414.	4784-86-5	1	0	0	1,3-Cyclopentadiene, 1,2-dimethyl-		1.12
2415.	4045-53-8	1	0	0	1,3-Cyclopentadiene, 1,3-dimethyl-		1.12
2416.	96-39-9	1	0	0	1,3-Cyclopentadiene, 1-methyl-		1.12
2417.	96-38-8	1	0	0	1,3-Cyclopentadiene, 5-methyl-		1.12
2418.	497-20-1	1	0	0	1,3-Cyclopentadiene, 5-methylene- {fulvene}		1.12
2419.		1	0	0	2,4-Cyclopentadien-1-one, 2,3-dimethyl-4-hydroxy-		2.5, 3.13
2420.	94618-71-0	1	0	0	2,4-Cyclopentadien-1-one, 2-methyl-		3.13
2421.	193-54-4	1	0	0	Cyclopenta[*cd*]fluoranthene		1.20
2422.		1	1	1	Cyclopenta[*b*]furan, 3-acetyl-4-pentyl-		3.13, 10.2

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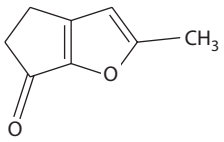
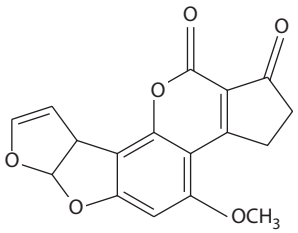
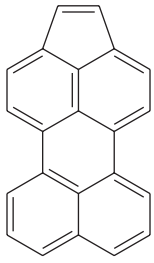
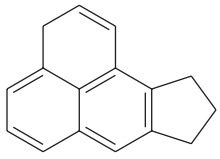
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2423.		1	1	1	Cyclopenta[*b*]furan-6-one, 4, 5-dihydro-2-methyl-		3.13, 10.2
2424.	1162-65-8	0	1	0	Cyclopenta[*c*]furo[3′,2′:4,5]furo [2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_1}		3.13, 6.3, 10.2
2425.	7220-81-7	0	1	0	Cyclopenta[*c*]furo[3′,2′:4,5] furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,8,9,9a-hexahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_2}		3.13, 6.3, 10.2
2426.	287-92-3	1	0	0	Cyclopentane {pentamethylene}		1.12
2427.	2452-99-5	1	0	0	Cyclopentane, 1,2-dimethyl-, *cis*-		1.12
2428.	822-50-4	1	0	0	Cyclopentane, 1,2-dimethyl-, *trans*-		1.12
2429.	96-37-7	1	0	0	Cyclopentane, methyl-		1.12
2430.	53366-54-4	1	0	0	Cyclopentane, (2-methylbutylidene)-		1.12
2431.	53366-58-8	1	0	0	Cyclopentane, (2-methylpropylidene)-		1.12
2432.	79637-61-9	1	0	0	Cyclopentane, propenyl-		1.12
2433.	2040-96-2	1	0	0	Cyclopentane, propyl-		1.12
2434.	30498-64-7	1	0	0	Cyclopentane, trimethyl-		1.12
2435.	1211-29-6	0	1	0	Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester {methyl jasmonate}		3.13, 5.3
2436.	20497-93-2	0	1	0	Cyclopentanecarboxaldehyde, 2-hydroxy-1-methyl- {two isomers}		2.5, 3.12
2437.	3400-45-1	0	1	0	Cyclopentanecarboxylic acid {cyclopentanoic acid}		4.3
2438.	38655-27-5	0	1	0	Cyclopentanecarboxylic acid, 1-methyl-3-(1-methylethenyl)-		4.3
2439.	66016-71-5	0	1	0	1,2-Cyclopentanedicarboxylic acid, 1-methyl-3-(1-methylethyl)-		4.3
2440.	28473-29-2	1	0	0	Cyclopentanedione {two isomers}		3.13
2441.	3008-40-0	1	1	1	1,2-Cyclopentanedione		3.13
2442.		0	1	0	1,2-Cyclopentanedione, 4-acetyl-		3.13
2443.		1	0	0	1,2-Cyclopentanedione, 3,4-diethyl-		3.13
2444.	54362-49-1	1	0	0	1,2-Cyclopentanedione, 3,5-diethyl-		3.13
2445.	72692-92-3	1	1	1	1,2-Cyclopentanedione, 3,3-dimethyl-		3.13
2446.	13494-06-9	1	1	1	1,2-Cyclopentanedione, 3,4-dimethyl-		3.13, 24.3, 25.29
2447.	13494-07-0	1	1	1	1,2-Cyclopentanedione, 3,5-dimethyl-		3.13, 24.3
2448.	13494-08-1	1	0	0	1,2-Cyclopentanedione, 3-ethyl-		3.13
2449.		1	0	0	1,2-Cyclopentanedione, 3-ethyl-3-methyl-		3.13
2450.		1	0	0	1,2-Cyclopentanedione, 3-ethyl-4-methyl-		3.13
2451.	71608-11-2	1	0	0	1,2-Cyclopentanedione, 3-ethyl-5-methyl- = 1,2-cyclopentanedione, 5-ethyl-3-methyl-		3.13

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2452.		1	0	0	1,2-Cyclopentanedione, hydroxy-		2.5, 3.13
2453.	765-70-8	1	1	1	1,2-Cyclopentanedione, 3-methyl- {cyclotene}		3.13, 25.29
2454.	60386-55-2	1	0	0	1,2-Cyclopentanedione, 3-(1-methylethyl)-		3.13
2455.	72693-09-5	1	0	0	1,2-Cyclopentanedione, 4-(1-methylethyl)-		3.13
2456.	71608-12-3	1	0	0	1,2-Cyclopentanedione, 3-methyl-5-propyl-		3.13
2457.	69745-71-7	1	0	0	1,2-Cyclopentanedione, 3-phenyl-		3.13
2458.	4542-64-7	1	0	0	1,2-Cyclopentanedione, 4-phenyl-		3.13
2459.	23747-37-7	1	0	0	1,2-Cyclopentanedione, 3-propyl-		3.13
2460.	3859-41-4	1	1	1	1,3-Cyclopentanedione		3.13
2461.	34598-80-6	1	0	0	1,3-Cyclopentanedione, 2,4-dimethyl-		3.13
2462.	823-36-9	1	0	0	1,3-Cyclopentanedione, 2-ethyl-		3.13
2463.	765-69-5	1	0	0	1,3-Cyclopentanedione, 2-methyl-		3.13
2464.		1	0	0	1,4-Cyclopentanedione, 2-hydroxy-3,5,5-trimethyl-		2.5, 3.13
2465.	120-92-3	1	1	1	Cyclopentanone {adipic ketone}		3.13
2466.	55713-44-5	0	1	0	Cyclopentanone, 2,2-dimethyl-4-(2-oxopropyl)-		3.13
2467.	1121-33-1	1	0	0	Cyclopentanone, 2,4-dimethyl-		3.13
2468.	20030-85-7	1	0	0	Cyclopentanone, 2,4-dimethyl- {isomer}		3.13
2469.	4041-09-2	1	0	0	Cyclopentanone, 2,5-dimethyl-		3.13
2470.	4971-18-0	1	0	0	Cyclopentanone, 2-ethyl-		3.13
2471.	10264-55-8	1	0	0	Cyclopentanone, 3-ethyl-		3.13
2472.		1	0	0	Cyclopentanone, 2-ethylidene-		3.13
2473.	473-84-7	1	0	0	Cyclopentanone, 2-hydroxy-		2.5, 3.13
2474.	28631-88-1	1	0	0	Cyclopentanone, methyl-		3.13
2475.	1120-72-5	1	0	0	Cyclopentanone, 2-methyl-		3.13
2476.		1	0	0	Cyclopentanone, 2-(1-methylpropyl)-		3.13
2477.	1757-42-2	1	0	0	Cyclopentanone, 3-methyl-		3.13
2478.		1	0	0	Cyclopentanone, 3-methyl- {isomer}		3.13
2479.	189-01-5	1	0	0	Cyclopenta[*cd*]perylene		1.20
2480.		1	0	0	Cyclopenta[*cd*]perylene, methyl-		1.20
2481.	211-95-0	1	0	0	Cyclopenta[*a*]phenalene		1.20
2482.	61261-04-9	1	0	0	Cyclopentaphenanthrene		1.20
2483.	80455-52-3	1	0	0	Cyclopentaphenanthrene {at least two isomers in MSS}		1.20
2484.		1	0	0	Cyclopentaphenanthrene, methyl- {at least two isomers in MSS}		1.20

(*continued*)

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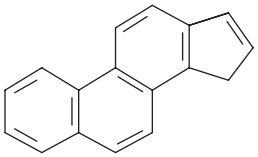
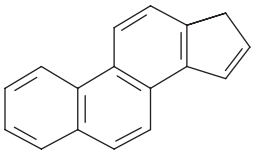
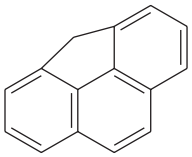
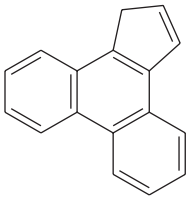
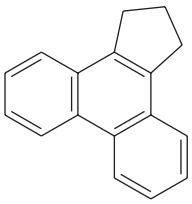
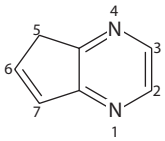
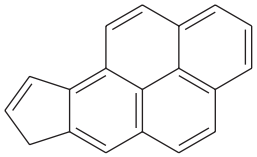
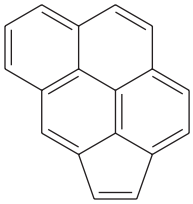
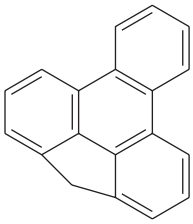
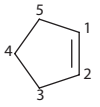
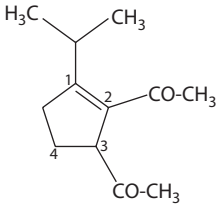
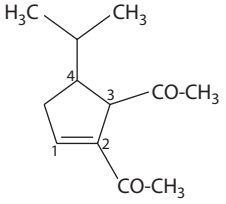
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2485.	219-07-8	1	0	0	15*H*-Cyclopenta[*a*]phenanthrene		1.20
2486.	482-66-6	1	0	0	15*H*-Cyclopenta[*a*]phenanthrene, 16,17-dihydro-		1.20
2487.	219-08-9	1	0	0	17*H*-Cyclopenta[*a*]phenanthrene		1.20
2488.	71277-92-4	1	0	0	17*H*-Cyclopenta[*a*]phenanthrene, ethyl-		1.20
2489.	71277-93-5	1	0	0	17*H*-Cyclopenta[*a*]phenanthrene, methyl-		1.20
2490.	203-64-5	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene {4,5-methylenephenanthrene}		1.20
2491.	71277-91-3	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene, dimethyl-		1.20
2492.	65319-51-9	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene, ethyl-		1.20
2493.	58548-39-3	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene, methyl-		1.20
2494.	235-92-7	1	0	0	1*H*-Cyclopenta[*l*]phenanthrene		1.20
2495.		1	0	0	Cyclopenta[*l*]phenanthrene, dihydro-		1.20
2496.	723-98-8	1	0	0	1*H*-Cyclopenta[*l*]phenanthrene, 2,3-dihydro-		1.20
2497.	25042-83-5	1	0	0	5*H*-Cyclopentapyrazine		17.7, 17.21
2498.	23747-47-9	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-		17.7, 17.21
2499.	38917-63-4	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-2, 3-dimethyl-		17.7, 17.21
2500.		1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5, 7-dimethyl-		17.7, 17.21
2501.	38917-60-1	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-ethyl-		17.7, 17.21
2502.	52517-53-0	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-ethyl-		17.7, 17.21
2503.	23747-46-8	1	1	1	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-methyl-		17.7, 17.21

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2504.	23747-48-0	1	1	1	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-methyl-		17.7, 17.21
2505.	61891-57-4	1	0	0	5*H*-Cyclopentapyrazine, dimethyl-		17.7, 17.21
2506.	61929-05-3	1	0	0	5*H*-Cyclopentapyrazine, 2,3-dimethyl-		17.7, 17.21
2507.	65129-00-2	1	0	0	5*H*-Cyclopentapyrazine, 2-ethyl-		17.7, 17.21
2508.	42315-22-0	1	0	0	Cyclopenta[*a*]pyrene		1.20
2509.		1	0	0	Cyclopenta[*a*]pyrene, 3,4-dihydro- {sometimes listed as 3,4-trimethylenepyrene}		1.20
2510.		1	0	0	Cyclopenta[*a*]pyrene, 3,4-dihydromethyl-		1.20
2511.	27208-37-3	1	0	0	Cyclopenta[*c,d*]pyrene {pyrene, 3.4-dimethylene}		1.20
2512.	25732-74-5	1	0	0	Cyclopenta[*cd*]pyrene, 3,4-dihydro-		1.20
2513.		1	0	0	Cyclopenta[*cd*]pyrene, 3, 4-dihydrodimethyl-		1.20
2514.	64760-18-5	1	0	0	Cyclopenta[*cd*]pyrene, 3,4-dihydromethyl-		1.20
2515.	23992-32-7	1	0	0	4*H*-Cyclopenta[*def*]triphenylene {4,5-methylenetriphenylene}		1.20
2516.	142-29-0	1	0	0	Cyclopentene		1.12
2517.		0	1	0	Cyclopentene, 2-acetyl-4-hydroxy-4-(1-methylethyl)-		2.5, 3.13
2518.		0	1	0	Cyclopentene, 2,3-diacetyl-1-(1-methylethyl)-		3.13
2519.		0	1	0	Cyclopentene, 2,3-diacetyl-4-(1-methylethyl)-		3.13

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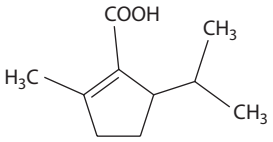
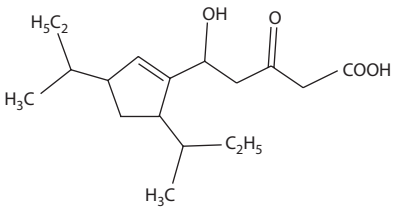
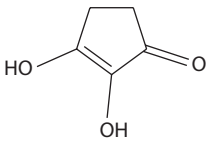
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2520.	54140-30-6	1	0	0	Cyclopentene, ethenyl-		1.12
2521.	28638-58-6	1	0	0	Cyclopentene, 1-ethenyl-		1.12
2522.	30233-85-3	1	0	0	Cyclopentene, ethyl-		1.12
2523.	2146-38-5	1	0	0	Cyclopentene, 1-ethyl-		1.12
2524.		1	0	0	Cyclopentene, methyl-		1.12
2525.	693-89-0	1	0	0	Cyclopentene, 1-methyl-		1.12
2526.	1120-62-3	1	0	0	Cyclopentene, 3-methyl-		1.12
2527.	1759-81-5	1	0	0	Cyclopentene, 4-methyl-		1.12
2528.		1	0	0	Cyclopentene, 3-(1-methylethyl)-		1.12
2529.	3074-61-1	1	0	0	Cyclopentene, 1-propyl-		1.12
2530.	56169-12-1	0	1	0	1-Cyclopentene-1-carboxylic acid, 2-methyl-5-(1-methylethyl)-		4.3
2531.	28750-51-8	1	1	1	3-Cyclopentene-1,2-dione		3.13
2532.		1	0	0	3-Cyclopentene-1,2-dione, 3,4-dimethyl-		3.13
2533.	2687-69-6	1	0	0	3-Cyclopentene-1,2-dione, 3,5-dimethyl-		3.13
2534.		1	0	0	3-Cyclopentene-1,2-dione, 3-ethyl-4-methyl-		3.13
2535.	10130-95-7	1	0	0	3-Cyclopentene-1,2-dione, 3-methyl-		3.13
2536.	66309-79-3	1	0	0	3-Cyclopentene-1,2-dione, 4-methyl-		3.13
2537.	930-60-9	0	1	0	4-Cyclopentene-1,3-dione		3.13
2538.		1	0	0	4-Cyclopentene-1,3-dione, 2,4-dimethyl-		3.13
2539.	18515-43-0	1	0	0	4-Cyclopentene-1,3-dione, 4,5-dimethyl-		3.13
2540.	53109-18-5	0	1	0	1-Cyclopentene-1-pentanoic acid, δ-hydroxy-3,5-bis(1-methylpropyl)-β-oxo-		2.5, 3.13
2541.	28982-58-3	1	0	0	Cyclopentenone		3.13
2542.	930-30-3	1	0	0	2-Cyclopenten-1-one {cyclopenten-3-one}		3.13
2543.		1	0	0	2-Cyclopenten-1-one, C_3-alkyl-		3.13
2544.		1	0	0	2-Cyclopenten-1-one, C_4-alkyl-		3.13
2545.	72692-71-8	1	0	0	2-Cyclopenten-1-one, dimethyl-		3.13
2546.	65462-39-7	1	0	0	2-Cyclopenten-1-one, ethyl-		3.13
2547.	61205-39-8	1	0	0	2-Cyclopenten-1-one, ethyl-2-hydroxy-		2.5, 3.13
2548.		1	0	0	2-Cyclopenten-1-one, ethylmethyl-		3.13
2549.	65452-01-9	1	0	0	2-Cyclopenten-1-one, methyl-		3.13
2550.		1	0	0	2-Cyclopenten-1-one, phenyl-		3.13
2551.	65436-85-3	1	0	0	2-Cyclopenten-1-one, propyl-		3.13
2552.	82000-05-3	1	0	0	2-Cyclopenten-1-one, trimethyl-		3.13
2553.	17190-74-8	0	1	0	2-Cyclopenten-1-one, 2-(2-butenyl)-4-hydroxy-3-methyl-		2.5, 3.13
2554.	78210-65-8	1	0	0	2-Cyclopenten-1-one, 2-(2-furanyl)-		3.13, 10.2
2555.	61892-84-0	1	0	0	2-Cyclopenten-1-one, 2-(2-oxopropyl)-		3.13
2556.	80-72-8	1	0	0	2-Cyclopenten-1-one, 2,3-dihydroxy- {reductic acid}		2.5, 3.13

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2557.	1121-05-7	1	1	1	2-Cyclopenten-1-one, 2,3-dimethyl-		3.13
2558.	3779-64-4	1	0	0	2-Cyclopenten-1-one, 2,3-dimethyl-4-(1-methylethyl)-		3.13
2559.	61893-14-9	0	1	0	2-Cyclopenten-1-one, 2,3-dimethyl-5-(1-methylethyl)-		3.13
2560.	28790-86-5	1	0	0	2-Cyclopenten-1-one, 2,3,4-trimethyl-		3.13
2561.	54562-24-2	1	0	0	2-Cyclopenten-1-one, 2,3,5-trimethyl-		3.13
2562.	66309-82-8	1	0	0	2-Cyclopenten-1-one, 2,4,5-trimethyl-		3.13
2563.	23048-13-7	1	0	0	2-Cyclopenten-1-one, 2,4-dimethyl-		3.13
2564.	4041-11-6	1	0	0	2-Cyclopenten-1-one, 2,5-dimethyl-		3.13
2565.	2931-10-4	1	0	0	2-Cyclopenten-1-one, 2-ethyl-		3.13
2566.	5682-72-4	1	0	0	2-Cyclopenten-1-one, 2-ethyl-3-methyl-		3.13
2567.	78210-64-7	1	0	0	2-Cyclopenten-1-one, 2-ethyl-5-methyl-		3.13
2568.	10493-98-8	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-		2.5, 3.13
2569.	29798-72-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-butyl)-		2.5, 3.13
2570.	61364-95-2	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,4-diethyl-		2.5, 3.13
2571.	52808-97-6	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,5-diethyl-		2.5, 3.13
2572.	21835-00-7	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-		2.5, 3.13
2573.	21834-98-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,5-dimethyl-		2.5, 3.13
2574.	42348-12-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-ethyl-4-methyl-		2.5, 3.13
2575.	58228-72-1	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-ethyl-5-methyl-		2.5, 3.13
2576.	28017-62-1	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-ethyl-		2.5, 3.13
2577.	53263-58-4	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-5-ethyl-3-methyl-		2.5, 3.13
2578.	22323-97-3	1	0	0	2-Cyclopenten-1-one, 2-methoxy-		3.13, 10.2
2579.	80-71-7	1	1	1	2-Cyclopenten-1-one, 2-hydroxy-3-methyl- {methylcyclopentenolone}		2.5, 3.13, 24.3, 25.29
2580.	15899-72-6	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-		2.5, 3.13
2581.	55277-47-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylethyl)		2.5, 3.13
2582.	109682-92-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylbutyl)-		2.5, 3.13
2583.	109682-91-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(3-methylbutyl)-		2.5, 3.13
2584.	109682-81-7	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-(1-methylethyl)-		2.5, 3.13
2585.	55277-47-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylethyl)-		2.5, 3.13
2586.	29798-73-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylpropyl)-		2.5, 3.13
2587.	25684-05-3	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylpropyl)-		2.5, 3.13
2588.	109682-89-5	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-propyl-		2.5, 3.13
2589.	109682-85-1	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-5-propyl-		2.5, 3.13
2590.		1	0	0	2-Cyclopenten-1-one,2-hydroxy-4-methyl-		2.5, 3.13

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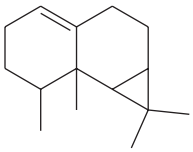
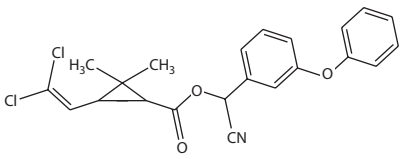
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2591.	109682-88-4	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-3-propyl-		2.5, 3.13
2592.	55007-08-4	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-pentyl-		2.5, 3.13
2593.	25684-04-2	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-propyl-		2.5, 3.13
2594.	82147-26-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-propyl-		2.5, 3.13
2595.	61205-40-1	1	1	1	2-Cyclopenten-1-one, 2-hydroxypropyl-		2.5, 3.13
2596.	109682-87-3	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl-		2.5, 3.13
2597.	24156-95-4	1	0	0	2-Cyclopenten-1-one, 3.5.5-trimethyl-		3.13
2598.		1	0	0	2-Cyclopenten-1-one, 2-methoxy-		3.13, 10.2
2599.	14189-85-6	1	0	0	2-Cyclopenten-1-one, 2-methoxy-3-methyl-		3.13, 10.2
2600.	1120-73-6	1	0	0	2-Cyclopenten-1-one, 2-methyl-		3.13
2601.	5760-58-7	1	0	0	2-Cyclopenten-1-one, 2-methyl-3-propyl-		3.13
2602.	61892-83-9	1	0	0	2-Cyclopenten-1-one, 2-methyl-4-(1-methylethyl)-		3.13
2603.	31089-17-5	1	0	0	2-Cyclopenten-1-one, 2-methyl-5-(1-methylethyl)-		3.13
2604.	66309-80-6	1	0	0	2-Cyclopenten-1-one, 2-methyl-5-methylene-		3.13
2605.	24105-07-5	1	1	1	2-Cyclopenten-1-one, 2-propyl-		3.13
2606.		1	0	0	2-Cyclopenten-1-one, 3-(2-furanyl)-		3.13, 10.2
2607.	1619-28-9	1	0	0	2-Cyclopenten-1-one, 3-(1-methylethyl)-		3.13
2608.		1	0	0	2-Cyclopenten-1-one, 3,4-diethyl-2-hydroxy-		2.5, 3.13
2609.	30434-64-1	1	0	0	2-Cyclopenten-1-one, 3,4-dimethyl-		3.13
2610.	21835-00-7	1	0	0	2-Cyclopenten-1-one, 3,4-dimethyl-2-hydroxy-		2.5, 3.13
2611.	72692-76-3	0	1	0	2-Cyclopenten-1-one, 3,4-dimethyl-2-(1-methylethyl)-		3.13
2612.		1	0	0	2-Cyclopenten-1-one, 3,5-diethyl-2-hydroxy-		2.5, 3.13
2613.	931-22-6	1	1	1	2-Cyclopenten-1-one, 3,5-dimethyl-		3.13
2614.	109682-90-8	1	0	0	2-Cyclopenten-1-one, 3,5-dimethyl-4-ethyl-2-hydroxy-		2.5, 3.13
2615.	21834-98-0	1	0	0	2-Cyclopenten-1-one, 3,5-dimethyl-2-hydroxy-		2.5, 3.13
2616.		0	1	0	2-Cyclopenten-1-one, 3,5-dimethyl-2-(1-methylethyl)-		3.13
2617.	5682-69-9	1	1	1	2-Cyclopenten-1-one, 3-ethyl-		3.13
2618.	21835-01-8	1	0	0	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- {ethylcyclopentenolone}		2.5, 3.13
2619.		1	0	0	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-4-methyl-		2.5, 3.13
2620.		1	0	0	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-5-methyl-		2.5, 3.13
2621.		1	0	0	2-Cyclopenten-1-one, 3-ethyl-2-methoxy-		3.13, 10.2
2622.	41496-77-9	1	1	1	2-Cyclopenten-1-one, 3-ethyl-2-methyl-		3.13
2623.	78210-63-6	1	0	0	2-Cyclopenten-1-one, 3-ethyl-4-hydroxy-		2.5, 3.13
2624.		1	0	0	2-Cyclopenten-1-one, 3-ethyl-4-methyl-		3.13
2625.		1	0	0	2-Cyclopenten-1-one, 3-ethyl-5-methyl-		3.13
2626.	5870-63-3	0	1	0	2-Cyclopenten-1-one, 3-hydroxy-2-methyl-		2.5, 3.13
2627.	2758-18-1	1	1	1	2-Cyclopenten-1-one, 3-methyl-		3.13

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2628.	3727-35-3	1	1	1	2-Cyclopenten-1-one, 3-methyl-2-(2-oxopropyl)-		3.13
2629.		1	0	0	2-Cyclopenten-1-one, 3-methyl-2-(1,3-pentadienyl)-		3.13
2630.	488-10-8	0	1	0	2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (*Z*)-		3.13
2631.		1	0	0	2-Cyclopenten-1-one, 3-(2-oxopropyl)-		3.13
2632.	3810-26-2	1	0	0	2-Cyclopenten-1-one, 3-phenyl-		3.13
2633.	35953-18-5	1	0	0	2-Cyclopenten-1-one, 3-propyl-		3.13
2634.	30434-65-2	0	1	0	2-Cyclopenten-1-one, 3,4,4-trimethyl-		3.13
2635.		1	0	0	2-Cyclopenten-1-one, 4-acetoxy-3-methyl-		3.13, 5.3
2636.		1	0	0	2-Cyclopenten-1-one, 4-acetyl-3,5,5-trimethyl-		3.13
2637.	28017-62-1	1	0	0	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-		2.5, 3.13
2638.	71387-71-8	1	0	0	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-3-methyl-		2.5, 3.13
2639.	71278-13-2	1	0	0	2-Cyclopenten-1-one, 4-ethyl-2-methyl-		3.13
2640.	30434-68-5	1	0	0	2-Cyclopenten-1-one, 4-ethyl-3-methyl-		3.13
2641.	10288-24-1	1	0	0	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-		2.5, 3.13
2642.	23415-96-7	1	0	0	2-Cyclopenten-1-one, 4-methyl-		3.13
2643.	66309-81-7	1	0	0	2-Cyclopenten-1-one, 4-methyl-3-(1-propenyl)-		3.13
2644.		1	0	0	2-Cyclopenten-1-one, 5-ethyl-2-hydroxy-3-methyl-		2.5, 3.13
2645.	70919-26-5	1	0	0	2-Cyclopenten-1-one, 5-hydroxy-		2.5, 3.13
2646.	70919-27-6	1	0	0	2-Cyclopenten-1-one, 5-hydroxy-3-methyl-		2.5, 3.13
2647.	14963-40-7	1	0	0	2-Cyclopenten-1-one, 5-methyl-		3.13
2648.	14320-37-7	1	0	0	3-Cyclopenten-1-one		3.13
2649.		0	1	0	3-Cyclopenten-1-one, 3-(1-methylethyl)-		3.13
2650.	17334-55-3	0	1	0	1aH-Cyclopropa[a]naphthalene, 1,1,7,7a-tetramethyl-2,3,5,6,7,7b-hexahydro {1(10)-aristolene, (+)}		1.12
2651.	1630-94-0	1	0	0	Cyclopropane, 1,1-dimethyl-		1.12
2652.	2511-95-7	1	0	0	Cyclopropane, 1,2-dimethyl-		1.12
2653.	930-18-7	1	0	0	Cyclopropane, 1,2-dimethyl-, (*Z*)-		1.12
2654.	2402-06-4	1	0	0	Cyclopropane, 1,2-dimethyl-, (*E*)-		1.12
2655.	22059-21-8	0	1	0	Cyclopropanecarboxylic acid, 1-amino-		4.3, 12.2
2656.	91465-08-6	1	1	1	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl) methyl ester {λ-Cyhalothrin®}		5.3, 11.2, 18.4, 21.3
2657.	52315-07-8	1	1	1	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl) methyl ester {Cypermethrin®}		5.3, 10.2, 11.2, 18.4, 21.3, 25.29

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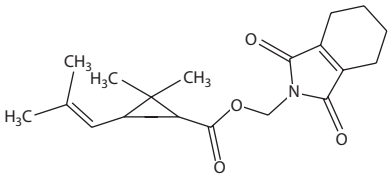
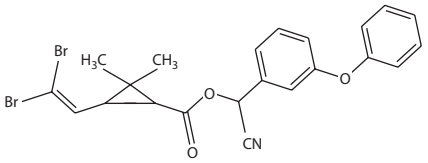
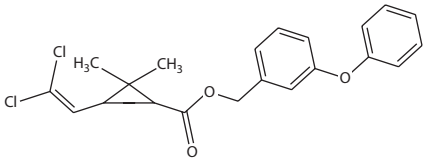
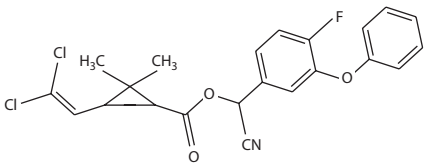
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2658.	67375-30-8	1	1	1	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl) methyl ester {α-Cypermethrin®}		5.3, 10.2, 11.2, 18.4, 21.3
2659.	121-29-9	0	1	0	Cyclopropanecarboxylic acid, 2, 2-dimethyl-3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {Pyrethrin II®}		5.3, 21.3
2660.	7696-12-0	0	1	0	Cyclopropanecarboxylic acid, 2, 2-dimethyl-3-(2-methyl-1-propenyl)-, (1-cyclohexene-1,2-dicarboximido) methyl ester {Tetramethrin®}		5.3, 21.3
2661.	121-21-1	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {Pyrethrin I®}		5.3, 21.3
2662.	10453-86-8	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, (5-phenylmethyl-3-furanyl)methyl ester {Resmethrin®}		5.3, 21.3
2663.	52918-63-5	1	1	1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl)methyl ester {Deltamethrin®}		5.3, 10.2, 11.2, 18.4, 21.3, 25.29
2664.	52645-53-1	0	1	0	Cyclopropanecarboxylic acid, 2, 2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl)methyl ester {Permethrin®, Spartan®}		5.3, 10.2, 18.4, 21.3, 25.29
2665.	68359-37-5	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl) methyl ester {Cyfluthrin®}		5.3, 10.2, 11.2, 18.4, 21.3
2666.	97-41-6	1	1	1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ethyl ester		5.3
2667.	5460-63-9	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, methyl ester		5.3
2668.	25402-06-6	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 3-(2-butenyl)-2-methyl-4-oxo-2-cyclopenten-1-yl ester {Cinerin I®}		5.3, 21.3
2669.	4466-14-2	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester {Jasmolin 1®}		5.3, 21.3

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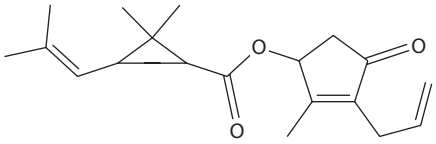
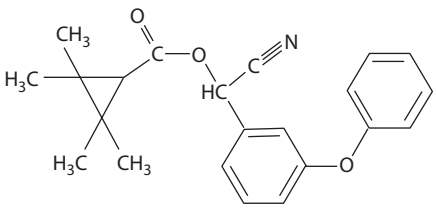
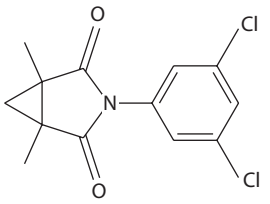
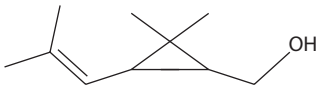
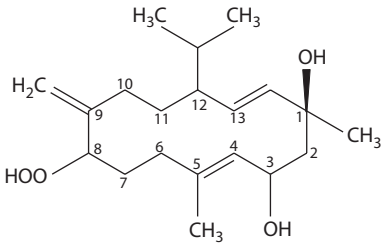
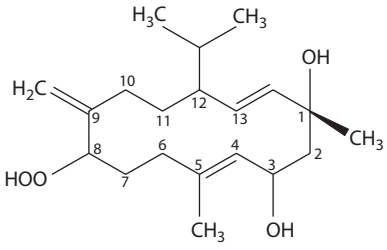
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2670.	584-79-2	0	1	0	Cyclopropanecarboxylic acid, 2, 2-dimethyl-3-(2-methylpropenyl)-, 2-(1-propenyl)-4-hydroxy-3-methyl-2-cyclopenten-1-one ester {Allethrin®}		5.3, 21.3
2671.	66841-25-6	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-, cyano(3-phenoxyphenyl)methyl ester {Tralomethrin®}		5.3, 11.2, 18.4, 21.3
2672.	39515-41-8	1	1	1	Cyclopropanecarboxylic acid, 2,2,3,3-tetramethyl cyano (3-phenoxyphenyl)methyl ester {Fenpropathrin®, Danitol®}		5.3, 11.2, 21.3
2673.	82657-04-3	0	1	0	Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-trifluoro-1-propenyl]-2, 2-dimethyl-, (2-methyl[1,1′-biphenyl]-3-yl)methyl ester, (1R,3R)-rel- {Bifenthrin®, Biphenthrin®}		5.3, 18.4, 21.3
2674.	17219-23-7	0	1	0	Cyclopropanecarboxylic acid, 2,3-dimethyl-		4.3
2675.	32809-16-8	0	1	0	1,2-Cyclopropanedicarboximide, *N* (3,5-dichlorophenyl)-1,2-dimethyl- {Procymidone®}		18.4, 21.3, 25.29
2676.	2516-33-8	0	1	0	Cyclopropanemethanol		2.5
2677.	18383-59-0	0	1	0	Cyclopropanemethanol, 2,2-dimethyl-3-(2-methylpropenyl)- {chrysanthemyl alcohol}		2.5
2678.	50906-50-8	0	1	0	9,19-Cyclostigmast-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24Z)-		2.5, 2.7
2679.	89288-59-5	0	1	0	4,13-Cyclotetradecadiene-1,3-diol, 8-hydroperoxy-1, 5-dimethyl-9-methylene-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8R*,12R*,13*E*)]-		2.5
2680.	89362-05-0	0	1	0	4,13-Cyclotetradecadiene-1, 3-diol, 8-hydroperoxy-1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,8S*,12S*,13*E*)]-		2.5

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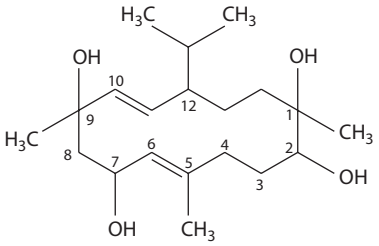
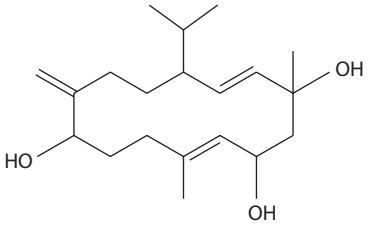
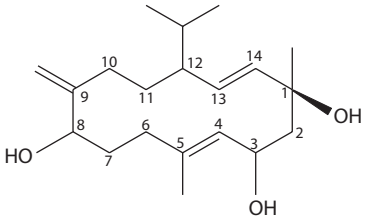
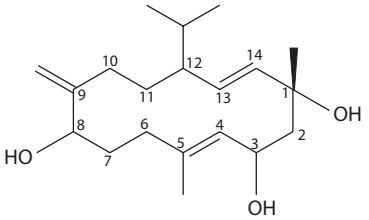
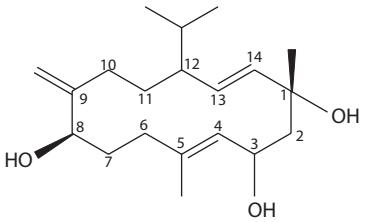
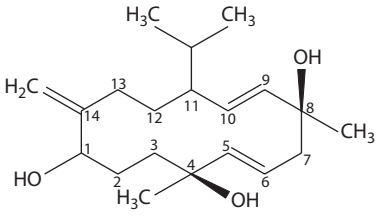
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2681.	102734-57-6	0	1	0	5,10-Cyclotetradecadiene-1,2,7,9-tetrol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,2R*,5*E*,7S*,9R*,10*E*,12R*)]-		2.5
2682.	89362-08-3	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-		2.5
2683.	89362-09-4	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,8S*,12S*,13*E*)]-		2.5
2684.	91200-13-4	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8S*,12R*,13*E*)]-		2.5
2685.	80802-00-2	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-		2.5
2686.	91163-46-1	0	1	0	5,9-Cyclotetradecadiene-1,4,8-triol, 4,8-dimethyl-14-methylene-11-(1-methylethyl)-, [1S-(1R*,4R*,5*E*,8S*,9*E*,11R*)]-		2.5
2687.	90660-18-7	0	1	0	4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-(1-methylethyl)-, [6R-(4*E*,6R*,		2.5, 3.13
2688.	119613-98-8	0	1	0	5,10-Cyclotetradecadien-1-one, 7,9-dihydroxy-7,11-dimethyl-4-(1-methylethyl)-, [4S-(4R*,5*E*,7R*,9S*,10*E*)]-		2.5, 3.13

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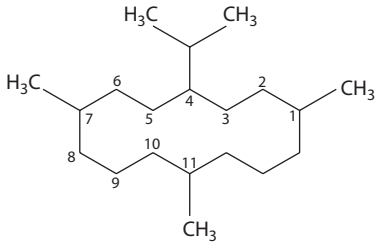
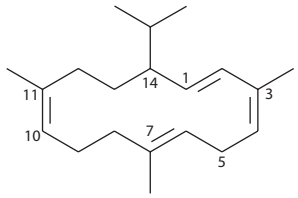
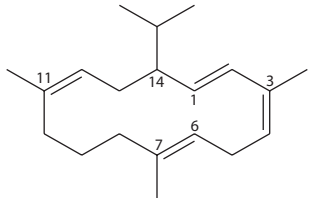
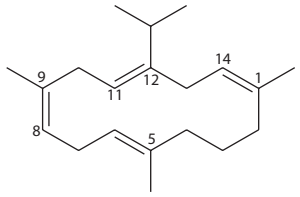
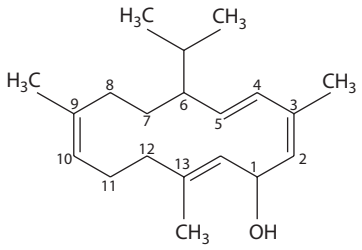
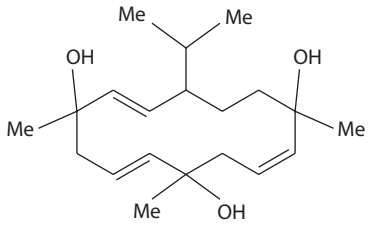
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2689.	1786-12-5	0	1	0	Cyclotetradecane, 1,7,11-trimethyl-4-(1-methylethyl)-		1.12
2690.	150405-76-8	0	1	0	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-		1.12
2691.	101159-08-4	1	1	1	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)- {cembrene}		1.12
2692.	1898-13-1	0	1	0	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(*E,Z,E,E*)]-		1.12
2693.		0	1	0	1,3,6,11-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-		1.12
2694.		0	1	0	5,8,11,14-Cyclotetradecatetraene, 1.5.9-trimethyl-12-(1-methylethyl)-		1.12
2695.	101159-07-3	0	1	0	1,4,7,10-Cyclotetradecatetraene, 1,7,11-trimethyl-4-(1-methylethenyl)-		1.12
2696.	39815-66-2	0	1	0	2,4,9,13-Cyclotetradecatetraen-1-ol, 3,9,13-trimethyl-6-(1-methylethyl)-		2.5
2697.	95334-70-6	0	1	0	2,6,10-Cyclotetradecatriene-1,5,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-		2.5

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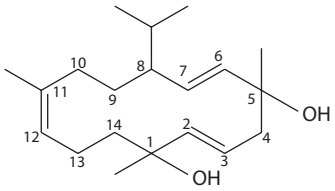
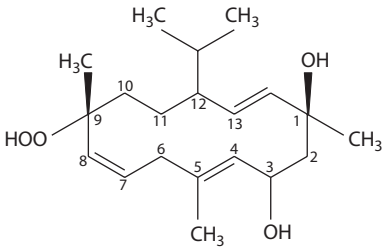
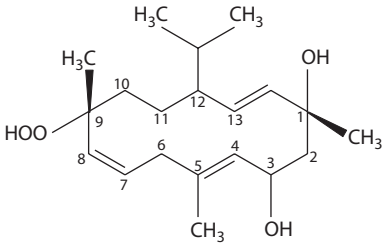
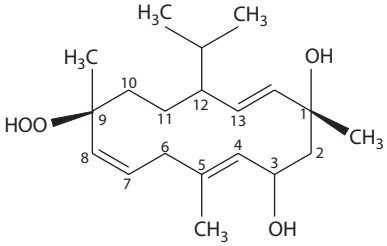
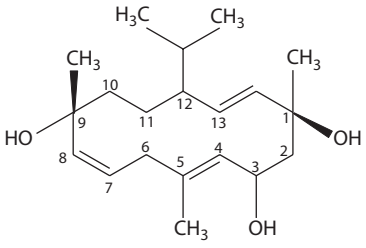
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2698.	59284-88-7	1	1	1	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, (1S,2*E*,5R,6*E*,8S,11*E*) {β-3,8,13-duvatriene-1,5-diol}		2.5
2699.	57688-99-0 59284-87-6	1	0	0	2,6,11-Cyclotetradecatriene-1, 5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-		2.5
2700.	84367-90-8	1	1	1	2,6,11-Cyclotetradecatriene-1, 5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1S-(1R*,2*E*,5R*,6*E*,8R*,11*E*)]-		2.5
2701.	84367-92-0	0	1	0	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8S*,11*E*)]-		2.5
2702.	89288-60-8	0	1	0	4,7,13-Cyclotetradecatriene-1, 3-diol, 9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*, 7*E*,9R*,12R*,13*E*)]-		2.5
2703.	89362-06-1	0	1	0	4,7,13-Cyclotetradecatriene-1, 3-diol, 9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*, 4*E*,7*E*,9S*,12R*,13*E*)]-		2.5
2704.	89362-07-2	0	1	0	4,7,13-Cyclotetradecatriene-1, 3-diol, 9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7*E*, 9S*,12S*,13*E*)]-		2.5
2705.	82003-46-1	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*, 4*E*,7*E*,9R*,12R*,13*E*)]-		2.5

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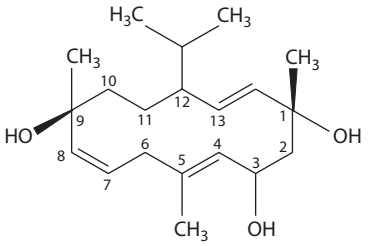
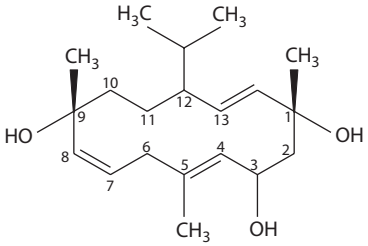
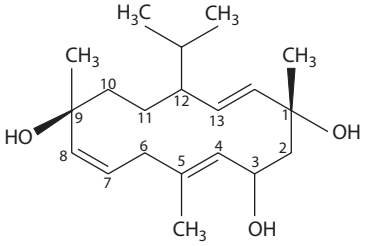
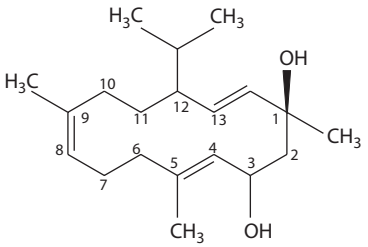
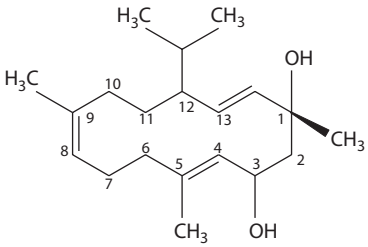
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2706.	89362-10-7	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7*E*,9R*,12R*,13*E*)]-		2.5
2707.	89362-11-8	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7*E*,9R*,12R*,13*E*)]-		2.5
2708.	91200-14-5	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7*E*,9R*,12R*,13*E*)]-		2.5
2709.	116348-80-2	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-		2.5
2710.	121916-90-3	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3R*,4*E*,8*E*,12S*,13*E*)]-		2.5
2711.	122620-36-4	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, (1R*,3R*,4*E*,8*E*,12S*,13*E*)-(±)-		2.5
2712.	57605-80-8	1	1	1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-		2.5, 26.9
2713.	57605-81-9	1	1	1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-1R*,3R*,4*E*,8*E*,12S*,13*E*)]-		2.5, 26.9

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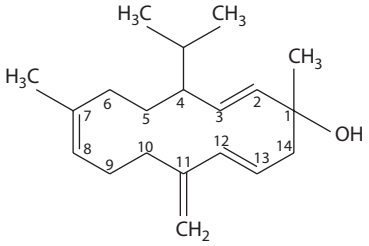
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2714.	87554-04-9	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*Z*)]-		2.5
2715.	7220-78-2	1	1	1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-		2.5
2716.	2043-08-1	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, 3-acetate, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-		2.5
2717.	146564-67-2	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 9-(hydroxymethyl)-1,5-dimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*Z*,12R*,13*E*)]-		2.5
2718.	149403-67-8	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7S*,8*E*,12R*)]-		2.5
2719.	149403-68-9	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7R*,8*E*,12R*)]-		2.5
2720.	149403-69-0	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7R*,8*E*,12S*)]-		2.5
2721.	149403-70-3	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7S*,8*E*,12S*)]-		2.5
2722.	149403-71-4	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7S*,8*Z*,12S*)]-		2.5
2723.	146564-66-1	0	1	0	4,9,13-Cyclotetradecatriene-1,3,8-triol, 3,9,13-trimethyl-6-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,6S*,8R*,9*E*,13*E*)]-		2.5
2724.	146609-95-2	0	1	0	4,9,13-Cyclotetradecatriene-1,3,8-triol, 3,9,13-trimethyl-6-(1-methylethyl)-, [1R-(1R*,3S*,4*E*,6S*,8R*,9*E*,13*E*)]-		2.5
2725.	60026-11-1	0	1	0	2,7,12-Cyclotetradecatrien-1-ol, 1,7-dimethyl-11-methylene-4-(1-methylethyl)- *Chem. Abstracts numbering*	 *Chem. Abstracts numbering*	2.5
2726.	87387-80-2	0	1	0	2,6,12-Cyclotetradecatrien-1-ol, 3,7,13-trimethyl-10-(1-methylethenyl)-		2.5
2727.	119864-28-7	0	1	0	2,7,10-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1R-(1R*,2*E*,4S*,7*E*,10*E*)]-		2.5
2728.	119944-62-6	0	1	0	2,7,10-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1S-(1R*,2*E*,4R*,7*E*,10*E*)]-		2.5

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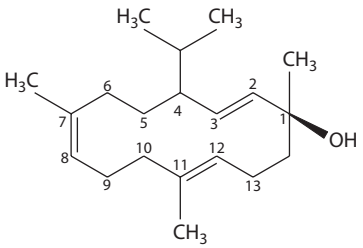
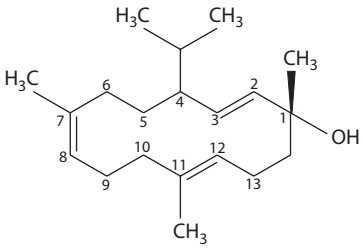
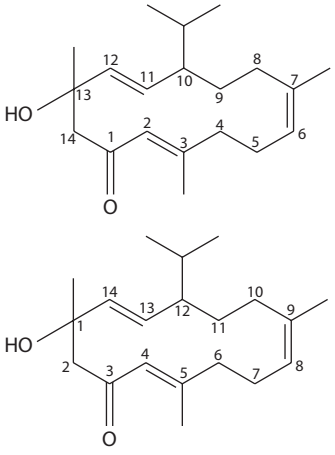
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2729.	25269-17-4	1	1	1	2,7,11-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1R-(1R*,2*E*,4S*,7*E*,11*E*)]-		2.5
2730.	80126-41-6	0	1	0	2,7,11-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1S-(1R*,2*E*,4R*,7*E*,11*E*)]-		2.5
2731.	149312-90-3	0	1	0	2,6,11-Cyclotetradecatrien-1-one, 5, 13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-, [5S-(2*E*,5R*,6*E*,10R*,11*E*,13R*)]-		2.5, 3.13
2732.	98064-74-5	0	1	0	2,5,11-Cyclotetradecatrien-1-one, 7,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-, [7S-(2*E*,5*E*,7R*,10R*,11*E*,13R*)]-		2.5, 3.13
2733.	149312-89-0	0	1	0	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-, [6S-(2*E*,6R*,7*E*,9R*,11S*,12*E*)]-		2.5, 3.13
2734.	149403-72-5	0	1	0	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-, [6S-(2*E*,6R*,7*E*,9S*,11S*,12*E*)]-		2.5, 3.13
2735.	41429-54-3	1	1	1	2,6,11-Cyclotetradecatrien-1-one, 13-hydroxy-3,7,13-trimethyl-10-(1-methylethyl)- = 4,8,13-cyclotetradecatrien-1-ol-3-one-1,5,9-trimethyl-12-(1-methylethyl)-		2.5, 3.13

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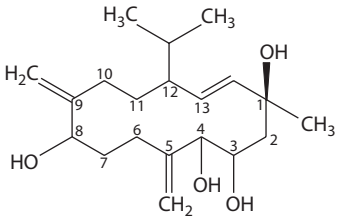
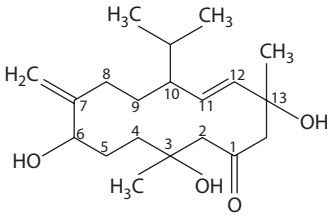
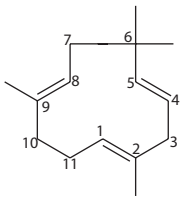
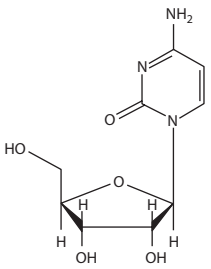
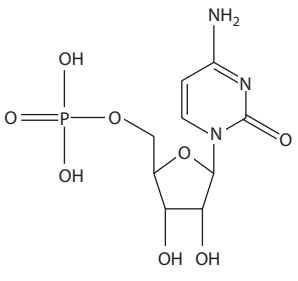
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2736.		0	1	0	13-Cyclotetradecene-1,3,4,8-tetrol-1-methyl-5,9-dimethylene-12-(1-methylethyl)-		2.5
2737.		0	1	0	1-Cyclotetradecen-1-one, 3,6,13-triol-3,13-dimethyl-7-methylene-10-(1-methylethyl)-		2.5, 3.13
2738.	62376-15-2	1	0	0	Cycloundecane, 1,1,2-trimethyl-		1.12
2739.	6753-98-6	0	1	0	1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (*E,E,E*)-		1.12
2740.	498-40-8	0	1	0	Cysteic acid	$HO\text{-}SO_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 18.1
2741.	52-90-4	1	1	1	*L*-Cysteine {propanoic acid, 2-amino-3- mercapto- (R)}	$HS\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 18.1, 24.3, 25.29, 26.9
2742.	636-58-8	0	1	0	*L*-Cysteine, *N*-*L*-γ-glutamyl-		4.3, 4.10, 12.2, 18.1
2743.	24645-67-8	0	1	0	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-}	$\{S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH\}_2$	0.4, 4.3, 4.10, 12.2, 18.1, 25.29
2744.	56-89-3 13028-62-1	0	1	0	*L*-Cystine		0.4, 4.3, 4.10, 12.2, 18.1
2745.	65-46-3	0	1	0	Cytidine {2(1*H*)-pyrimidinone, 4-amino-1-β-*D*-ribofuranosyl-}		2.5, 10.2, 12.2, 17.7
2746.	65-47-4	0	1	0	Cytidine 5′-(tetrahydrogen triphosphate)		2.5, 10.2, 12.2, 17.7
2747.	63-37-6	0	1	0	5′-Cytidylic acid		2.5, 5.3, 10.2, 12.2, 17.7

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2748.	9044-61-5	0	1	0	Cytochrome b 559		22.2
2749.	9035-46-5	0	1	0	Cytochrome c6		22.2
2750.	62168-75-6	0	1	0	Deacylase		22.2
2751.	2363-88-4	0	1	0	2,4-Decadienal		3.12
2752.	25152-84-5	1	1	1	2,4-Decadienal, (*E,E*)-		3.12, 24.3
2753.	63889-75-8	0	1	0	Decadienoic acid {sebacic acid}		4.3
2754.	59286-28-1	0	1	0	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*Z,E*)-		3.13, 4.3
2755.	58315-84-7	0	1	0	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, [S-(*E,E*)]-		3.13, 4.3
2756.	59262-52-1	0	1	0	2,7-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*E,E*)-		3.13, 4.3
2757.	158815-70-4	0	1	0	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-		2.5, 4.3, 6.3
2758.	160115-53-7	0	1	0	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-, methyl ester		2.5, 5.3, 6.3
2759.	112-31-2	1	1	1	Decanal {capraldehyde}	$H_3C\text{-}(CH_2)_8\text{-}CH{=}O$	3.12, 24.3, 25.29
2760.	2016-57-1	1	0	0	1-Decanamine		12.2
2761.	124-18-5	1	1	1	Decane	$H_3C\text{-}(CH_2)_8\text{-}CH_3$	1.10
2762.	61193-21-3	1	0	0	Decane, methyl-	$C_{10}H_{21}\text{-}CH_3$	1.10
2763.	6975-98-0	0	1	0	Decane, 2-methyl-	$H_3C\text{-}CH(CH_3)\text{-}(CH_2)_7\text{-}CH_3$	1.10
2764.	13151-34-3	1	0	0	Decane, 3-methyl-	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_6\text{-}CH_3$	1.10
2765.	13151-35-4	1	0	0	Decane, 5-methyl-	$H_3C\text{-}(CH_2)_4\text{-}CH(CH_3)\text{-}(CH_2)_3\text{-}CH_3$	1.10
2766.	111-20-6	1	1	1	Decanedioic acid	$HOOC\text{-}(CH_2)_8\text{-}COOH$	4.3
2767.	110-40-7	0	1	0	Decanedioic acid, diethyl ester	$H_5C_2\text{-}OOC\text{-}(CH_2)_8\text{-}COO\text{-}C_2H_5$	5.3
2768.	334-48-5	1	1	1	Decanoic acid {capric acid}	$H_3C\text{-}(CH_2)_8\text{-}COOH$	0.4, 4.3, 21.3, 24.3, 25.29
2769.	110-38-3	1	1	1	Decanoic acid, ethyl ester {ethyl caprate}	$H_3C\text{-}(CH_2)_8\text{-}COO\text{-}C_2H_5$	5.3, 24.3, 25.29
2770.		1	1	1	Decanoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-		2.5, 3.13, 4.3
2771.	5601-60-5	0	1	0	Decanoic acid, 8-methyl-		4.3
2772.	110-42-9	0	1	0	Decanoic acid, methyl ester	$H_3C\text{-}(CH_2)_8\text{-}COO\text{-}CH_3$	5.3
2773.	70898-23-6	1	1	1	Decanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester, (all-*E*)- {solanesyl decanoate}		5.3
2774.	70898-24-7	0	1	0	Decanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-	$H_3C\text{-}(CH_2)_8\text{-}COOCH_2\text{-}CH{=}C(CH_3)\text{-}CH_2\text{-}[CH_2CH_2CH(CH_3)CH_2]_3\text{-}H$	5.3
2775.	112-30-1	1	1	1	1-Decanol {capric alcohol}	$H_3C\text{-}(CH_2)_8\text{-}CH_2OH$	2.5, 21.3, 24.3, 25.29
2776.	693-54-9	1	1	1	2-Decanone {methyl octyl ketone}	$H_3C\text{-}(CH_2)_7\text{-}CO\text{-}CH_3$	3.13
2777.	9027-22-9	0	1	0	Decarboxylase		22.2
2778.	9036-20-8	0	1	0	Decarboxylase, adenosylmethionine		22.2
2779.	9024-77-5	0	1	0	Decarboxylase, arginine		22.2
2780.	9024-58-2	0	1	0	Decarboxylase, glutamate		22.2
2781.	37259-67-9	0	1	0	Decarboxylase, glycine		22.2
2782.	37205-42-8	0	1	0	Decarboxylase, α-ketoglutaric acid		0.4, 22.2

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2783.	9024-60-6	0	1	0	Decarboxylase, ornithine		22.2
2784.	9001-04-1	0	1	0	Decarboxylase, pyruvate		22.2
2785.	9024-70-8	0	1	0	Decarboxylase, uroporphyrinogen		22.2
2786.	63892-04-6	0	1	0	2,7,9-Decatrienoic acid, 3,9-dimethyl-6-(1-methylethyl)-, (*E,E*)-		4.3
2787.	2497-25-8	0	1	0	2-Decenal, (*Z*)-	H_3C-$(CH_2)_6$-CH═CH-CH═O	3.12
2788.	3913-71-1	0	1	0	2-Decenal, (*E*)-		3.12
2789.	58474-80-9	0	1	0	3-Decenal	H_3C-$(CH_2)_5$-CH═CH-CH_2-CH═O	3.12
2790.	30390-50-2	0	1	0	4-Decenal		3.12
2791.	21662-09-9	0	1	0	4-Decenal, (*Z*)-		3.12
2792.	872-05-9	1	1	1	1-Decene	H_2C═CH-$(CH_2)_7$-CH_3	1.11
2793.		1	0	0	1-Decene, 5-methyl-	H_2C═CH-$(CH_2)_2$-$CH(CH_3)$-$(CH_2)_4$-CH_3	1.11
2794.	6816-17-7	0	1	0	2-Decene	H_3C-CH═CH-$(CH_2)_6$-CH_3	1.11
2795.	26446-27-5 72881-27-7	0	1	0	Decenoic acid {three isomers detected}		4.3
2796.	60924-66-5	0	1	0	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-		2.5, 3.13, 4.3
2797.	129777-23-7	0	1	0	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-, [R-[R*,S*-(*E*)]]-		2.5, 3.13, 4.3
2798.	77288-98-3	0	1	0	6-Decen-2-one, 8,10-dihydroxy-8-methyl-5-(1-methylethyl)-		2.5, 3.13
2799.	9001-03-0	0	1	0	Dehydratase, carbonate		22.2
2800.	9024-34-4	0	1	0	Dehydratase, threonine		22.2
2801.	9035-82-9	0	1	0	Dehydrogenase		22.2
2802.	9031-72-5	0	1	0	Dehydrogenase, alcohol		22.2
2803.	9001-40-5	0	1	0	Dehydrogenase, glucose 6-phosphate		22.2
2804.	9029-12-3	0	1	0	Dehydrogenase, glutamate (nicotinamide adenine dinucleotide (phosphate))		22.2
2805.	9001-46-1	0	1	0	Dehydrogenase, glutamic acid		22.2
2806.	9026-38-4	0	1	0	Dehydrogenase, glutathione (ascorbate)		18.1, 22.2
2807.	9001-50-7	0	1	0	Dehydrogenase, glyceraldehyde phosphate		22.2
2808.	9028-13-1	0	1	0	Dehydrogenase, homoserine		22.2
2809.	9001-58-5	0	1	0	Dehydrogenase, isocitrate		22.2
2810.	9028-48-2	0	1	0	Dehydrogenase, isocitrate (nicotinamide adenine dinucleotide phosphate)		22.2
2811.	9001-64-3	0	1	0	Dehydrogenase, malate		22.2
2812.	56941-16-3	0	1	0	Dehydrogenase, malate (decarboxylating) (nicotinamide adenine dinucleotide (phosphate))		22.2
2813.	37250-19-4	0	1	0	Dehydrogenase, malate (nicotinamide adenine dinucleotide phosphate)		22.2
2814.	9028-47-1	0	1	0	Dehydrogenase, malate (oxalacetate-decarboxylating) (nicotinamide adenine dinucleotide phosphate)		22.2
2815.	9029-14-5	0	1	0	Dehydrogenase, methylenetetrahydrofolate		22.2
2816.	37256-31-8	0	1	0	Dehydrogenase, nicotine		22.2
2817.	9001-82-5	0	1	0	Dehydrogenase, phosphogluconate		22.2

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2818.	9073-95-4	0	1	0	Dehydrogenase, phosphogluconate (decarboxylating)		22.2
2819.	9050-70-8	0	1	0	Dehydrogenase, proline		22.2
2820.	9028-28-8	0	1	0	Dehydrogenase, quinate		22.2
2821.	9079-67-8	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide		22.2
2822.	9032-20-6	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide (phosphate) (quinone)		22.2
2823.	37256-36-3	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide (quinone)		22.2
2824.	37256-37-4	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide phosphate (quinone)		22.2
2825.	9001-68-7	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide phosphate		22.2
2826.	9026-87-3	0	1	0	Dehydrogenase, shikimate		22.2
2827.	9002-02-2	0	1	0	Dehydrogenase, succinate		22.2
2828.	9054-84-6	0	1	0	Dehydrogenase, xanthine		22.2
2829.		0	1	0	*Deinococcus-Thermus*, *Thermus*		22.2
2830.	97162-77-1	0	1	0	Demethylase, nicotine		22.2
2831.	9007-49-2	0	1	0	Deoxyribonucleic acid		0.4, 22.2
2832.	159844-35-6	0	1	0	Deoxyribonucleic acid (*Arabidopsis thaliana* clone TAY029 gene UbcAt3 ubiquitin-carrier enzyme E 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2833.	141712-74-5	0	1	0	Deoxyribonucleic acid (*Arabidopsis thaliana* strain Heynhold glycerol phosphate acyltransferase messenger RNA complementary)		22.2
2834.	140812-74-4	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* gene pma1 plus 5′- and 3′-flanking region fragment)		22.2
2835.	130061-32-4	0	1	0	Deoxyribonucleic acid (*Nicotiana sylvestris* clone NySS4 ribulose diphosphate carboxylase small subunit gene)		22.2
2836.	144997-82-0	0	1	0	Deoxyribonucleic acid (*Nicotiana sylvestris* clone yaDC12/yaDC17 gene psaDa protein D 2 messenger RNA complementary)		22.2
2837.	155317-25-2	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A11 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2838.	155317-10-5	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A13 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2839.	155317-11-6	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A14 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2840.	155317-12-7	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A15 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2841.	155317-13-8	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A6 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2842.	155317-14-9	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A7 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2843.	155317-15-0	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone NeIF-4A9 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2844.	160074-66-8	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* clone Ubi.U4 gene Ubi.U4 polyubiquitin plus 5′- and 3′-flanking region fragment)		22.2
2845.	160075-53-6	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* cv. SR1 leaf clone Ntfad3 ω-3 fatty acid desaturase mRNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2846.	131553-16-7	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun 16.5 kDa protein messenger RNA complementary)		22.2
2847.	131553-15-6	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun chitinase isoenzyme messenger RNA complementary)		22.2
2848.	143514-65-2	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun clone NeIF-5A3 protein formation initiation factor eIF 5A isoform gene)		22.2
2849.	141093-81-4	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun clone pMOG404 osmotin messenger RNA complementary)		22.2
2850.	143638-33-9	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun clone pTOL1 osmotin messenger RNA complementary)		22.2
2851.	143341-52-0	0	1	0	Deoxyribonucleic acid (tobacco 1-109-extensin-like protein precursor-specifying)		22.2

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2852.	152619-15-3	0	1	0	Deoxyribonucleic acid (tobacco chitinase acidic isoenzyme III messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2853.	152619-16-4	0	1	0	Deoxyribonucleic acid (tobacco chitinase basic isoenzyme III messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2854.	142978-98-1	0	1	0	Deoxyribonucleic acid (tobacco chloroplast clone L27-1 ribosome protein L 27 messenger RNA complementary)		22.2
2855.	139872-58-5	0	1	0	Deoxyribonucleic acid (tobacco clone lambda 5A gene RB7 plus 5′- and 3′-flanking region fragment)		22.2
2856.	139872-57-4	0	1	0	Deoxyribonucleic acid (tobacco clone lambda 5A gene RB7)		22.2
2857.	128284-58-2	0	1	0	Deoxyribonucleic acid (tobacco clone lambda CHN17 chitinase basic isoenzyme gene)		22.2
2858.	156553-68-3	0	1	0	Deoxyribonucleic acid (tobacco clone 59 gene chi-V chitinase plus 5′- and 3′-flanking region fragment)		22.2
2859.	156553-69-4	0	1	0	Deoxyribonucleic acid (tobacco clone cA-3 gene chi-V chitinase messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2860.	155663-09-5	0	1	0	Deoxyribonucleic acid (tobacco clone cpb20-52 antifungal protein CPB 20 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2861.	124757-79-5	0	1	0	Deoxyribonucleic acid (tobacco clone E22 protein PR 5 gene)		22.2
2862.	148757-18-0	0	1	0	Deoxyribonucleic acid (tobacco clone G27.1/G27.2 gene Npg1 plus 5′- and 3′-flanking region fragment)		22.2
2863.	158928-85-9	0	1	0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 1 fragment)		22.2
2864.	158928-86-0	0	1	0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 2 fragment)		22.2
2865.	158928-87-1	0	1	0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 3 fragment)		22.2
2866.	145137-42-4	0	1	0	Deoxyribonucleic acid (tobacco clone NtDAHPS-1 phospho-2-keto-3-deoxyheptonate aldolase messenger RNA complementary)		22.2
2867.	151876-45-8	0	1	0	Deoxyribonucleic acid (tobacco clone OMT3.4 catechol methyltransferase isoenzyme II messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2868.	128512-15-2	0	1	0	Deoxyribonucleic acid (tobacco clone pBSGlu39.1 endo-1,3-β-glucanase isoenzyme gene coding region)		22.2
2869.	128512-16-3	0	1	0	Deoxyribonucleic acid (tobacco clone pBSGlu39.3 endo-1,3-β-glucanase isoenzyme gene coding region)		22.2
2870.	147626-92-4	0	1	0	Deoxyribonucleic acid (tobacco clone pcGS2-17 glutamine synthetase isoenzyme 2 messenger RNA complementary)		22.2
2871.	128512-19-6	0	1	0	Deoxyribonucleic acid (tobacco clone pGL31 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)		22.2
2872.	128512-20-9	0	1	0	Deoxyribonucleic acid (tobacco clone pGL36 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)		22.2
2873.	128512-21-0	0	1	0	Deoxyribonucleic acid (tobacco clone pGL43 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)		22.2
2874.	103469-25-6	0	1	0	Deoxyribonucleic acid (tobacco clone PROB12 protein TL messenger RNA complementary)		22.2
2875.	158928-82-6	0	1	0	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 1 fragment)		22.2
2876.	158928-83-7	0	1	0	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 2 fragment)		22.2
2877.	158928-84-8	0	1	0	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 3 fragment)		22.2
2878.	141002-75-7	0	1	0	Deoxyribonucleic acid (tobacco clone pVK5 osmotin messenger RNA complementary)		22.2
2879.	150001-42-6	0	1	0	Deoxyribonucleic acid (tobacco clone TSC81 ribosome protein L 17 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2880.	128512-25-4	0	1	0	Deoxyribonucleic acid (tobacco endo-1,3-β-glucanase isoenzyme messenger RNA complementary)		22.2
2881.	143341-55-3	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 107-amino acid fragment-specifying)		22.2
2882.	143341-56-4	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 81-amino acid fragment-specifying)		22.2
2883.	160936-44-7	0	1	0	Deoxyribonucleic acid (tobacco leaf curl virus coat protein gene)		22.2
2884.	141004-11-7	0	1	0	Deoxyribonucleic acid (tobacco ribosome protein L 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2885.	143513-68-2	0	1	0	Deoxyribonucleic acid (tobacco strain NK326 gene oee2-A plus 5′- and 3′-flanking region fragment)		22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
2886.	143513-69-3	0	1	0	Deoxyribonucleic acid (tobacco strain NK326 gene oee2-A)		22.2
2887.	149309-58-0	0	1	0	Deoxyribonucleic acid (tobacco thioredoxin h2 gene plus 5′- and 3′-flanking region fragment)		18.1, 22.2
2888.	140114-22-3	0	1	0	Deoxyribonucleic acid (tobacco thioredoxin messenger RNA complementary plus 5′- and 3′-flanking region fragment)		18.1, 22.2
2889.	141712-75-6	0	1	0	Deoxyribonucleic acid (*Arabidopsis thaliana* strain Heynhold glycerol phosphate acyltransferase messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2890.	148037-15-4	0	1	0	Deoxyribonucleic acid (*Arabidopsis thaliana* thioredoxin h messenger RNA complementary plus 5′- and 3′-flanking region fragment)		18.1, 22.2
2891.	147533-09-3	0	1	0	Deoxyribonucleic acid (*Nicotiana alata* clone NaPRP3g12 proline-rich protein PRP 3 gene plus 5′- and 3′-flanking region fragment)		22.2
2892.	139860-37-0	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-4A2 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′-and 3′-flanking region fragment)		22.2
2893.	146150-24-5	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-4A2 protein formation initiation factor eIF 4A messenger RNA complementary)		22.2
2894.	140095-89-2	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-4A3 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′-and 3′-flanking region fragment)		22.2
2895.	146150-26-7	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-4A3 protein formation initiation factor eIF 4A messenger RNA complementary)		22.2
2896.	140360-04-9	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-5A2 protein formation initiation factor eIF 5A isoform messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2897.	143514-64-1	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-5A2 protein formation initiation factor eIF 5A isoform messenger RNA complementary)		22.2

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2898.	141374-52-9	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone pSOD3 copper–zinc superoxide dismutase messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2899.	143348-77-0	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone pSOD3 copper–zinc superoxide dismutase messenger RNA complementary)		22.2
2900.	144997-81-9	0	1	0	Deoxyribonucleic acid (*Nicotiana sylvestris* clone yaDC12/yaDC17 gene psaDa protein D 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2901.	140110-39-0	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun clone NeIF-5A3 protein formation initiation factor eIF 5A isoform gene plus 5′- and 3′-flanking region fragment)		22.2
2902.	141093-82-5	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun clone pMOG404 osmotin messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2903.	141093-84-7	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun clone pMOG4041-226-osmotin-specifying plus 5′- and 3′-flanking region fragment)		22.2
2904.	142978-99-2	0	1	0	Deoxyribonucleic acid (tobacco chloroplast clone L27-1 ribosome protein L 27 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2905.	145093-14-7	0	1	0	Deoxyribonucleic acid (tobacco clone EPSPS-1 5-enolpyruvoylshikimate 3-phosphate synthase messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2906.	139837-73-3	0	1	0	Deoxyribonucleic acid (tobacco clone NtDAHPS-1 phospho-2-keto-3-deoxyheptonate aldolase messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2907.	128512-17-4	0	1	0	Deoxyribonucleic acid (tobacco clone pBSGlu39.1 endo-1,3-β-glucanase isoenzyme gene coding region plus 5′- and 3′-flanking region fragment)		22.2
2908.	128512-18-5	0	1	0	Deoxyribonucleic acid (tobacco clone pBSGlu39.3 endo-1,3-β-glucanase isoenzyme gene coding region plus 5′- and 3′-flanking region fragment)		22.2
2909.	145735-56-4	0	1	0	Deoxyribonucleic acid (tobacco clone pcGS2-17 glutamine synthetase isoenzyme 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2910.	128512-22-1	0	1	0	Deoxyribonucleic acid (tobacco clone pGL31 endo-1,3-β- glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2911.	128512-23-2	0	1	0	Deoxyribonucleic acid (tobacco clone pGL36 endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2912.	128512-24-3	0	1	0	Deoxyribonucleic acid (tobacco clone pGL43 endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2913.	143341-58-6	0	1	0	Deoxyribonucleic acid (tobacco clone pMG15 extensin-like protein messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2914.	128512-26-5	0	1	0	Deoxyribonucleic acid (tobacco endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)		22.2
2915.	143341-53-1	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 171-amino acid C-terminal fragment-specifying plus 3′-flanking region fragment)		22.2
2916.	143341-54-2	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 264-amino acid C-terminal fragment-specifying plus 3′-flanking region fragment)		22.2
2917.	143341-57-5	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 393-amino acid C-terminal fragment-specifying plus 3′-flanking region fragment)		22.2
2918.	139637-37-9	0	1	0	Deoxyribonucleic acid, d(A-T-G-T-T-C-T-C-T-C-T-T-T-T-A-A-T-G-G-T-G-G-T-T-C-T-T-T-A-G)		22.2
2919.	152789-83-8	0	1	0	Deoxyribonucleic acid, d(C-A-T-C-A-C-G-T-G-A-G-A-T-A-A-G-A-G-C-C-G-C-C-A), double-stranded complementary		22.2
2920.	152789-84-9	0	1	0	Deoxyribonucleic acid, d(T-A-A-A-G-T-C-A-A-A-G-A-A-T-T-T-C-A-A-T-G-T-C-A-C-A), double-stranded complementary		22.2
2921.	67880-95-9	0	1	0	Desaturase, fatty acid ω3-		22.2
2922.	159965-67-0	0	1	0	Desaturase, fatty acid ω3- (tobacco clone Ntfad3)		22.2
2923.	107544-21-8	0	1	0	Desaturase, phytoene		22.2
2924.	9004-53-9	0	1	0	Dextrin		0.4, 2.5, 8.3, 24.3, 25.29
2925.		0	1	0	*Dialister*		22.2

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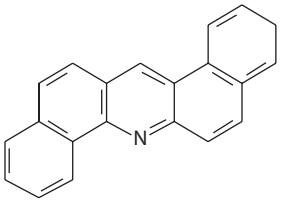
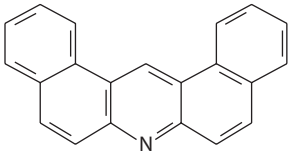
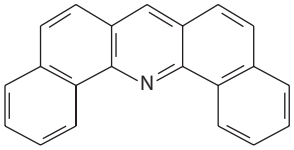
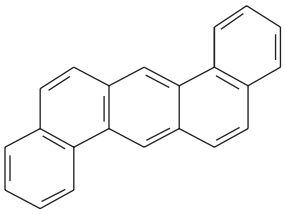
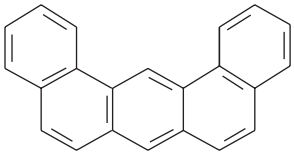
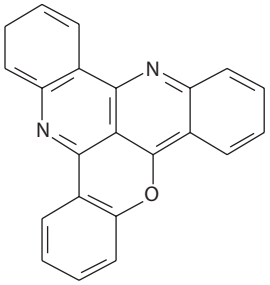
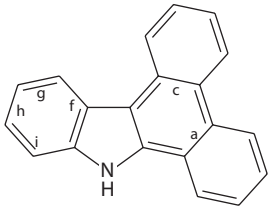
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2926.	37340-89-9	0	1	0	Diaphorase		22.2
2927.	5385-75-1	1	0	0	Dibenz[*a,e*]aceanthrylene {dibenzo[*a,e*]fluoranthene}		1.20
2928.	189-75-3	1	0	0	Dibenz[*j,mno*]aceanthrylene		1.20
2929.	71630-69-8	1	0	0	Dibenz[*j,mno*]aceanthrylene, methyl-		1.20
2930.	226-36-8	1	0	0	Dibenz[*a,h*]acridine		17.21, 23.5
2931.	226-92-6	1	0	0	Dibenz[*a,i*]acridine		17.21
2932.	224-42-0	1	0	0	Dibenz[*a,j*]acridine		17.21, 23.5
2933.	224-53-3	1	0	0	Dibenz[*c,h*]acridine		17.21
2934.	67775-07-9	1	0	0	Dibenzanthracene		1.20
2935.	53-70-3	1	1	1	Dibenz[*a,h*]anthracene {DB[*a,h*]A}		1.20, 23.5
2936.	224-41-9	1	0	0	Dibenz[*a,j*]anthracene		1.20
2937.	4607-33-4	1	0	0	Dibenzo[*b,h*][1]benzopyrano[2,3,4-*de*][1,6]naphthyridine		17.23
2938.	34442-52-9	1	0	0	1*H*-Dibenzo[*a,c*]carbazole		17.21

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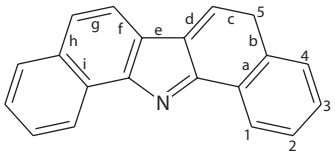
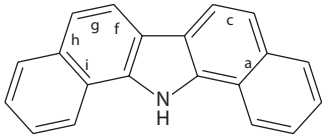
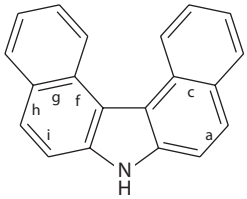
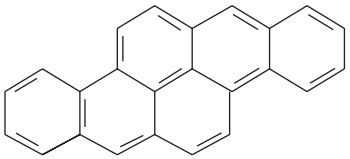
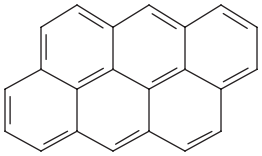
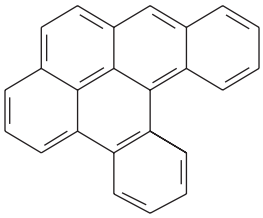
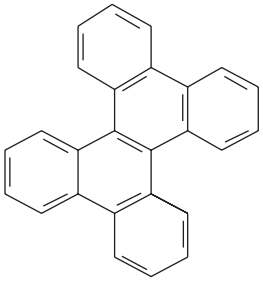
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2939.	207-84-1	0	1	0	7*H*-Dibenzo[*a,g*]carbazole		17.21
2940.	239-63-4	1	0	0	5*H*-Dibenzo[*a,i*]carbazole		17.21
2941.	239-64-5	1	0	0	13*H*-Dibenzo[*a,i*]carbazole		17.21
2942.	194-59-2	1	0	0	7*H*-Dibenzo[*c,g*]carbazole		17.21, 23.5
2943.	28641-62-5	1	0	0	5*H*-Dibenzo[*c,g*]carbazole		17.21
2944.	189-64-0	1	0	0	Dibenzo[*b,def*]chrysene {dibenzo[*a,h*]pyrene}		1.20, 23.5
2945.	191-26-4	1	0	0	Dibenzo[*def,mno*]chrysene {anthanthrene}		1.20
2946.	64760-24-3	1	0	0	Dibenzo[*def,mno*]chrysene, dimethyl- {at least two isomers in MSS}		1.20
2947.	41699-10-9	1	0	0	Dibenzo[*def,mno*]chrysene, methyl- {at least two, possibly three, isomers in MSS}		1.20
2948.	31927-64-7	1	0	0	Dibenzo[*def,mno*]chrysene, 6-methyl-		1.20
2949.	191-30-0	1	0	0	Dibenzo[*def,p*]chrysene {dibenzo[*a,l*]pyrene}		1.20, 23.5
2950.	191-68-4	1	0	0	Dibenzo[*g,p*]chrysene		1.20

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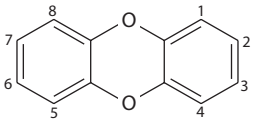
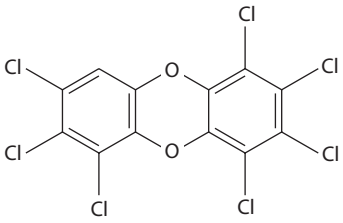
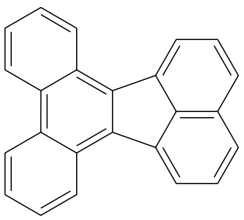
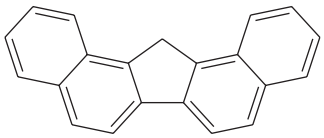
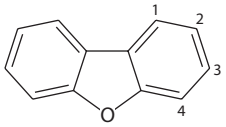
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2951.	1210-35-1	1	0	0	5*H*-Dibenzo[*a,d*]cyclohepten-5-one, 10,11-dihydro-		3.13
2952.	262-12-4	1	0	0	Dibenzo[*b,e*][1,4]dioxin		10.2
2953.		1	0	0	Dibenzo[*b,e*][1,4]dioxin, polychloro-		10.2, 18.4, 26.9
2954.	35822-46-9	1	1	1	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,8-heptachloro-		10.2, 18.4
2955.	58200-70-7	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,9-heptachloro-		10.2, 18.4
2956.	39227-28-6	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,7,8-hexachloro-		10.2, 18.4
2957.	57653-85-7	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,6,7,8-hexachloro-		10.2, 18.4
2958.	19408-74-3	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8,9-hexachloro-		10.2, 18.4
2959.	40321-76-4	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8-pentachloro-		10.2, 18.4
2960.	1746-01-6	1	1	1	Dibenzo[*b,e*][1,4]dioxin, 2,3,7,8-tetrachloro-		10.2, 18.4
2961.	37871-00-4	1	0	0	Dibenzo[*b,e*][1,4]dioxin, heptachloro-		10.2, 18.4
2962.	34465-46-8	1	0	0	Dibenzo[*b,e*][1,4]dioxin, hexachloro-		10.2, 18.4
2963.	3268-87-9	1	0	0	Dibenzo[*b,e*][1,4]dioxin, octachloro-		10.2, 18.4
2964.	36088-22-9	1	0	0	Dibenzo[*b,e*][1,4]dioxin, pentachloro-		10.2, 18.4
2965.	41903-57-5	1	0	0	Dibenzo[*b,e*][1,4]dioxin, tetrachloro-		10.2, 18.4
2966.	60382-88-9	1	0	0	Dibenzofluoranthene {at least two isomers in MSS}		1.20
2967.	203-18-9	1	0	0	Dibenzo[*j,l*]fluoranthene		1.20
2968.	239-60-1	1	0	0	13*H*-Dibenzo[*a,i*]fluorene		1.20
2969.	132-64-9	1	1	1	Dibenzofuran {2,2′-biphenylene oxide}		10.2
2970.	29062-95-1	1	0	0	Dibenzofuran, dimethyl-		10.2
2971.	38998-75-3	1	0	0	Dibenzofuran, heptachloro-		10.2, 18.4
2972.	55684-94-1	1	0	0	Dibenzofuran, hexachloro-		10.2, 18.4
2973.	60826-62-2	1	0	0	Dibenzofuran, methyl-		10.2

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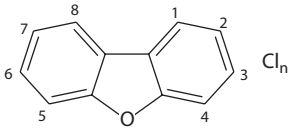
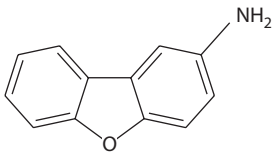
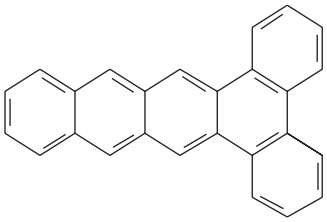
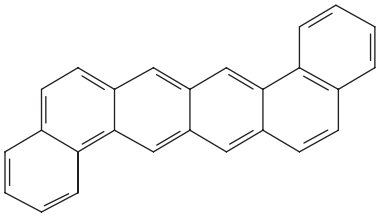
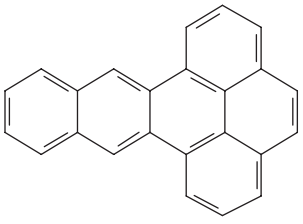
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2974.	39001-02-0	1	0	0	Dibenzofuran, octachloro-		10.2, 18.4
2975.	30402-15-4	1	0	0	Dibenzofuran, pentachloro-		10.2, 18.4
2976.	30402-14-3	1	0	0	Dibenzofuran, tetrachloro-		10.2, 18.4
2977.		1	0	0	Dibenzofuran, polychloro-		10.2, 18.4
2978.	67562-39-4	1	1	1	Dibenzofuran, 1,2,3,4,6,7,8-heptachloro-		10.2, 18.4
2979.	55673-89-7	1	0	0	Dibenzofuran, 1,2,3,4,7,8,9-heptachloro-		10.2, 18.4
2980.	70648-26-9	1	0	0	Dibenzofuran, 1,2,3,4,7,8-hexachloro-		10.2, 18.4
2981.	91538-84-0	1	0	0	Dibenzofuran, 1,2,3,4,7,9-hexachloro-		10.2, 18.4
2982.	67517-48-0	1	0	0	Dibenzofuran, 1,2,3,4,8-pentachloro-		10.2, 18.4
2983.	57117-44-9	1	0	0	Dibenzofuran, 1,2,3,6,7,8-hexachloro-		10.2, 18.4
2984.	72918-21-9	1	0	0	Dibenzofuran, 1,2,3,7,8,9-hexachloro-		10.2, 18.4
2985.	57117-41-6	1	0	0	Dibenzofuran, 1,2,3,7,8-pentachloro-		10.2, 18.4
2986.	60851-34-5	1	0	0	Dibenzofuran, 2,3,4,6,7,8-hexachloro-		10.2, 18.4
2987.	57117-31-4	1	0	0	Dibenzofuran, 2,3,4,7,8-pentachloro-		10.2, 18.4
2988.	83704-32-9	1	0	0	Dibenzofuran, 2,3,4,8-tetrachloro-		10.2, 18.4
2989.	51207-31-9	1	0	0	Dibenzofuran, 2,3,7,8-tetrachloro-		10.2, 18.4
2990.	7320-50-5	1	0	0	Dibenzofuran, 1-methyl-		10.2
2991.	7320-51-6	1	0	0	Dibenzofuran, 2-methyl-		10.2
2992.	7320-52-7	1	0	0	Dibenzofuran, 3-methyl-		10.2
2993.	7320-53-8	1	0	0	Dibenzofuran, 4-methyl-		10.2
2994.	3693-22-9	1	0	0	2-Dibenzofuranamine		10.2, 12.2
2995.	4106-66-5	1	0	0	3-Dibenzofuranamine		10.2, 12.2
2996.	216-00-2	1	0	0	Dibenzo[*a,c*]naphthacene		1.20
2997.	227-04-3	1	0	0	Dibenzo[*a,j*]naphthacene		1.20
2998.	193-09-9	1	0	0	Dibenzo[*de,qr*]naphthacene {naphtho[2,3-*d*]pyrene}		1.20

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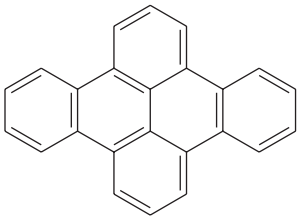
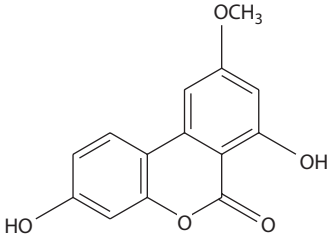
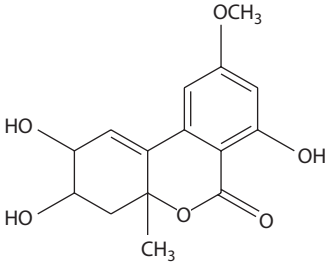
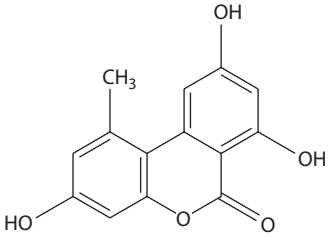
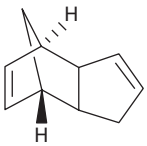
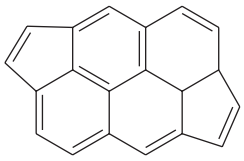
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
2999.	192-51-8	1	0	0	Dibenzo[*fg,op*]naphthacene {dibenzo[*e,l*]pyrene}		1.20
3000.	26894-49-5	0	1	0	6*H*-Dibenzo[*b,d*]pyran-6-one,3,7(3,9or7,9)-dihydroxy-9(7 or 3)-methoxy-1-methyl-		6.3, 9.22, 10.2
3001.	29752-43-0	0	1	0	6*H*-Dibenzo[*b,d*]pyran-6-one, 9-methoxy-4a-methyl-2,3,4,4a-tetrahydro-2,3, 7-trihydroxy- (2α,3β,4aβ)-		6.3, 9.22, 10.2
3002.	641-38-3	0	1	0	6*H*-Dibenzo[*b,d*]pyran-6-one, 1-methyl-3,7,9-trihydroxy-		6.3, 9.22
3003.	58615-36-4	1	0	0	Dibenzopyrene		1.20
3004.	132-65-0	1	1	1	Dibenzothiophene		18.1
3005.	70021-47-5	0	1	0	Dibenzothiophene, dimethyl- {at least four isomers detected}		18.1
3006.	30995-64-3	1	1	1	Dibenzothiophene, methyl- {at least four isomers detected}		18.1
3007.	77-73-6	1	0	0	Dicyclopentadiene		1.12
3008.	98791-43-6	1	0	0	Dicyclopenta[*cd,jk*]pyrene		1.20
3009.	98791-44-7	1	0	0	Dicyclopenta[*cd,jk*]pyrene, 1,2-dihydro-		1.20

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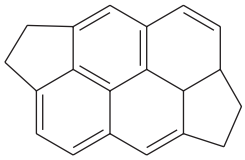
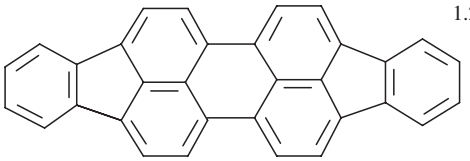
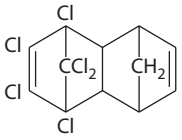
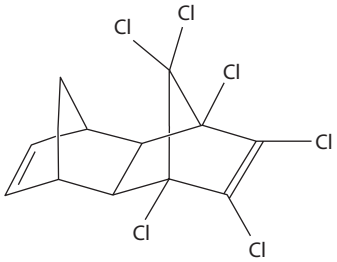
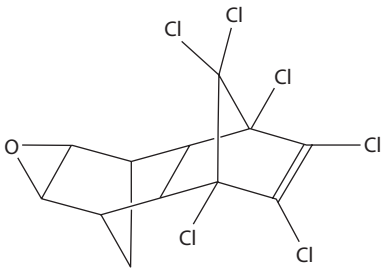
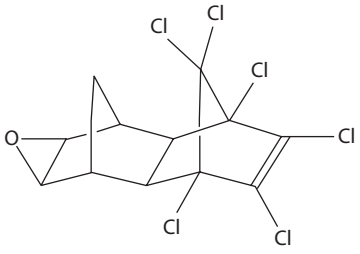
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3010.	98791-45-8	1	0	0	Dicyclopenta[*cd,jk*]pyrene, 1,2,3,4-tetrahydro-		1.20
3011.	5894-59-7	0	1	0	Digalacturonic acid		2.5, 4.3, 10.2
3012.	188-94-3	1	0	0	Diindeno[1,2,3-*cd*:1′,2′,3′-*lm*]perylene		1.20
3013.	309-00-2	1	1	1	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5α,8α,8aβ)- [endo, endo] {Aldrin®}		18.4, 21.3
3014.	465-73-6	0	1	0	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10, 10-hexachloro- 1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5β,8β,8aβ)- [endo, exo] {Isodrin®}		18.4, 21.3
3015.	60-57-1	1	1	1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro- 1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aα,3β,6β,6aα,7β,7aα)- {Dieldrin®}		10.2, 18.4, 21.3
3016.	72-20-8	1	1	1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6, 6a,7,7a-octahydro-, (1aα,2β,2aβ,3α,6α,6aβ,7β,7aα)- {Endrin®}		10.2, 18.4, 21.3
3017.	119973-29-4	1	0	0	26,27-Dinorergosta-3,5-diene		1.12, 2.7
3018.	119973-31-8	1	0	0	26,27-Dinorergosta-3,5,22-triene, (22E)-		1.12, 2.7
3019.	119973-30-7	1	0	0	26,27-Dinorergost-3-ene, (5α)-		1.12, 2.7
3020.	117210-53-4	0	1	0	2,7-Dioxabicyclo[2.2.1]heptane, 1,3-dimethyl-3-(4-methyl-3-pentenyl)-, endo-		10.2
3021.	117305-90-5	0	1	0	2,7-Dioxabicyclo[2.2.1]heptane, 1,3-dimethyl-3-(4-methyl-3-pentenyl)-, exo-		10.2

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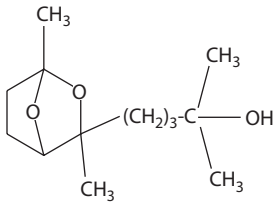
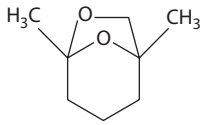
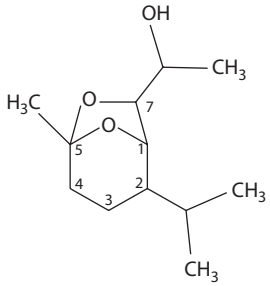
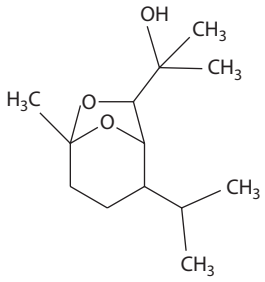
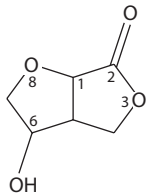
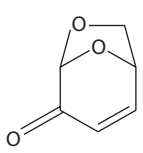
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3022.	117210-54-5	0	1	0	2,7-Dioxabicyclo[2.2.1]heptane-3-butanol, α,α,1,3-tetramethyl-		2.5, 10.2
3023.	121927-15-9	0	1	0	13,14-Dioxabicyclo[10.2.2]hexadec-6-ene-2,3,5-triol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2S*,3R*,5S*,		2.5, 10.2
3024.	52886-15-4	0	1	0	2,9-Dioxabicyclo[3.3.1]nonan-4-ol, 1,3,3-trimethyl-6-(1-methylethyl)- {two isomers reported}		2.5, 10.2
3025.	28401-39-0	0	1	0	6,8-Dioxabicyclo[3.2.1]octane, 1,5-dimethyl- {frontalin}		10.2
3026.	58001-00-6	0	1	0	6,8-Dioxabicyclo[3.2.1] octane-7-methanol, 2-(1-methylethyl)-α,5-dimethyl- [1α,2β,5α,7α(R*)]		2.5, 10.2
3027.	58001-10-8	0	1	0	6,8-Dioxabicyclo[3.2.1] octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-, (2-endo,7-exo)-(±)-		2.5, 10.2
3028.	52992-36-6	0	1	0	6,8-Dioxabicyclo[3.2.1] octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-		2.5, 10.2
3029.	110053-63-9	1	0	0	3,8-Dioxabicyclo[3.3.0]octan-2-one, 6-hydroxy-		2.5, 6.3, 10.2
3030.	37112-31-5	1	1	1	6,8-Dioxabicyclo[3.2.1]oct-2-en-4-one,(1S)- {levoglucosenone}		3.13, 10.2

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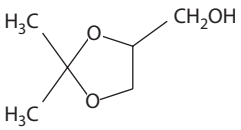
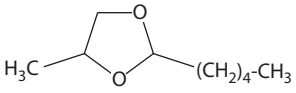
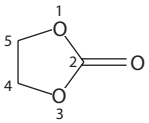
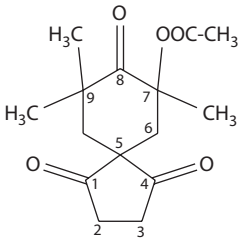
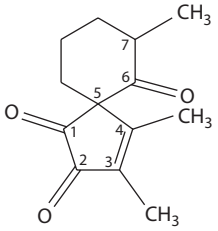
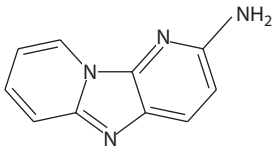
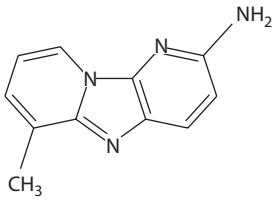
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3031.		1	0	0	1,3-Dioxalane, 4-methyl-		10.2
3032.		1	0	0	1,3-Dioxalane, 4-methyl- {isomer}		10.2
3033.	5464-28-8	1	0	0	1,3-Dioxalane-4-methanol		2.5, 10.2
3034.	100-79-8	1	0	0	1,3-Dioxalane-4-methanol, 2,2-dimethyl-		2.5, 10.2
3035.	26563-74-6	1	0	0	1,3-Dioxolane, 4-methyl-2-pentyl-, (*Z*)-		10.2
3036.	96-49-1	1	0	0	1,3-Dioxalan-2-one {ethylene glycol carbonate}		5.3
3037.	931-40-8	1	0	0	1,3-Dioxalan-2-one, 4-(hydroxymethyl)- {glycerol carbonate}		2.5, 5.3
3038.	108-32-7 9005-37-2	1	1	1	1,3-Dioxalan-2-one, 4-methyl- {1,2-propylene glycol carbonate}		5.3
3039.	505-22-6	1	0	0	1,3-Dioxane		10.2
3040.	86687-05-0	1	0	0	1,3-Dioxane, 5-hydroxy-		10.2
3041.	123-91-1	1	0	0	1,4-Dioxane		10.2
3042.	16279-34-8	1	0	0	1,4-Dioxane, 2-methyl-		10.2
3043.	162188-91-2	1	0	0	1,4-Dioxaspiro[4.5]decan-8-one, 7-(acetyloxy)-7,9,9-trimethyl-, (±)-		3.13, 5.3
3044.	41059-94-3 51607-05-7	0	1	0	1,6-Dioxaspiro[4.5]dec-3-en-2-one, 3,4,7-trimethyl-		3.13
3045.	9025-33-6	0	1	0	Dipeptidase, prolyl		22.2
3046.	67730-10-3	1	0	0	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine {Glu-P-2}		12.2, 17.29, 23.5
3047.	67730-11-4	1	0	0	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 6-methyl- {Glu-P-1}		12.2, 17.29, 23.5

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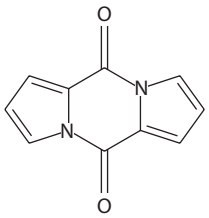
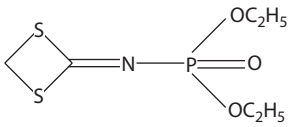
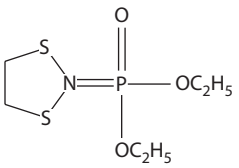
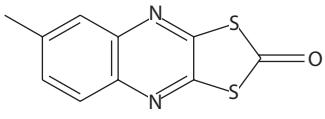
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3048.	484-73-1	1	1	1	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione {pyrocoll}		17.23
3049.	59017-02-6	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, 1,2,3,5a,8,10a-hexahydro-, (5aS-*cis*)-		17.23
3050.		1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione, 1,2,3,5a,8,10a-hexahydro-3-methyl-		17.23
3051.	71277-95-7	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione, methyl-		17.23
3052.	6708-06-1 36588-48-4	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*] pyrazine-5,10-dione, octahydro-		17.23
3053.	9054-89-1	0	1	0	Dismutase, superoxide		22.2
3054.	143352-40-3	0	1	0	Dismutase, superoxide (*Nicotiana plumbaginifolia* clone pSOD3 copper–zinc protein moiety reduced)		22.2
3055.	5905-46-4	1	0	0	Disulfide, 1-propenyl propyl		18.1
3056.	110-81-6	1	0	0	Disulfide, diethyl	$H_3C\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_3$	18.1
3057.	624-92-0	1	1	1	Disulfide, dimethyl	$H_3C\text{-}S\text{-}S\text{-}CH_3$	18.1
3058.	20333-39-5	1	0	0	Disulfide, ethyl methyl		18.1
3059.	5905-47-5	1	0	0	Disulfide, methyl 1-propenyl		18.1
3060.	2179-58-0	1	0	0	Disulfide, methyl 2-propen-1-yl		18.1
3061.	2179-59-1	1	0	0	Disulfide, propyl 2-propen-1-yl		18.1
3062.	2179-60-4	1	0	0	Disulfide, methyl propyl		18.1
3063.	21548-32-3	0	1	0	1,3-Dithietan-2-ylidenephosphoramidic acid, diethyl ester {Fosthietan®}		5.3, 18.1, 21.3
3064.	947-02-4	0	1	0	Dithiolan-2-ylidenephosphoramidic acid, diethyl ester {Cyolane®, Phosfolan®}		5.3, 18.1, 21.3
3065.	2439-01-2	0	1	0	1,3-Dithiolo[4,5-*b*]quinoxalin-2-one, 6-methyl- {Quinomethionate®}		18.1, 21.3
3066.	29564-66-7	0	1	0	Docosadienoic acid, (*Z*,*Z*)-		4.3
3067.	629-97-0	1	1	1	Docosane	$H_3C\text{-}(CH_2)_{20}\text{-}CH_3$	1.10, 25.29
3068.	1560-81-2	1	1	1	Docosane, 2-methyl-	$(H_3C)\text{=}CH\text{-}(CH_2)_{19}\text{-}CH_3$	1.10
3069.	72227-00-0	1	1	1	Docosane, 3-methyl-	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{18}\text{-}CH_3$	1.10
3070.	112-85-6	1	1	1	Docosanoic acid {behenic acid}	$H_3C\text{-}(CH_2)_{20}\text{-}COOH$	4.3
3071.	17671-27-1	1	1	1	Docosanoic acid, docosyl ester	$H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	5.3
3072.	42233-07-8	1	1	1	Docosanoic acid, dodecyl ester	$H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	5.3
3073.	42233-14-7	1	1	1	Docosanoic acid, eicosyl ester	$H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	5.3
3074.	5908-87-2	1	0	0	Docosanoic acid, ethyl ester	$H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}CH_2\text{-}CH_3$	5.3
3075.	42233-15-8	1	1	1	Docosanoic acid, heneicosyl ester	$H_3C\text{-}(CH_2)_{20}\text{-}COO\text{-}(CH_2)_{20}\text{-}CH_3$	5.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
3076.	121877-99-4	1	1	1	Docosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{26}$-CH_3	5.3
3077.	42233-12-5	1	1	1	Docosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{16}$-CH_3	5.3
3078.	55136-77-1	1	1	1	Docosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{25}$-CH_3	5.3
3079.	42233-11-4	1	1	1	Docosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{15}$-CH_3	5.3
3080.	42233-13-6	1	1	1	Docosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{18}$-CH_3	5.3
3081.	21511-31-9	1	1	1	Docosanoic acid, octacosyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{27}$-CH_3	5.3
3082.	24271-12-3	1	1	1	Docosanoic acid, octadecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{17}$-CH_3	5.3
3083.		1	1	1	Docosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{24}$-CH_3	5.3
3084.	42233-10-3	1	1	1	Docosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{14}$-CH_3	5.3
3085.	42233-17-0	1	1	1	Docosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{23}$-CH_3	5.3
3086.	42233-09-0	1	1	1	Docosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{13}$-CH_3	5.3
3087.	127353-53-1	1	0	0	Docosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl docosanoate}		5.3
3088.	42233-16-9	1	1	1	Docosanoic acid, tricosyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{32}$-CH_3	5.3
3089.	42233-08-9	1	1	1	Docosanoic acid, tridecyl ester	H_3C-$(CH_2)_{20}$-COO-$(CH_2)_{12}$-CH_3	5.3
3090.	36332-95-3	0	1	0	Docosanoic acid, 20-methyl-	H_3C-CH_2 $CH(CH_3)$-$(CH_2)_{18}$-COOH	4.3
3091.	121877-76-7	1	1	1	Docosanoic acid, 20-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{18}$-COO-$(CH_2)_{21}$-CH_3	5.3
3092.	121877-62-1	1	1	1	Docosanoic acid, 20-methyl-, eicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{18}$-COO-$(CH_2)_{19}$-CH_3	5.3
3093.	121877-71-2	1	1	1	Docosanoic acid, 20-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{18}$-COO-$(CH_2)_{20}$-CH_3	5.3
3094.	59708-74-6	0	1	0	Docosanoic acid, 21-methyl-	$(H_3C)_2$=CH-$(CH_2)_{19}$-COOH	4.3
3095.	30303-65-2	0	1	0	Docosanol		2.5
3096.	661-19-8	1	1	1	1-Docosanol {behenyl alcohol}	H_3C-$(CH_2)_{20}$-CH_2OH	2.5
3097.		0	1	0	1-Docosanol, 20-methyl-		2.5
3098.		0	1	0	1-Docosanol, 21-methyl-		2.5
3099.	29730-67-4	1	0	0	Docosene		1.11
3100.	1599-67-3	1	0	0	1-Docosene	H_3C-$(CH_2)_{19}$-CH=CH_2	1.11
3101.		1	0	0	1-Docosene, 2-methyl-	H_2C=$C(CH_3)$-$(CH_2)_{19}$-CH_3	1.11
3102.		1	0	0	2-Docosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{18}$-CH_3	1.11
3103.		1	0	0	2-Docosene, (*E*)-		1.11
3104.		1	0	0	2-Docosene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{18}$-CH_3	1.11
3105.		1	0	0	2-Docosene, 20-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{16}$-$CH(CH_3)$-CH_2-CH_3	1.11
3106.		1	0	0	2-Docosene, 20-methyl-, (*E*)-		1.11
3107.		1	0	0	2-Docosene, 21-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{17}$-$CH(CH_3)_2$	1.11
3108.		1	0	0	2-Docosene, 21-methyl-, (*E*)-		1.11
3109.	112-86-7	0	1	0	13-Docosenoic acid, (*Z*)-		4.3
3110.	65596-29-4	0	1	0	3,6-Dodecadienedioic acid, 10-hydroxy-4,9-dimethyl-		2.5, 4.3
3111.	40596-69-8	1	1	1	2,4-Dodecadienoic acid, 11-methoxy-3,7,11-trimethyl-, 1-methylethyl ester, (*E,E*)- {Methoprene®, Altosid®}		5.3, 21.3, 24.3
3112.		0	1	0	2,4-Dodecadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-		3.13, 4.3
3113.	7226-86-0	1	0	0	2,6-Dodecadien-1-ol, 3,7,11-trimethyl-		2.5
3114.	117232-64-1	0	1	0	5,10-Dodecadien-2-one, 9-hydroxy-6,11-dimethyl-		2.5, 3.13
3115.	112-54-9	0	1	0	Dodecanal	H_3C-$(CH_2)_{10}$-CH=O	3.12
3116.	14995-49-4	1	0	0	Dodecanamide, *N*-(1-methylethyl)-		13.1
3117.	112-18-5	1	0	0	Dodecanamine, *N,N*-dimethyl-		12.2

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
3118.	112-40-3	1	1	1	Dodecane	H_3C-$(CH_2)_{10}$-CH_3	1.10
3119.	1560-97-0	1	0	0	Dodecane, 2-methyl-	H_3C-$(CH_2)_9$-$CH{=}(CH_3)_2$	1.10
3120.	17312-57-1	1	1	1	Dodecane, 3-methyl-	H_3C-$(CH_2)_8$-$CH(CH_3)$-CH_2-CH_3	1.10
3121.	3891-98-3	1	1	1	Dodecane, 2,6,10-trimethyl- (farnesane)		1.10
3122.	693-23-2	1	0	0	Dodecanedioic acid	HOOC-$(CH_2)_{10}$-COOH	4.3
3123.	143-07-7	1	1	1	Dodecanoic acid {lauric acid}	H_3C-$(CH_2)_{10}$-COOH	0.4, 4.3, 21.3, 24.3, 25.29
3124.	71278-23-4	1	1	1	Dodecanoicacid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl dodecanoate}		5.3
3125.	71278-24-5	1	0	0	Dodecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester		5.3
3126.	36617-18-2	1	1	1	Dodecanoic acid, eicosyl ester	H_3C-$(CH_2)_{10}$-COO-$(CH_2)_{19}$-CH_3	5.3
3127.	106-33-2	0	1	0	Dodecanoic acid, ethyl ester {ethyl laurate}	H_3C-$(CH_2)_{10}$-COO-C_2H_5	5.3, 24.3, 25.29
3128.	111-82-0	1	1	1	Dodecanoic acid, methyl ester	H_3C-$(CH_2)_{10}$-COO-CH_3	5.3
3129.	7416-57-1	0	1	0	Dodecanoic acid, 10-methyl-	H_3C-CH_2 $CH(CH_3)$-$(CH_2)_8$-COOH	4.3
3130.	121877-15-4	1	1	1	Dodecanoic acid, 10-methyl-, eicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_8$-COO-$(CH_2)_{19}$-CH_3	5.3
3131.	121877-10-9	1	1	1	Dodecanoic acid, 11-methyl-, eicosyl ester	$(H_3C)_2{=}CH$-$(CH_2)_9$-COO-$(CH_2)_{19}$-CH_3	5.3
3132.	27342-88-7	1	0	0	Dodecanol		2.5
3133.	112-53-8	1	1	1	1-Dodecanol {lauryl alcohol}	H_3C-$(CH_2)_{10}$-CH_2OH	2.5, 21.3, 25.29
3134.	6750-34-1	0	1	0	1-Dodecanol, 3,7,11-trimethyl- {hexahydrofarnesol}		2.5
3135.	6175-49-1	0	1	0	2-Dodecanone	H_3C-$(CH_2)_9$-CO-CH_3	3.13
3136.	502-61-4	1	0	0	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (*E,E*)- {α-farnesene}		1.11
3137.		1	0	0	2,6,9,11-Dodecatetraen-1-ol, 2,6,10-trimethyl-, (2*E*,6*E*,9*E*)- {α-sinensol}		2.5
3138.		1	0	0	2,6,10,?-Dodecatetraenol {dehydrofarnesol}		2.5
3139.	18794-84-8	1	0	0	1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (*E*)- {β-farnesene}		1.11
3140.	3899-18-1	1	0	0	2,6,10-Dodecatriene, 2,6,10-trimethyl-, (*E,E*)-		1.11
3141.		1	0	0	2,6,10-Dodecatriene, 3,7,11-trimethyl- = 2,6,10-dodecatriene, 2,6,10-trimethyl-		1.11
3142.	7548-13-2	0	1	0	2,6,10-Dodecatrienoic acid, 3,7,11-trimethyl-		4.3
3143.	7212-44-4	1	1	1	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- {nerolidol}		2.5, 24.3, 25.29
3144.	142-50-7	0	1	0	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, [S-(*Z*)]-		2.5
3145.		1	1	1	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate, (*Z*)- {*cis*-nerolidol acetate}		5.3
3146.		1	1	1	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate, (*E*)- {*trans*-nerolidol acetate}		5.3
3147.	4602-84-0 3790-71-4	1	1	1	2,6,10-Dodecatrien-1-ol,3,7,11-trimethyl- {sinensol, farnesol}		2.5, 21.3, 24.3, 25.29

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3148.	106-28-5	1	0	0	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (*E*)- {farnesol isomer}		2.5
3149.	29548-30-9	1	1	1	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, acetate {farnesyl acetate}		5.3
3150.		0	1	0	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, formate {farnesyl formate}		5.3
3151.	25378-22-7	1	0	0	Dodecene		1.11
3152.	112-41-4	1	0	0	1-Dodecene	$H_2C{=}CH\text{-}(CH_2)_9\text{-}CH_3$	1.11
3153.	16435-49-7	1	0	0	1-Dodecene, 2-methyl-	$H_2C{=}C(CH_3)\text{-}(CH_2)_9\text{-}CH_3$	1.11
3154.		1	0	0	2-Dodecene, 2-methyl-	$H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_8\text{-}CH_3$	1.11
3155.		1	0	0	2-Dodecene, 10-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_6\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1.11
3156.		1	0	0	2-Dodecene, 10-methyl-, (*E*)-		1.11
3157.		1	0	0	2-Dodecene, 11-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}CH(CH_3)_2$	1.11
3158.		1	0	0	2-Dodecene, 11-methyl-, (*E*)-		1.11
3159.	1289-45-8	1	0	0	Dodecenoic acid		4.3
3160.	4412-16-2	0	1	0	2-Dodecenoic acid		4.3
3161.	544-85-4	1	1	1	Dotriacontane	$H_3C\text{-}(CH_2)_{30}\text{-}CH_3$	1.10, 25.29
3162.	1720-11-2	1	1	1	Dotriacontane, 2-methyl-	$H_3C\text{-}(CH_2)_{29}\text{-}CH{=}(CH_3)_2$	1.10
3163.	20129-49-1	1	1	1	Dotriacontane, 3-methyl-	$H_3C\text{-}(CH_2)_{28}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1.10
3164.	16753-27-8	1	1	1	Dotriacontane-16,17-$^{14}C_2$, labeled with ^{14}C		1.10
3165.	3625-52-3	1	0	0	Dotriacontanoic acid	$H_3C\text{-}(CH_2)_{30}\text{-}COOH$	4.3
3166.	121878-06-6	1	1	1	Dotriacontanoic acid, eicosyl ester	$H_3C\text{-}(CH_2)_{30}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	5.3
3167.	110053-56-0	1	0	0	2,6,10,14,18,22,26,30-Dotriacontaoctaene, 3,7,11,15,19,23,27-heptamethyl-		1.11
3168.	66309-89-5	1	0	0	2,6,10,14,18,22,26,30-Dotriacontaoctaene, 2,6,10,14,18,22,26,30-octamethyl-, (all-*E*)-		1.11
3169.	85792-05-8	1	0	0	Dotriacontene		1.11
3170.	18435-55-7	1	0	0	1-Dotriacontene	$H_2C{=}CH\text{-}(CH_2)_{29}\text{-}CH_3$	1.11
3171.		1	0	0	2-Dotriacontene, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{28}\text{-}CH_3$	1.11
3172.		1	0	0	2-Dotriacontene, (*E*)-		1.11
3173.	7429-91-6	1	1	1	Dysprosium	Dy	20.5
3174.	9007-57-2	0	1	0	Edestin		18.1, 22.2
3175.	25448-01-5	0	1	0	Eicosadienoic acid		4.3
3176.	2400-66-0	0	1	0	Eicosanal	$H_3C\text{-}(CH_2)_{18}\text{-}CH{=}O$	3.12
3177.	112-95-8	1	1	1	Eicosane	$H_3C\text{-}(CH_2)_{18}\text{-}CH_3$	1.10
3178.		0	1	0	Eicosane, methyl-		1.10
3179.	1560-84-5 52845-08-6	1	0	0	Eicosane, 2-methyl- {isoheneicosane}	$H_3C\text{-}(CH_2)_{17}\text{-}CH{=}(CH_3)_2$	1.10
3180.	6418-46-8	0	1	0	Eicosane, 3-methyl-	$H_3C\text{-}(CH_2)_{16}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1.10
3181.	4616-73-3	1	0	0	Eicosanenitrile	$H_3C\text{-}(CH_2)_{18}\text{-}CN$	11.2
3182.	506-30-9	1	1	1	Eicosanoic acid {arachidic acid}	$H_3C\text{-}(CH_2)_{18}\text{-}COOH$	4.3
3183.	42232-87-1	1	1	1	Eicosanoic acid, docosyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	5.3
3184.	42232-82-6	1	1	1	Eicosanoic acid, dodecyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{11}\text{-}CH_3$	5.3
3185.	22432-80-0	1	1	1	Eicosanoic acid, eicosyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	5.3
3186.	42218-26-8	1	1	1	Eicosanoic acid, heneicosyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{20}\text{-}CH_3$	5.3
3187.	121877-87-0	1	1	1	Eicosanoic acid, heptacosyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{26}\text{-}CH_3$	5.3
3188.	36610-58-9	1	1	1	Eicosanoic acid, heptadecyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{16}\text{-}CH_3$	5.3
3189.	17318-45-5	1	1	1	Eicosanoic acid, hexacosyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{25}\text{-}CH_3$	5.3
3190.	22413-05-4	1	1	1	Eicosanoic acid, hexadecyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{15}\text{-}CH_3$	5.3
3191.	1120-28-1	1	0	0	Eicosanoic acid, methyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}CH_3$	5.3
3192.	36610-60-3	1	1	1	Eicosanoic acid, nonadecyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{18}\text{-}CH_3$	5.3
3193.	55309-61-0	1	1	1	Eicosanoic acid, octacosyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{27}\text{-}CH_3$	5.3
3194.	22432-79-7	1	1	1	Eicosanoic acid, octadecyl ester	$H_3C\text{-}(CH_2)_{18}\text{-}COO\text{-}(CH_2)_{17}\text{-}CH_3$	5.3

(*continued*)

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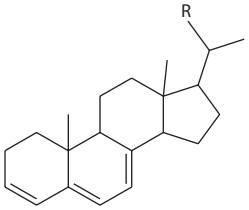
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3195.	121877-79-0	1	1	1	Eicosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{24}$-CH_3	5.3
3196.	36665-69-7	1	1	1	Eicosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{14}$-CH_3	5.3
3197.	42232-89-3	1	1	1	Eicosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{23}$-CH_3	5.3
3198.	22413-04-3	1	1	1	Eicosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{13}$-CH_3	5.3
3199.	71278-14-3	1	0	0	Eicosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester		5.3
3200.	42232-88-2	1	1	1	Eicosanoic acid, tricosyl ester	H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{32}$-CH_3	5.3
3201.	36610-55-6	1	1	1	Eicosanoic acid, tridecyl ester	H_3C-$(CH_2)_{18}$-COO-$(CH_2)_{12}$-CH_3	5.3
3202.	36332-93-1	1	1	1	Eicosanoic acid, 18-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{16}$-COOH	4.3
3203.	121877-60-9	1	1	1	Eicosanoic acid, 18-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{16}$-COO-$(CH_2)_{21}$-CH_3	5.3
3204.	59708-73-5	0	1	0	Eicosanoic acid, 19-methyl-	$(H_3C)_2$=CH-$(CH_2)_{17}$-COOH	4.3
3205.	28679-05-2	0	1	0	Eicosanol		2.5
3206.	629-96-9	1	1	1	1-Eicosanol {arachic alcohol}	H_3C-$(CH_2)_{18}$-CH_2OH	2.5
3207.		0	1	0	1-Eicosanol, 18-methyl-		2.5
3208.		0	1	0	1-Eicosanol, 19-methyl-		2.5
3209.	4340-76-5	1	0	0	2-Eicosanol		2.5
3210.	7431-92-7	1	0	0	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl-, (all-*E*)-	H-[CH_2-C(CH_3)=CH-CH_2]$_5$-H	1.11
3211.	75581-03-2	1	0	0	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl-		1.11
3212.		1	0	0	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl- {isomer}		1.11
3213.	506-32-1	1	1	1	5,8,11,14-Eicosatetraenoic acid, (all-*Z*)- {arachidonic acid}		4.3
3214.	55682-88-7	0	1	0	11,14,17-Eicosatrienoic acid, methyl ester		5.3
3215.	27400-78-8	1	0	0	Eicosene		1.11
3216.	3452-07-1	1	1	1	1-Eicosene	H_2C=CH-$(CH_2)_{17}$-CH_3	1.11
3217.		1	0	0	1-Eicosene, 2-methyl-	H_2C=C(CH_3)-$(CH_2)_{17}$-CH_3	1.11
3218.		1	0	0	2-Eicosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{16}$-CH_3	1.11
3219.	42448-85-2	1	0	0	2-Eicosene, (*E*)-		1.11
3220.		1	0	0	2-Eicosene, 2-methyl-	H_3C-C(CH_3)=CH-$(CH_2)_{16}$-CH_3	1.11
3221.		1	0	0	2-Eicosene, 18-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{14}$-$CH(CH_3)$-CH_2-CH_3	1.11
3222.		1	0	0	2-Eicosene, 18-methyl-, (*E*)-		1.11
3223.		1	0	0	2-Eicosene, 19-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{15}$-$CH(CH_3)_2$	1.11
3224.		1	0	0	2-Eicosene, 19-methyl-, (*E*)-		1.11
3225.	26764-41-0	1	1	1	Eicosenoic acid		4.3
3226.	22104-85-4	0	1	0	2-Eicosen-1-ol	H_3C-$(CH_2)_{16}$-CH=CH-CH_2OH	2.5
3227.		0	1	0	*Enterococcus gallinarum*		22.2
3228.	159844-36-7	0	1	0	Enzyme E 2 (*Arabidopsis thaliana* clone TAY029 gene UbcAt3 ubiquitin-carrier)		22.2
3229.	38419-69-1	0	1	0	6*H*-3,10b-Epoxy-1*H*-naphtho[2,1-*b*] pyran, decahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]-		10.2
3230.	7440-52-0	1	1	1	Erbium		20.5
3231.	474-60-2	0	1	0	Ergostan-3-ol,(3β,5α,24R)- {campestanol}		2.5, 2.7
3232.	77327-07-2	1	0	0	Ergosta-3,5,7-triene, (24ξ)-	 R=-$(CH_2)_2$-$CH(CH_3)$-$CH(CH_3)_2$	1.12, 2.7

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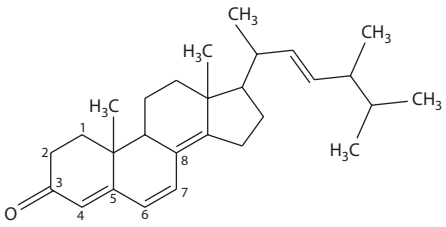
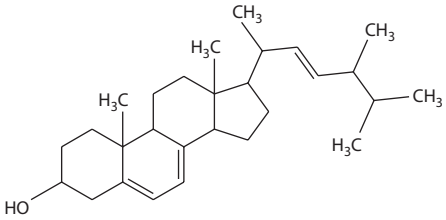
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3233.	19254-69-4	0	1	0	Ergosta-4,6,8(14),22-tetraen-3-one,(22*E*)-		2.7, 3.13
3234.	474-67-9	0	1	0	Ergosta-5,22-dien-3-ol, (3β,22*E*)-		2.5, 2.7
3235.	474-63-5	0	1	0	Ergosta-5,24(28)-dien-3-ol, (3β)-		2.5, 2.7
3236.	52936-69-3	0	1	0	Ergosta-5,25-dien-3-ol, (3β)-		2.5, 2.7
3237.	21490-25-5	0	1	0	Ergosta-7,24(28)-dien-3β-ol, 4β-methyl-		2.5, 2.7
3238.	474-68-0	0	1	0	Ergosta-7,24(28)-dien-3-ol, (3β,5α)-		2.5, 2.7
3239.	1176-52-9	0	1	0	Ergosta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α)-		2.5, 2.7
3240.	23839-47-6	0	1	0	Ergosta-8,14-dien-3-ol, (3β,5α)-		2.5, 2.7
3241.	33886-74-7	0	1	0	Ergosta-8,24(28)-dien-3-ol, 14-methyl-, (3β,5α)-		2.5, 2.7
3242.	16910-32-0	0	1	0	Ergosta-8,24(28)-dien-3-ol, 4, 14-dimethyl-, (3β,4α,5α)-		2.5, 2.7
3243.	57-87-4	1	1	1	Ergosta-5,7,22-trien-3-ol, (3β,22*E*)- {ergosterol}		2.5, 2.7
3244.	74635-33-9	0	1	0	Ergosta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-		2.5, 2.7
3245.	80736-41-0	0	1	0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R, 23R,24S)-		2.5, 2.7, 3.13
3246.	121468-15-3	0	1	0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3β,5α,22R,23R,24S)-		2.5, 2.7, 3.13
3247.	92751-21-8	0	1	0	Ergostan-6-one, 3,22,23-trihydroxy-, (3β,5α,22R,23R,24S)-		2.5, 2.7, 3.13
3248.	87734-68-7	0	1	0	Ergostan-6-one, 3,22,23-trihydroxy-, (3α,5α,22R,23R,24S)-		2.5, 2.7, 3.13
3249.	20304-54-5	0	1	0	Ergost-4-en-3-ol, (24R)- {campest-7-en-3-β-ol}		2.5, 2.7
3250.	474-62-4	1	1	1	Ergost-5-en-3-ol, (3β,24R)- {campesterol}		2.5, 2.7
3251.	26047-31-4	0	1	0	Ergost-7-en-3-ol, (3β)-		2.5, 2.7
3252.	17105-75-8	1	0	0	Ergost-7-en-3-ol, (3β,24ξ)-		2.5, 2.7
3253.	33860-48-9	0	1	0	Ergost-8-en-3-ol, 14-methyl-, (3β,5α)-		2.5, 2.7
3254.	16910-33-1	0	1	0	Ergost-8-en-3-ol, 4,14-dimethyl-, 3β,4α,5α)-		2.5, 2.7
3255.	70116-48-2	0	1	0	Ergost-8-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-		2.5, 2.7
3256.		0	1	0	*Escherichia coli K12*		22.2
3257.	9013-79-0	0	1	0	Esterase		22.2
3258.	9025-98-3	0	1	0	Esterase, pectin {pectase}		0.4, 22.2
3259.	75-04-7	1	1	1	Ethanamine {ethylamine}	$H_3C\text{-}CH_2\text{-}NH_2$	0.4, 12.2

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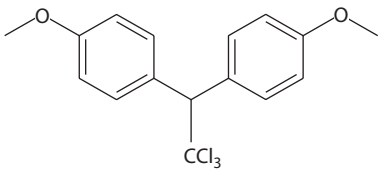
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3260.	51-75-2	1	0	0	Ethanamine, 2-chloro-*N*-(2-chloroethyl)-*N*-methyl-	$(Cl\text{-}CH_2\text{-}CH_2)_2{=}N\text{-}CH_3$	12.2, 18.4
3261.	121-44-8	1	1	1	Ethanamine, *N,N*-diethyl- {triethylamine}	$(H_3C\text{-}CH_2)_3{\equiv}N$	12.2
3262.	30533-08-5	1	0	0	Ethanamine, *N*,1-dimethyl-*N*-nitroso-		12.2, 15.8
3263.	109-89-7	1	1	1	Ethanamine, *N*-ethyl- {diethylamine}	$(H_3C\text{-}CH_2)_2{=}NH$	12.2
3264.	55-18-5	1	1	1	Ethanamine, *N*-ethyl-*N*-nitroso- {NDEA}	$(H_3C\text{-}CH_2)_2{=}N\text{-}NO$	12.2, 15.8, 23.5
3265.	624-78-2	1	1	1	Ethanamine, *N*-methyl-	$H_3C\text{-}CH_2\text{-}NH\text{-}CH_3$	12.2
3266.	10595-95-6	1	1	1	Ethanamine, *N*-methyl-*N*-nitroso- {NEMA}	$H_3C\text{-}CH_2\text{-}N(NO)\text{-}CH_3$	12.2, 15.8, 23.5
3267.	97190-07-3	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monooctadecadienoate monooctadecatrienoate, (all-*Z*)-		2.5, 12.2
3268.	97190-09-5	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl] oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecatrienoate, (*Z,Z,Z*)-		2.5, 12.2
3269.	97190-10-8	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl] oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecadienoate, (*Z,Z*)-		2.5, 12.2
3270.	97190-12-0	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy) hydroxyphosphinyl] oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monooctadecadienoate		2.5, 12.2
3271.	62-49-7 123-41-1	0	1	0	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl- {choline}	$HO\text{-}(CH_2)_2\text{-}N^{+}{\equiv}(CH_3)_3$	0.4, 2.5, 12.2
3272.	8002-43-5	0	1	0	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl-, phosphatidyl- {lecithin}		0.4, 12.2
3273.	74-84-0	1	0	0	Ethane	$H_3C\text{-}CH_3$	1.10
3274.	530-45-0	0	1	0	Ethane, bis(4-methylphenyl)-		1.13
3275.	354-53-0	1	1	1	Ethane, 1-chloro-2-bromotetrafluoro- {Freon® 114b1}	$ClF_2C\text{-}CF_2Br$	18.4
3276.	75-88-7	1	1	1	Ethane, 1-chloro-2,2,2-trifluoro- {Freon® 133a}	$ClCH_2\text{-}CF_3$	18.4
3277.	534-15-6	1	0	0	Ethane, 1,1-dimethoxy-		10.2
3278.	67-72-1	1	0	0	Ethane, hexachloro-		18.4
3279.	624-89-5	1	0	0	Ethane, (methylthio)-		18.1
3280.	60-29-7	1	1	1	Ethane, 1,1′-oxybis- {ethyl ether}		10.2
3281.	352-93-2	1	0	0	Ethane, 1,1′-thiobis-		18.1
3282.	106-93-4	0	1	0	Ethane, 1,2-dibromo- {ethylene dibromide, EDB®, Bromofume®}	$Br\text{-}CH_2\text{-}CH_2\text{-}Br$	18.4, 21.3

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3283.	107-06-2	1	0	0	Ethane, 1,2-dichloro-		18.4
3284.	306-83-2	1	1	1	Ethane, 2,2-dichloro-1,1,1-trifluoro- {Freon® 123}	$Cl_2CH\text{-}CF_3$	18.4
3285.	104-66-5	0	1	0	Ethane, 1,2-diphenoxy-	$C_6H_5\text{-}O\text{-}CH_2CH_2\text{-}OC_6H_5$	10.2
3286.	75-00-3	1	0	0	Ethane, chloro-	$C_2H_5\text{-}Cl$	18.4
3287.	540-67-0	1	0	0	Ethane, methoxy-	$C_2H_5\text{-}O\text{-}CH_3$	10.2
3288.	79-24-3	1	0	0	Ethane, nitro-	$C_2H_5\text{-}NO_2$	16.1
3289.	811-97-2	1	1	1	Ethane, 1,1,1,2-tetrafluoro- {Freon® 134a}	$FCH_2\text{-}CF_3$	18.4
3290.	71-55-6	1	0	0	Ethane, 1,1,1-trichloro-	$H_3C\text{-}C{\equiv}Cl_3$	18.4
3291.	72-43-5	0	1	0	Ethane, 1,1,1-trichloro-2,2-bis (4-methoxyphenyl)- {Methoxychlor®}		10.2, 18.4, 21.3
3292.	25323-89-1	0	1	0	Ethane, 1,2,2-trichloro-		18.4, 21.3
3293.	151-67-7	1	1	1	Ethane,1,1,1-trifluoro-2-bromo-2-chloro- {Freon® 123b1, Halothane}	$ClBrCH\text{-}CF_3$	18.4
3294.	107-22-2	1	1	1	Ethanedial {glyoxal}	O═CH-CH═O	3.12, 25.29
3295.	460-19-5	1	0	0	Ethanedinitrile {cyanogen}	NC-CN	0.4, 11.2, 19.5
3296.		0	1	0	Ethanedioate {oxalate}		20.6
3297.	144-62-7	1	1	1	Ethanedioic acid {oxalic acid}	HOOC-COOH	0.4, 4.3, 25.29
3298.	43058-40-8	1	1	1	Ethanedioic acid, labeled with ^{14}C {oxalic acid-^{14}C}		4.3, 25.29
3299.	14258-49-2	0	1	0	Ethanedioic acid, ammonium salt		20.6
3300.	17787-48-3	0	1	0	Ethanedioic acid, calcium salt (1:1), hydrate (2:5)		20.6
3301.	563-72-4 25454-23-3	0	1	0	Ethanedioic acid, calcium salt		0.4, 20.6
3302.	95-92-1	0	1	0	Ethanedioic acid, diethyl ester		5.3
3303.	583-52-8	0	1	0	Ethanedioic acid, dipotassium salt		20.6
3304.	6018-94-6	0	1	0	Ethanedioic acid, nickel salt		20.6
3305.	17480-26-1	0	1	0	Ethanedioic acid, tin salt {stannous oxalate}		20.6
3306.	542-10-9	1	0	0	1,1-Ethanediol, diacetate		5.3
3307.	107-21-1	1	1	1	1,2-Ethanediol {ethylene glycol}	$HOCH_2\text{-}CH_2OH$	0.4, 2.5
3308.	111-55-7	1	0	0	1,2-Ethanediol, diacetate		5.3
3309.	534-82-7	0	1	0	1,2-Ethanediol, 1-(4-hydroxy-3-methoxyphenyl)-		2.5, 9.22, 10.2
3310.	542-59-6	1	0	0	1,2-Ethanediol, monoacetate {acetic acid, 2-hydroxyethyl ester}	$HO\text{-}(CH_2)_2\text{-}OOC\text{-}CH_3$	2.5, 5.3
3311.	134-81-6	1	0	0	Ethanedione, diphenyl- {benzil}	$C_6H_5\text{-}CO\text{-}CO\text{-}C_6H_5$	3.13
3312.	107-35-7	0	1	0	Ethanesulfonic acid, 2-amino- {taurine}	$H_2N\text{-}(CH_2)_2\text{-}SO_3H$	12.2, 18.1
3313.	75-08-1	1	0	0	Ethanethiol {ethyl mercaptan}	$C_2H_5\text{-}SH$	18.1
3314.	40460-44-4	0	1	0	1,1,2-Ethanetriol		2.5
3315.	23135-22-0	0	1	0	Ethanimidothioic acid, 2-(dimethylamino)-*N*-[[(methylamino)carbonyl] oxy]-2-oxo-, methyl ester {Oxamyl®}	$(H_3C)_2{=}N\text{-}CO\text{-}C(S\text{-}CH_3){=}N\text{-}OOC\text{-}NH\text{-}CH_3$	5.3, 18.1, 21.3
3316.	59669-26-0	0	1	0	Ethanimidothioic acid, *N′*,*N′*-(thiobis ((methylimino)carbonyloxy))bis-, dimethyl ester {Thiodicarb®}	$S{=}[NH\text{-}COO\text{-}N{=}C(CH_3)\text{-}SCH_3]_2$	5.3, 18.1, 21.3

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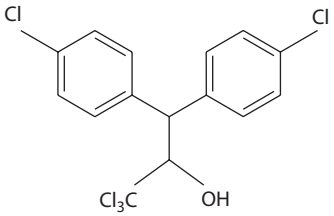
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
3317.	64-17-5	1	1	1	Ethanol {ethyl alcohol}	$H_3C\text{-}CH_2OH$	0.4, 2.5, 24.3, 25.29, 26.9
3318.		1	1	1	1-^{14}C-Ethanol {ethyl alcohol-^{14}C}		2.5, 25.29
3319.	107-07-3	1	1	1	Ethanol, 2-chloro- {chlorohydrin}		2.5, 18.4
3320.	108-01-0	1	0	0	Ethanol, 2-(dimethylamino)-	$(H_3C)_2{=}N\text{-}CH_2\text{-}CH_2OH$	2.5, 12.2
3321.	109-83-1	0	1	0	Ethanol, 2-(methylamino)-	$H_3C\text{-}NH\text{-}CH_2\text{-}CH_2OH$	2.5, 12.2
3322.	1116-54-7	1	1	1	Ethanol, 2,2′-(nitrosoimino) bis- {NDELA}	$(HO\text{-}CH_2CH_2)_2{=}N\text{-}NO$	2.5, 12.2, 25.8, 23.5
3323.	112-27-6	1	1	1	Ethanol, 2,2′-(1,2-ethanediylbis(oxy)) bis- {triethylene glycol}	$HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$	2.5, 10.2, 25.29
3324.	111-21-7	1	1	1	Ethanol, 2,2′-[1,2-ethanediylbis (oxy)]bis-, diacetate		5.3, 10.2
3325.	112-60-7	0	1	0	Ethanol, 2,2′-[oxybis(2,1-ethanediyloxy)] bis- {tetraethylene glycol}	$HO\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}O\text{-}(CH_2)_2\text{-}OH$	2.5, 10.2
3326.	30934-97-5	1	0	0	Ethanol, 2,2-dimethoxy-		2.5, 10.2
3327.	111-42-2	1	1	1	Ethanol, 2,2′-iminobis- {diethanolamine}	$(HO\text{-}CH_2CH_2)_2{=}NH$	2.5, 12.2
3328.	111-46-6	1	1	1	Ethanol, 2,2′-oxybis- {diethylene glycol}	$(HO\text{-}CH_2CH_2)_2{=}O$	0.4, 2.5, 10.2
3329.	141-43-5	0	1	0	Ethanol, 2-amino- {ethanolamine}	$HO\text{-}CH_2CH_2\text{-}NH_2$	2.5, 12.2
3330.	1071-23-4	0	1	0	Ethanol, 2-amino-, dihydrogen phosphate (ester)		5.3, 12.2
3331.	78-51-3	1	0	0	Ethanol, 2-butoxy-, phosphate (3:1)	$[H_3C\text{-}(CH_2)_3\text{-}O\text{-}(CH_2)_2]_3{\equiv}P{=}O$	5.3, 10.2
3332.	110-80-5	1	1	1	Ethanol, 2-ethoxy-	$HO\text{-}CH_2CH_2\text{-}O\text{-}CH_2CH_3$	2.5, 10.2
3333.	109-86-4	1	1	1	Ethanol, 2-methoxy-	$HO\text{-}CH_2CH_2\text{-}O\text{-}CH_3$	2.5, 10.2
3334.	122-99-6	0	1	0	Ethanol, 2-phenoxy-	$C_6H_5O\text{-}CH_2CH_2\text{-}OH$	2.5, 10.2
	1321-27-3	0	0	0	Ethanol, phenyl- Previously listed as 60-12-8 Benzeneethanol		2.5
3335.	115-32-2	0	1	0	Ethanol, 2,2,2-trichloro-1,1-bis (4-chlorophenyl)- {Dicofol®}		2.5, 18.4, 21.3
3336.		1	0	0	Ethanone, 1-(alkyl-1*H*-pyrrolyl)-		3.13, 17.4
3337.	6004-60-0	1	0	0	Ethanone, 1-cyclopentyl-		3.13
3338.	765-43-5	1	0	0	Ethanone, 1-cyclopropyl-		3.13
3339.	78210-69-2	1	0	0	Ethanone, 1-(1,2-dihydro-2-methyl-3-pyridinyl)-		3.13, 17.7
3340.		1	0	0	Ethanone, 1-(1,2-dihydro-1*H*-pyrrolyl)-		3.13, 17.4
3341.	117210-49-8	0	1	0	Ethanone, 1-(1,4,4a,5,6,7,8,8a-octahydro-4a,8,8-trimethyl-2-naphthalenyl)-, (4aR-*trans*)-		3.13
3342.	932-66-1	1	0	0	Ethanone, 1-(1-cyclohexen-1-yl)-		3.13
3343.		1	0	0	Ethanone, 1-(dimethylphenyl)- {dimethylacetophenone}		3.13
3344.	937-30-4	1	0	0	Ethanone, 1-(4-ethylphenyl)-		3.13
3345.		1	0	0	Ethanone, 1-(1-ethyl-1*H*-pyrrol-3-yl)-		3.13, 17.4
3346.	26444-19-9	1	0	0	Ethanone, 1-(methylphenyl)- {methylacetophenone}		3.13
3347.		1	0	0	Ethanone, 1-(methyl-1*H*-pyrrolyl)-		3.13, 17.4

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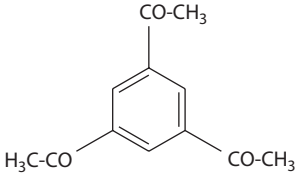
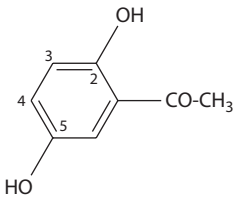
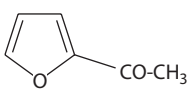
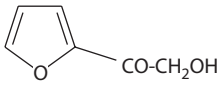
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3348.	941-98-0	1	0	0	Ethanone, 1-(1-naphthalenyl) {1′-acetonaphthone}		3.13
3349.	20583-33-9	0	1	0	Ethanone, 1-(1*H*-pyrazol-3-yl)-		3.13, 17.4
3350.	25016-16-4	0	1	0	Ethanone, 1-(1*H*-pyrazol-4-yl)-		3.13, 17.4
3351.	1072-83-9	1	1	1	Ethanone, 1-(1*H*-pyrrol-2-yl)- {2-acetylpyrrole, methyl 2-pyrrolyl ketone}		3.13, 17.4, 24.3, 25.29
3352.	1072-82-8	1	1	1	Ethanone, 1-(1*H*-pyrrol-3-yl)- {3-acetylpyrrole, methyl 3-pyrrolyl ketone}		3.13, 17.4
3353.	711-79-5	1	1	1	Ethanone, 1-(1-hydroxy-2-naphthalenyl)-		3.13, 9.22
3354.	20970-50-7	1	0	0	Ethanone, 1-(1-methyl-1 *H*-imidazol-5-yl)-		3.13, 17.4
3355.	37687-18-6	1	0	0	Ethanone, 1-(1-methyl-1*H*-pyrazol-4-yl)-		3.13, 17.4
3356.	932-16-1	1	1	1	Ethanone, 1-(1-methyl-1*H*-pyrrol-2-yl)-		3.13, 17.4
3357.	932-62-7	1	1	1	Ethanone, 1-(1-methyl-1*H*-pyrrol-3-yl)-		3.13, 17.4
3358.	70987-81-4	1	1	1	Ethanone, 1-(1,2,3-trimethyl-2-cyclopenten-2-yl)-		3.13
3359.	779-90-8	0	1	0	Ethanone, 1,1′,1″-(1,3,5-benzenetriyl)tris- {1,3,5-triacetylbenzene}		3.13
3360.		1	0	0	Ethanone, 1-(2-alkylphenyl)-		3.13
3361.	55041-85-5	1	1	1	Ethanone, 1-(2,3-dihydro-1 *H*-pyrrolizin-5-yl)-		3.13, 17.4
3362.		1	0	0	Ethanone, 1-(2,3-dihydrothiophen-2-yl)-		3.13, 18.1
3363.	19005-95-9	1	0	0	Ethanone, 1-(2,4,5-trimethyl-1 *H*-pyrrol-3-yl)-		3.13, 17.4
3364.	1667-01-2	0	1	0	Ethanone, 1-(2,4,6-trimethylphenyl)-		3.13
3365.	85213-22-5	0	1	0	Ethanone, 1-(2,5-dihydro-pyrrol-2-yl)- {2-acetylpyrroline}		3.13, 17.4
3366.		1	0	0	Ethanone, 1-(2,5-dihydro-5-methyl-1 *H*-pyrrol-3-yl)-		3.13, 17.4
3367.	490-78-8	1	0	0	Ethanone, 1-(2,5-dihydroxyphenyl)-		3.13, 9.22
3368.	1500-94-3	1	0	0	Ethanone, 1-(2,5-dimethyl-1*H*-pyrrol-3-yl)-		3.13, 17.4
3369.	1197-92-8	0	1	0	Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-		3.13
3370.	699-83-2	1	0	0	Ethanone, 1-(2,6-dihydroxyphenyl)-		3.13, 9.22
3371.	1192-62-7	1	1	1	Ethanone, 1-(2-furanyl)- {2-acetylfuran}		3.13, 10.2
3372.	19859-79-1	1	0	0	Ethanone, 1-(2-furanyl)-2-(acetyloxy)-		3.13, 5.3, 10.2
3373.	17678-19-2	1	1	1	Ethanone, 1-(2-furanyl)-2-hydroxy-		2.5, 3.13, 10.2

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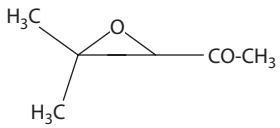
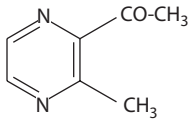
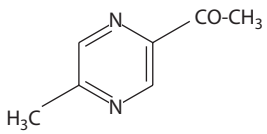
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3374.	703-98-0	1	0	0	Ethanone, 1-(2-hydroxy-3-methoxyphenyl)-		3.13, 9.22, 10.2
3375.	6921-64-8	0	1	0	Ethanone, 1-(2-hydroxy-4-methylphenyl)-		3.13, 9.22
3376.	1450-72-2	1	1	1	Ethanone, 1-(2-hydroxy-5-methylphenyl)-		3.13, 9.22
3377.	703-23-1	1	0	0	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-		3.13, 9.22, 10.2
3378.		0	1	0	Ethanone, 1-(2-hydroxy-6-methylphenyl)-		3.13, 9.22
3379.	118-93-4	1	1	1	Ethanone, 1-(2-hydroxyphenyl)-		3.13, 9.22
3380.	78210-66-9	1	0	0	Ethanone, 1-(2-methyl-1*H*-imidazol-4-yl)-		3.13, 17.4
3381.	577-16-2	1	1	1	Ethanone, 1-(2-methylphenyl)- {2-methylacetophenone}		3.13
3382.		0	1	0	Ethanone, 1-[2-methyl-5-(1-methylethyl)-phenyl]-		3.13
3383.	1122-62-9	1	1	1	Ethanone, 1-(2-pyridinyl)- {2-acetylpyridine}		3.13, 17.7, 24.3
3384.	60026-20-2	1	1	1	Ethanone, 1-(2-pyrrolidinyl)- {2-acetylpyrrolidine}		3.13, 17.4
3385.	24295-03-2	0	1	0	Ethanone, 1-(2-thiazolyl)- {2-acetylthiazole}		3.13, 18.1
3386.	88-15-3	0	1	0	Ethanone, 1-(2-thienyl)- {2-acetylthiophene}		3.13, 18.1
3387.		0	1	0	Ethanone, 1-[2,3-dihydro-2-(1-methylethyl)-inden-4-yl]-		3.13
3388.		0	1	0	Ethanone, 1-[3,4-dihydro-6-(1-methylethyl)-inden-4-yl]-pyran-2-yl-		3.13, 10.2
3389.		0	1	0	Ethanone, 1-(3,4-dihydro-4-methylpyrazin-2-yl)-		3.13, 17.7
3390.	1197-09-7	1	0	0	Ethanone, 1-(3,4-dihydroxyphenyl)-		3.13, 9.22
3391.	1131-62-0	1	0	0	Ethanone, 1-(3,4-dimethoxyphenyl)-		3.13
3392.	4478-63-1	0	1	0	Ethanone, 1-(3,3-dimethyloxiranyl)- {mesityl oxide epoxide}		3.13, 10.2
3393.	89-74-7	0	1	0	Ethanone, 1-(2,4-dimethylphenyl)-		3.13
3394.	3637-01-2	1	0	0	Ethanone, 1-(3,4-dimethylphenyl)-		3.13
3395.	51863-60-6	0	1	0	Ethanone, 1-(3,5-dihydroxyphenyl)-		3.13, 9.22
3396.	117210-50-1	0	1	0	Ethanone, 1-(3a,4,5,6,7,7a-hexahydro-3a,7,7-trimethyl-1*H*-inden-2-yl)-, (3aR-*trans*)-		3.13
3397.	66611-15-2	1	0	0	Ethanone, 1-(3-benzofuranyl)-		3.13, 10.2
3398.	22699-70-3	1	0	0	Ethanone, 1-(3-ethylphenyl)-		3.13
3399.	14313-09-8	1	0	0	Ethanone, 1-(3-furanyl)-		3.13, 10.2
3400.	3420-59-5	0	1	0	Ethanone, 1-(3-hydroxy-2-furanyl)- {isomaltol}		2.5, 3.13, 10.2
3401.		1	0	0	Ethanone, 1-(3-hydroxy-2-methoxyphenyl)-		3.13, 9.22, 10.2
3402.	6100-74-9	1	0	0	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-		3.13, 9.22, 10.2
3403.	33414-49-2	1	0	0	Ethanone, 1-(3-hydroxy-4-methylphenyl)-		3.13, 9.22
3404.	121-71-1	1	0	0	Ethanone, 1-(3-hydroxyphenyl)-		3.13, 9.22
3405.	586-37-8	1	0	0	Ethanone, 1-(3-methoxyphenyl)-		3.13, 10.2
3406.	72693-15-3	1	0	0	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-		3.13, 17.4
3407.	72709-76-3	1	0	0	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-		3.13, 17.4
3408.	585-74-0	1	1	1	Ethanone, 1-(3-methylphenyl)- {3-methylacetophenone}		3.13

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
3409.	23787-80-6	1	1	1	Ethanone, 1-(3-methylpyrazinyl)- {2-acetyl-3-methylpyrazine}		3.13, 17.7
3410.	350-03-8	1	1	1	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine or methyl 3-pyridyl ketone}		0.4, 3.13, 17.7, 24.3
3411.	25343-57-1	0	1	0	Ethanone,1-[3-(1,4,5,6-tetrahydropyridinyl)]-		3.13, 17.7
3412.	27300-27-2	0	1	0	Ethanone,1-[3-(3,4,5,6-tetrahydropyridinyl)]-		3.13, 17.7
3413.	59576-31-7	1	0	0	Ethanone, 1-(4,6-dimethyl-2-pyridinyl)-		3.13, 17.7
3414.	37920-25-5	1	0	0	Ethanone, 1-(4-butylphenyl)-		3.13
3415.	1676-63-7	1	0	0	Ethanone, 1-(4-ethoxyphenyl)-		3.13, 10.2
3416.	66309-77-1	1	0	0	Ethanone,1-(4-ethyl-2,3-dimethylphenyl)-		3.13
3417.	493-33-4	1	0	0	Ethanone,1-(4-hydroxy-2-methoxyphenyl)-		3.13, 9.22, 10.2
3418.	2478-38-8	1	0	0	Ethanone,1-(4-hydroxy-3,5-dimethoxyphenyl)-		3.13, 9.22, 10.2
3419.	498-02-2	1	1	1	Ethanone,1-(4-hydroxy-3-methoxyphenyl)- {acetovanillone}		3.13, 9.22, 10.2
3420.	99-93-4	1	1	1	Ethanone, 1-(4-hydroxyphenyl)-		3.13, 9.22
3421.	100-06-1	1	1	1	Ethanone, 1-(4-methoxyphenyl)- {acetanisole}		3.13, 10.2, 24.3, 25.29
3422.	2524-90-5	1	0	0	Ethanone,1-(4-methyl-1*H*-imidazol-2-yl)-		3.13, 17.4
3423.	122-00-9	1	1	1	Ethanone, 1-(4-methylphenyl)- {4-methylacetophenone}		3.13, 24.3, 25.29
3424.	59576-26-0	1	0	0	Ethanone, 1-(4-methyl-2-pyridinyl)-		3.13, 17.7
3425.	1122-54-9	1	1	1	Ethanone, 1-(4-pyridinyl)- {4-acetylpyridine}		3.13, 17.7
3426.	38205-66-2	1	0	0	Ethanone, 1-(4-thiazolyl)- {4-acetylthiazole}		3.13, 18.1
3427.	32974-92-8	0	1	0	Ethanone, 1-(5-ethylpyrazinyl)-		3.13, 17.7
3428.	23328-91-8	1	0	0	Ethanone, 1-(5-methyl-1*H*-imidazol-2-yl)-		3.13, 17.4
3429.	6982-72-5	1	1	1	Ethanone, 1-(5-methyl-1*H*-pyrrol-2-yl)- {2-acetyl-5-methylpyrrole}		3.13, 17.4
3430.	1193-79-9	1	1	1	Ethanone, 1-(5-methyl-2-furanyl)- {2-acetyl-5-methylfuran}		3.13, 10.2, 24.3
3431.		1	0	0	Ethanone, 1-(5-methyl-2-furanyl)-2-hydroxy-		2.5, 3.13, 10.2
3432.	102518-81-0	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-		3.13, 10.2
3433.	102518-82-1	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-, (exo,exo)-(±)-		3.13, 10.2
3434.	42972-46-3	1	1	1	Ethanone, 1-(5-methyl-3-pyridinyl)-		3.13, 17.7
3435.	22047-27-4	1	1	1	Ethanone, 1-(5-methylpyrazinyl)- {2-acetyl-5-methylpyrazine}		3.13, 17.7
3436.	78210-67-0	1	0	0	Ethanone, 1-(5-propyl-1*H*-imidazol-4-yl)-		3.13, 17.4
3437.	6940-57-4	1	0	0	Ethanone, 1-(6-methyl-2-pyridinyl)-		3.13, 17.7
3438.	36357-38-7	1	1	1	Ethanone, 1-(6-methyl-3-pyridinyl)-		3.13, 17.7
3439.	22047-26-3	1	1	1	Ethanone, 1-(6-methylpyrazinyl)- {2-acetyl-6-methylpyrazine}		3.13, 17.7
3440.	61891-76-7	1	0	0	Ethanone, 1-(dihydro-3,4-dimethylpyrrol-2-yl)-		3.13, 17.4
3441.	78249-86-2	1	0	0	Ethanone, 1-(dimethylpyridinyl)-		3.13, 17.7

(*continued*)

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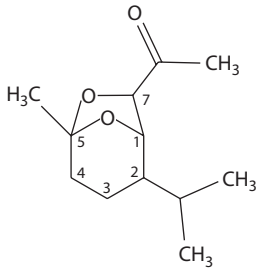
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3442.	25496-14-4	1	0	0	Ethanone, 1-(ethylphenyl)-		3.13
3443.	25154-45-4	1	0	0	Ethanone, 1-(furanyl)-		3.13, 10.2
3444.	692-73-0	1	0	0	Ethanone, 1-(hydroxymethylphenyl)-		2.5, 3.13
3445.	70587-92-7	1	0	0	Ethanone, 1-(hydroxyphenyl)-		3.13, 9.22
3446.	71278-10-9	1	0	0	Ethanone, 1-(methyl-2-furanyl)-		3.13, 10.2
3447.	74430-25-4	1	1	1	Ethanone, 1-(methylfuranyl)-		3.13, 10.2
3448.	78249-87-3	1	0	0	Ethanone, 1-(methylpyridinyl)- {two isomers}		3.13, 17.7
3449.	1333-52-4 93-08-3	1	1	1	Ethanone, 1-(2-naphthalenyl)- {methyl naphthyl ketone}		3.13, 24.3
3450.	25252-64-6	1	0	0	Ethanone, 1-(tetrahydro-2-furanyl)-		3.13, 10.2
3451.	121198-50-3	1	1	1	Ethanone, 1-(tetrahydrofuranyl)-		3.13, 10.2
3452.	13678-73-4	0	1	0	Ethanone, 1-[1-(2-furanylmethyl)-1*H*-pyrrol-2-yl]-		3.13, 10.2, 17.4
3453.	22583-61-5	1	0	0	Ethanone,1-[2-(1,1-dimethylethyl)phenyl]-		3.13
3454.	112523-81-6	0	1	0	Ethanone, 1-[2,3,3a,4,6a,7,8,9,9a, 9b-decahydro-5,9a-dimethyl-7-(1-methylethyl)-1*H*-cyclopent[*a*]azulen-3-yl]-, [3R-(3α,3aα,6aβ,7β,9aα,9bβ)]-		3.13
3455.	152186-01-1	0	1	0	Ethanone, 1-[2,3,3a,4,6a,7,8,9,9a, 9b-decahydro-5,9a-dimethyl-7-(1-methylethyl)-1*H*-cyclopent[*a*]azulen-3-yl]-, (3α,3aα,6aβ,7β,9aα,9bβ)-(±)-		3.13
3456.	1767-84-6	0	1	0	Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-		3.13
3457.	94390-73-5	1	0	0	Ethanone, 1-[2-methyl-5-(1-methylethyl)-2,5-cyclohexadien-1-yl]-		3.13
3458.	1202-08-0	0	1	0	Ethanone, 1-[2-methyl-5-(1-methylethyl)phenyl]-		3.13
3459.	51297-35-9	0	1	0	Ethanone, 1-[3-(1-ethyl-2-methylpropyl)oxiranyl]-		3.13, 10.2
3460.	38552-75-9	0	1	0	Ethanone, 1-[2-(1-methylethenyl) cyclopentyl]-		3.13
3461.	31577-86-3 43219-68-7	0	1	0	Ethanone, 1-[3-(1-methylethenyl) cyclopentyl]- {two isomers}		3.13
3462.	120056-06-6	0	1	0	Ethanone, 1-[3-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl) oxiranyl]-, [1S-[1α(2S*,3R*),2β,4a		2.5, 3.13, 10.2
3463.		1	0	0	Ethanone, 1-[4-(2,6-dimethylpyridinyl)]-		3.13, 17.7
3464.	55087-82-6	1	0	0	Ethanone, 1-[5-(hydroxymethyl)-2-furanyl]-		2.5, 3.13, 10.2
3465.	52812-41-6	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-		3.13, 10.2
3466.	57934-85-7	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-, (exo,exo)-(±)-		3.13, 10.2

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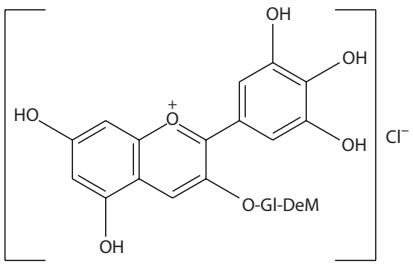
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3467.	123695-66-9	1	0	0	Ethanone, 1-[6-hydroxy-6-methyl-3-(1-methylethyl)-2-cyclohexen-1-yl]-		2.5, 3.13
3468.	823-76-7	0	1	0	Ethanone, 1-cyclohexyl-		3.13
3469.	57276-33-2	1	0	0	Ethanone, 1-cyclopropyl-2-(3-pyridinyl)-		3.13, 17.7
3470.	98-86-2	1	1	1	Ethanone, 1-phenyl- {acetophenone}		3.13, 24.3, 25.29
3471.	2243-35-8	0	1	0	Ethanone, 1-phenyl-2-(acetyloxy)-		3.13, 5.3
3472.	22047-25-2	1	1	1	Ethanone, 1-pyrazinyl- {acetylpyrazine}		3.13, 17.7, 24.3, 25.29
3473.	119-53-9	0	1	0	Ethanone, 1,2-diphenyl-2-hydroxy-	C_6H_5-CHOH-CO-C_6H_5	2.5, 3.13
3474.	574-06-1	1	0	0	Ethanone, 1,2-diphenyl-2-(acetyloxy)- {benzoin acetate}		3.13, 5.3
3475.	582-24-1	1	0	0	Ethanone, 2-hydroxy-1-phenyl-	C_6H_5-CO-CH_2OH	2.5, 3.13
3476.	593-67-9	1	1	1	Ethenamine	H_2C═CH-NH_2	12.2
3477.	74-85-1	1	1	1	Ethene {ethylene}	H_2C═CH_2	1.11, 21.3, 25.29
3478.	75-01-4	0	1	0	Ethene, chloro- {vinyl chloride}	H_2C═CH-Cl	18.4, 23.5
3479.	79-38-9	1	1	1	Ethene, chlorotrifluoro- {Freon® 1113}	ClFC═CF_2	18.4
3480.	79-35-6	1	1	1	Ethene, 1,1-dichloro-2,2-difluoro- {Freon® 1112a}	Cl_2C═CF_2	18.4
3481.	10083-24-6	0	1	0	Ethene, 1-(3,4-dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)- (*E*)- {*trans*-piceatannol}		9.22
3482.	501-36-0	0	1	0	Ethene, 1-(4-hydroxyphenyl)-2-(3,5-dihydroxyphenyl)-, (*E*)- {*trans*- resveratrol}		9.22
3483.	61434-67-1	0	1	0	Ethene, 1-(4-hydroxyphenyl)-2-(3,5-dihydroxyphenyl)-, (*Z*)- {*cis*-resveratrol}		9.22
3484.	102-61-4	0	1	0	Ethene, 1-(phenyl)-2-(3,5-dihydroxyphenyl)- {pinosylvin}		9.22
3485.	127-18-4	1	0	0	Ethene, tetrachloro-	Cl_2C═CCl_2	18.4
3486.	79-01-6	1	0	0	Ethene, trichloro-	Cl_2C═CHCl	18.4
3487.	463-51-4	1	0	0	Ethenone {ketene}	H_2C═CO	3.13
3488.	2154-50-9	1	0	0	Ethoxyl radical	OCH_2CH_3	27.1
3489.	74-86-2	1	0	0	Ethyne {acetylene}	HC≡CH	0.4, 1.11, 25.29
3490.	7440-53-1	1	1	1	Europium	Eu	20.5
3491.	378750-46-0	1	1	1	Europium, isotope of mass 152	^{152}Eu	20.5
3492.	9040-09-9	0	1	0	Ferredoxins		22.2
3493.		0	1	0	*Firmicutes*, *Bacilli*		22.2
3494.		0	1	0	*Firmicutes*, *Clostridia*		22.2
3495.	29732-48-7	0	1	0	Flavylium, 3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride		2.5, 8.3, 9.22, 10.2, 18.4
3496.		0	1	0	Flavylium, 3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-3′,4′,5,7-tetrahydroxy-, chloride		2.5, 8.3, 9.22, 10.2, 18.4

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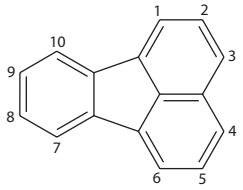
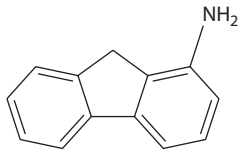
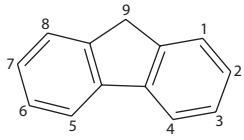
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3497.		1	0	0	Fluoraninene, ethylmethyl-		1.20
3498.	2693-46-1	1	0	0	3-Fluoranthenamine		12.2
3499.	206-44-0	1	1	1	Fluoranthene		1.20, 26.9
3500.		1	0	0	Fluoranthene, alkyl-		1.20
3501.	41593-24-2	1	0	0	Fluoranthene, dihydro-		1.20
3502.	71278-25-6	1	0	0	Fluoranthene, dihydromethyl-		1.20
3503.	60826-74-6	1	0	0	Fluoranthene, dimethyl- {at least four isomers in MSS}		1.20
3504.	23339-04-0	1	0	0	Fluoranthene, 2,3-dimethyl-		1.20
3505.	38048-87-2	1	0	0	Fluoranthene, 7,8-dimethyl-		1.20
3506.	22271-04-1	1	0	0	Fluoranthene, 7,10-dimethyl-		1.20
3507.	25889-63-8	1	0	0	Fluoranthene, 8,9-dimethyl-		1.20
3508.	55220-72-9	1	0	0	Fluoranthene, ethyl-		1.20
3509.	20496-16-6	1	0	0	Fluoranthene, 3-ethyl-		1.20
3510.	46864-87-3	1	0	0	Fluoranthene, 8-ethyl-		1.20
3511.	71277-96-8	1	0	0	Fluoranthene, ethylmethyl-		1.20
3512.	71277-97-9	1	0	0	Fluoranthene, hexamethyl-		1.20
3513.	30997-39-8	1	0	0	Fluoranthene, methyl-		1.20
3514.	25889-60-5	1	0	0	Fluoranthene, 1-methyl-		1.20
3515.	33543-31-6	1	1	1	Fluoranthene, 2-methyl-		1.20
3516.	1706-01-0	1	0	0	Fluoranthene, 3-methyl-		1.20
3517.	23339-05-1	1	0	0	Fluoranthene, 7-methyl-		1.20
3518.	20485-57-8	1	0	0	Fluoranthene, 8-methyl-		1.20
3519.	71277-98-0	1	0	0	Fluoranthene, pentamethyl- {at least two isomers in MSS}		1.20
3520.	55220-69-4	1	0	0	Fluoranthene, propyl-		1.20
3521.	71277-99-1	1	0	0	Fluoranthene, tetramethyl-		1.20
3522.	41637-87-0	1	0	0	Fluoranthene, trimethyl-		1.20
3523.		1	0	0	Fluorenamine		12.2
3524.	64294-96-8	1	0	0	9*H*-Fluorenamine		12.2
3525.	6344-63-4	1	0	0	9*H*-Fluoren-1-amine		12.2
3526.	153-78-6	1	0	0	9*H*-Fluoren-2-amine		12.2
3527.	7083-63-8	1	0	0	9*H*-Fluoren-4-amine		12.2
3528.	525-03-1	1	0	0	9*H*-Fluoren-9-amine		12.2
3529.	86-73-7	1	1	1	9*H*-Fluorene		1.20
3530.	30582-01-5	1	1	1	9*H*-Fluorene, dimethyl- {at least five isomers in MSS}		1.20
3531.		1	0	0	9*H*-Fluorene, ?,9-dimethyl-		1.20
3532.	17057-98-6	1	0	0	9*H*-Fluorene, 1,9-dimethyl-		1.20
3533.	4612-63-9	1	1	1	9*H*-Fluorene, 2,3-dimethyl-		1.20

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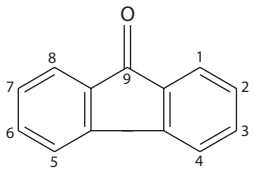
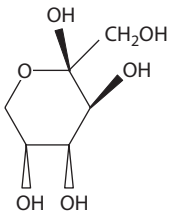
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3534.	4569-45-3	1	0	0	9*H*-Fluorene, 9,9-dimethyl-		1.20
3535.	71278-00-7	1	0	0	9*H*-Fluorene, dimethylethyl-		1.20
3536.	65319-49-5	1	0	0	9*H*-Fluorene, ethyl- {at least two isomers in MSS}		1.20
3537.	1207-20-1	1	0	0	9*H*-Fluorene, 2-ethyl-		1.20
3538.	2294-82-8	1	0	0	9*H*-Fluorene, 9-ethyl-		1.20
3539.	71278-01-8	1	0	0	9*H*-Fluorene, ethylmethyl- {at least two isomers in MSS}		1.20
3540.	26914-17-0	1	1	1	9*H*-Fluorene, methyl-		1.20
3541.	1730-37-6	1	0	0	9*H*-Fluorene, 1-methyl-		1.20
3542.	1430-97-3	1	0	0	9*H*-Fluorene, 2-methyl-		1.20
3543.	2523-39-9	1	0	0	9*H*-Fluorene, 3-methyl-		1.20
3544.	1556-99-6	1	0	0	9*H*-Fluorene, 4-methyl-		1.20
3545.	2523-37-7	1	0	0	9*H*-Fluorene, 9-methyl-		1.20
3546.	4425-82-5	1	0	0	9*H*-Fluorene, 9-methylene-		1.20
3547.	63372-50-9	1	0	0	9*H*-Fluorene, tetramethyl-		1.20
3548.	30582-02-6	1	0	0	9*H*-Fluorene, trimethyl-		1.20
3549.	6276-03-5	1	1	1	9*H*-Fluorene-1-carboxylic acid		4.3
3550.	27134-14-1	1	0	0	Fluoren-9-one, ethyl-		3.13
3551.	27134-15-2	1	0	0	Fluoren-9-one, ethylmethyl-		3.13
3552.	486-25-9	1	1	1	9*H*-Fluoren-9-one		3.13
3553.	27134-13-0	1	0	0	9*H*-Fluoren-9-one, dimethyl {five isomers detected}		3.13
3554.	79147-47-0	1	0	0	9*H*-Fluoren-9-one, methyl- {two isomers detected}		3.13
3555.	5501-37-1	1	0	0	9*H*-Fluoren-9-one, 1-methyl-		3.13
3556.	2840-51-9	1	1	1	9*H*-Fluoren-9-one, 2-methyl-		3.13
3557.	1705-89-1	1	0	0	9*H*-Fluoren-9-one, 3-methyl-		3.13
3558.	4269-05-0	1	0	0	9*H*-Fluoren-9-one, 4-methyl-		3.13
3559.	16984-48-8	1	0	0	Fluoride	F^{-1}	18.4, 20.5
3560.	7782-41-4	1	1	1	Fluorine	F_2	0.4, 18.4, 19.5, 20.5
3561.	50-00-0	1	1	1	Formaldehyde	H-CH=O	0.4, 3.12, 23.5
3562.	75-12-7	1	0	0	Formamide	$H\text{-}CO\text{-}NH_2$	13.1
3563.	871-71-6	1	0	0	Formamide, *N*-butyl-	$H\text{-}CO\text{-}NH\text{-}(CH_2)_3\text{-}CH_3$	13.1
3564.	68-12-2	1	1	1	Formamide, *N,N*-dimethyl-	$H\text{-}CO\text{-}N{=}(CH_3)_2$	13.1
3565.		1	0	0	Formamide, *N*-(3-methylpyrrolyl-2-ethyl)-		13.1, 17.9
3566.	72693-10-8	1	0	0	Formamide, *N*-(2-furanylmethyl)-		10.2, 13.1
3567.	123-39-7	1	0	0	Formamide, *N*-methyl-	$H\text{-}CO\text{-}NH\text{-}CH_3$	13.1
3568.	10285-87-7	1	0	0	Formamide, *N*-(3-methylbutyl)-		13.1
3569.	2591-79-9	1	0	0	Formamide, *N*-pentyl-	$H\text{-}CO\text{-}NH\text{-}(CH_2)_4\text{-}CH_3$	13.1
3570.	103-70-8	1	0	0	Formamide, *N*-phenyl-		13.1
3571.	6343-54-0	1	0	0	Formamide, *N*-(phenylmethyl)-		13.1
3572.	56625-04-8	1	0	0	Formamide, *N*-(3-pyridinylmethyl)-		13.1, 17.7
3573.	71-47-6	1	1	1	Formate		20.6
3574.	64-18-6	1	1	1	Formic acid	H-COOH	0.4, 4.3
3575.	592-84-7	0	1	0	Formic acid, butyl ester		5.3
3576.	105-86-2 23135-22-0	0	1	0	Formic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl formate}		5.3

(*continued*)

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3577.	692-45-5	1	0	0	Formic acid, ethenyl ester {vinyl formate}		5.3
3578.	109-94-4	1	0	0	Formic acid, ethyl ester	H-COO-CH_2-CH_3	5.3
3579.	629-33-4	0	1	0	Formic acid, hexyl ester	H-COO-$(CH_2)_5$-CH_3	5.3
3580.	107-31-3	1	1	1	Formic acid, methyl ester {methyl formate}	H-COO-CH_3	5.3
3581.	110-45-2	0	1	0	Formic acid, 3-methylbutyl ester		5.3, 24.3, 25.29
3582.	625-55-8	1	0	0	Formic acid, 1-methylethyl ester	H-COO-CH═$(CH_3)_2$	5.3
3583.	638-49-3	0	1	0	Formic acid, pentyl ester	H-COO-$(CH_2)_4$-CH_3	5.3
3584.	104-62-1	1	1	1	Formic acid, 2-phenylethyl ester	H-COO-$(CH_2)_2$-C_6H_5	5.3
3585.	104-57-4	1	1	1	Formic acid, phenylmethyl ester {benzyl formate}	H-COO-CH_2-C_6H_5	5.3, 24.3, 25.29
3586.	110-74-7	0	1	0	Formic acid, propyl ester		5.3
3587.	2597-44-6	1	0	0	Formyl radical	H-CO	27.1
3588.	9037-90-5	0	1	0	*D*-Fructan		2.5, 8.3, 10.2
3589.	10247-46-8	0	1	0	*D*-Fructofuranose		2.5, 8.3, 10.2
3590.	71385-82-5	0	1	0	β-*D*-Fructofuranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2.5, 8.3, 10.2, 17.9
3591.	79082-92-1	0	1	0	β-*D*-Fructofuranose, 2,6-bis(dihydrogen phosphate)		2.5, 5.3, 8.3, 10.2
3592.	9001-57-4	0	1	0	β-Fructofuranosidase {β-fructosidase, invertase}		0.4, 22.2
3593.	79886-47-8	0	1	0	β-*D*-Fructopyranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2.5, 8.3, 10.2, 17.9
3594.	57-48-7	1	1	1	*D*-Fructose {levulose}		0.4, 2.5, 8.3, 10.2, 24.3, 25.29
3595.	51767-72-7	0	1	0	*D*-Fructose, labeled with ^{13}C {*D*-fructose-^{13}C}		2.5, 8.3, 10.2
3596.		0	1	0	*D*-Fructose, labeled with ^{14}C {*D*-fructose-^{14}C}		2.5, 8.3, 10.2
3597.	29118-61-4	0	1	0	*D*-Fructose, 1-(2-carboxy-1-pyrrolidinyl)-1-deoxy-, (S)-		2.5, 8.3, 10.2, 17.4
3598.	488-69-7	0	1	0	*D*-Fructose, 1,6-bis(dihydrogen phosphate)		2.5, 5.3, 8.3, 10.2
3599.	70954-04-0	0	1	0	*D*-Fructose, 1-[(1-carboxy-2-hydroxypropyl)amino]-1-deoxy-, [R-(R*,S*)]-		2.5, 8.3, 10.2, 12.2
3600.	34393-27-6	0	1	0	*D*-Fructose, 1-[(3-amino-1-carboxy-3-oxopropyl)amino]-1-deoxy-, (S)-		2.5, 8.3, 10.2, 12.2
3601.	10003-63-1	0	1	0	*D*-Fructose, 1-[(3-carboxypropyl)amino]-1-deoxy-		2.5, 8.3, 10.2, 12.2
3602.	70906-15-9	0	1	0	*D*-Fructose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-		2.5, 8.3, 10.2, 17.9
3603.	643-13-0	0	1	0	*D*-Fructose, 6-(dihydrogen phosphate)		2.5, 5.3, 8.3, 10.2
3604.	36119-15-0	0	1	0	*D*-Fructose, mono(dihydrogen phosphate)		2.5, 5.3, 8.3, 10.2
3605.	9033-47-0	0	1	0	Fructosidase {polyfructosidase}		22.2

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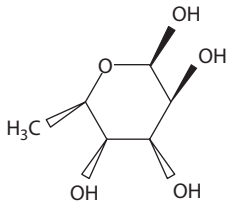
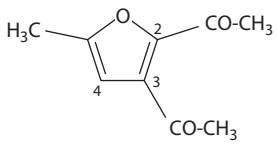
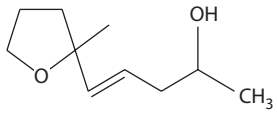
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3606.	2438-80-4	0	1	0	Fucose		2.5, 8.3, 10.2
3607.	110-00-9	1	0	0	Furan		10.2, 23.5
3608.		0	1	0	Furan, C_3-alkyl- {three isomers detected}		10.2
3609.	64079-00-1	0	1	0	Furan, butyl-		10.2
3610.		0	1	0	Furan, 2,3-diacetyl-5-methyl-		3.13, 10.2
3611.	28802-49-5	1	0	0	Furan, dimethyl-		10.2
3612.	31093-57-9	1	0	0	Furan, ethenyl-		10.2
3613.		1	0	0	Furan, ethenylmethyl-		10.2
3614.	27252-25-1	0	1	0	Furan, ethyl-		10.2
3615.	12758-54-2	1	0	0	Furan, hexenyl-methyl-		10.2
3616.	27137-41-3	1	0	0	Furan, methyl-		10.2
3617.	64079-01-2	0	1	0	Furan, pentyl-		10.2
3618.	27252-26-2	0	1	0	Furan, propyl-		10.2
3619.	109-99-9	1	1	1	Furan, tetrahydro-		10.2
3620.	41239-48-9	0	1	0	Furan, tetrahydro-2,5-diethyl-		10.2
3621.		0	1	0	Furan, tetrahydro-2-methyl-2-(4-hydroxy-1-pentenyl)-		2.5, 10.2
3622.	3208-40-0	0	1	0	Furan, tetrahydro-2-(3-phenylpropyl)-		10.2
3623.	13678-51-8	1	0	0	Furan, 2-(2-furanylmethyl)-5-methyl-		10.2
3624.	10504-11-7	1	0	0	Furan, 2-(2-methyl-1-propenyl)-		10.2
3625.	60858-07-3	1	0	0	Furan, 2-(3-hexenyl)-5-methyl-		10.2
3626.	4868-20-6	1	0	0	Furan, 2-(3-hexenyl)-5-methyl-, (*Z*)-		10.2
3627.	1197-40-6	1	1	1	Furan, 2,2′-methylenebis-		10.2
3628.	110484-93-0	1	0	0	Furan, 2,2′-methylenebis[5-ethyl-		10.2
3629.	13679-43-1	1	0	0	Furan, 2,2′-methylenebis[5-methyl-		10.2
3630.	1191-99-7	1	0	0	Furan, 2,3-dihydro-		10.2
3631.	121213-25-0	1	1	1	Furan, 2,3-dihydro-2-methoxy-		10.2
3632.	1708-25-4	1	0	0	Furan, 2,3-dihydro-2-methyl-		10.2
3633.	34314-83-5	1	1	1	Furan, 2,3-dihydro-4-methyl-		10.2
3634.	14920-89-9	1	0	0	Furan, 2,3-dimethyl-		10.2
3635.	3710-43-8	1	0	0	Furan, 2,4-dimethyl-		10.2
3636.	1708-29-8	1	1	1	Furan, 2,5-dihydro-		10.2
3637.	13314-90-4	1	0	0	Furan, 2,5-dihydro-2,5-bis(methylene)-		10.2
3638.	332-77-4	1	0	0	Furan, 2,5-dihydro-2,5-dimethoxy-		10.2
3639.	13436-43-6	1	1	1	Furan, 2,5-dihydro-2-methoxy-		10.2
3640.	1708-30-1	1	0	0	Furan, 2,5-dihydro-2-methyl-		10.2
3641.	10504-06-0	0	1	0	Furan, 2,5-diethyl-		10.2

(*continued*)

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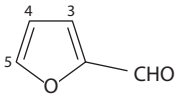
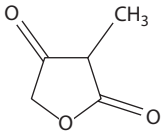
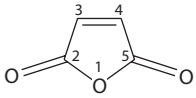
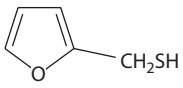
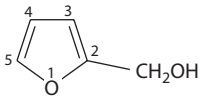
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3642.	625-86-5	1	1	1	Furan, 2,5-dimethyl-		10.2
3643.	110484-94-1	1	0	0	Furan, 2-[1-(5-ethyl-2-furanyl)ethyl]-5-methyl-		10.2
3644.	4466-24-4	1	1	1	Furan, 2-butyl-		10.2
3645.	1487-18-9	1	1	1	Furan, 2-ethenyl-		10.2
3646.	10504-13-9	1	0	0	Furan, 2-ethenyl-5-methyl- = furan, 5-ethenyl-2-methyl-		10.2
3647.	13679-86-2	0	1	0	Furan, 2-ethenyltetrahydro-2-methyl-5-(1-methylethenyl)-		10.2
3648.	3208-16-0	1	1	1	Furan, 2-ethyl-		10.2
3649.	1703-52-2	1	0	0	Furan, 2-ethyl-5-methyl-		10.2
3650.	534-22-5	1	1	1	Furan, 2-methyl-		10.2
3651.		0	1	0	Furan, 2-methyl-5 (1-methylethenyl)-		10.2
3652.	96-47-9	1	0	0	Furan, 2-methyltetrahydro-		10.2
3653.	3777-69-3	0	1	0	Furan, 2-pentyl-		10.2
3654.	17113-33-6	1	0	0	Furan, 2-phenyl-		10.2
3655.	55484-04-3	1	0	0	Furan, 2-(4-pyridyl)-		10.2, 17.7
3656.	42933-00-6 54869-11-3	1	1	1	Furan, 3-(4,8,12-trimethyltridecyl)- {phytofuran}		10.2
3657.	930-27-8	1	1	1	Furan, 3-methyl-		10.2
3658.	13423-15-9	1	1	1	Furan, 3-methyltetrahydro-		10.2
3659.	13679-41-9	0	1	0	Furan, 3-phenyl-		10.2
3660.	10504-04-8	1	0	0	Furan, 2,3,5-trimethyl-		10.2
3661.	2745-26-8	1	0	0	2-Furanacetic acid		4.3, 10.2
3662.	4915-21-3	1	0	0	2-Furanacetic acid, ethyl ester		5.3, 10.2
3663.	617-90-3	1	0	0	2-Furancarbonitrile		10.2, 11.2
3664.	13714-86-8	1	0	0	2-Furancarbonitrile, 5-methyl-		10.2, 11.2
3665.	39276-09-0	1	0	0	Furancarboxaldehyde		3.12, 10.2
3666.	98-01-1	1	1	1	2-Furancarboxaldehyde {furfural, 2-furaldehyde}		0.4, 3.12, 10.2
3667.		1	0	0	2-Furancarboxaldehyde, hydroxy-		2.5, 3.12, 10.2
3668.	25376-49-2	0	1	0	2-Furancarboxaldehyde, (hydroxymethyl)-		2.5, 3.12, 10.2
3669.	26895-04-5	1	0	0	2-Furancarboxaldehyde, methyl-		3.12, 10.2
3670.	33342-48-2	1	0	0	2-Furancarboxaldehyde, 3-methyl-		3.12, 10.2
3671.	32529-53-6	1	1	1	2-Furancarboxaldehyde, 5-acetyl-		3.12, 3.13, 10.2
3672.	10551-58-3	0	1	0	2-Furancarboxaldehyde, 5-[(acetyloxy) methyl]-		3.12, 5.3, 10.2
3673.	23074-10-4	1	0	0	2- Furancarboxaldehyde, 5-ethyl-		3.12, 10.2
3674.	67-47-0	1	1	1	2-Furancarboxaldehyde, 5-(hydroxymethyl)-		2.5, 3.12, 10.2
3675.	21300-07-2	0	1	0	2-Furancarboxaldehyde, 5-methoxy-		3.12, 10.2
3676.		0	1	0	2-Furancarboxaldehyde, 5-methoxy-?-methyl-		3.12, 10.2
3677.	1917-64-2	1	0	0	2-Furancarboxaldehyde, 5-(methoxymethyl)-		3.12, 10.2
3678.	620-02-0	1	1	1	2-Furancarboxaldehyde, 5-methyl-		3.12, 10.2
3679.		1	1	1	2-Furancarboxaldehyde, 5-(2-phenylethenyl)-		3.12, 10.2
3680.	498-60-2	1	1	1	3-Furancarboxaldehyde		3.12, 10.2
3681.	29988-76-9	1	1	1	Furancarboxamide		10.2, 13.1
3682.	609-38-1	1	1	1	2-Furancarboxamide		10.2, 13.1
3683.		1	1	1	2-Furancarboxamide, *N*-ethyl-		10.2, 13.1
3684.	61190-74-7	1	1	1	2-Furancarboxamide, *N*-(2-furanylmethyl)-		10.2, 13.1
3685.	26447-28-9	1	1	1	Furancarboxylic acid		4.3, 10.2
3686.	88-14-2	1	1	1	2-Furancarboxylic acid {furoic acid}		4.3, 10.2
3687.	61892-61-3	1	1	1	2-Furancarboxylic acid, 2-(acetyloxy)ethyl ester		5.3, 10.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3688.	3736-81-0	1	0	0	2-Furancarboxylic acid, 4-[(2,2-dichloroacetyl)-methylamino] phenyl ester		5.3, 10.2, 13.1, 18.4
3689.	614-99-3	0	1	0	2-Furancarboxylic acid, ethyl ester {ethyl 2-furoate}		5.3, 10.2
3690.	71278-16-5	1	1	1	2-Furancarboxylic acid, 3-hydroxy-		2.5, 4.3, 10.2
3691.	6338-41-6	1	0	0	2-Furancarboxylic acid, 5-(hydroxymethyl)-		2.5, 4.3, 10.2
3692.	1917-15-3	1	0	0	2-Furancarboxylic acid, 5-methyl-		4.3, 10.2
3693.	611-13-2	1	1	1	2-Furancarboxylic acid, methyl ester {methyl 2-furoate}		5.3, 10.2, 24.3
3694.	3885-29-8	1	0	0	2-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester		5.3, 6.3
3695.	488-93-7	1	0	0	3-Furancarboxylic acid		4.3, 10.2
3696.	6947-94-0	1	0	0	3-Furancarboxylic acid, 2-methyl-		4.3, 10.2
3697.	636-44-2	1	0	0	3-Furancarboxylic acid, 2,5-dimethyl-		4.3, 10.2
3698.	4412-96-8	1	0	0	3-Furancarboxylic acid, 3-methyl-		4.3, 10.2
3699.	21984-93-0	1	0	0	3-Furancarboxylic acid, 5-methyl-		4.3, 10.2
3700.	13129-23-2	0	1	0	3-Furancarboxylic acid, methyl ester		5.3, 10.2
3701.	5204-91-1	1	0	0	3-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester		5.3, 6.3
3702.	823-82-5	1	1	1	2,5-Furandicarboxaldehyde		3.12, 10.2
3703.	61892-94-2	1	0	0	3,4-Furandiol, tetrahydro-3-methyl-		2.5, 10.2
3704.	1192-51-4	1	0	0	2,4(3*H*,5*H*)-Furandione, 3-methyl-		3.13, 6.3
3705.	108-31-6	1	1	1	2,5-Furandione {maleic anhydride}		7.1, 26.9
3706.		1	1	1	2,5-^{14}C- 2,5-Furandione {maleic anhydride-2,5-^{14}C}		7.1, 25.29
3707.	28843-39-2	1	0	0	2,5-Furandione, 3,4-diethyl-		7.1
3708.	33765-37-6	0	1	0	2,5-Furandione, 3,4-diethyldihydro-, (*E*)-		7.1
3709.	108-30-5	1	1	1	2,5-Furandione, dihydro- {succinic anhydride}		7.1
3710.	17347-61-4	1	1	1	2,5-Furandione, dihydro-3,3-dimethyl-		7.1
3711.	7475-92-5	1	1	1	2,5-Furandione, dihydro-3,4-dimethyl-		7.1
3712.	4100-80-5	1	0	0	2,5-Furandione, dihydro-3-methyl-		7.1
3713.	83174-26-9	1	0	0	2,5-Furandione, dihydro-3-propyl-		7.1
3714.	766-39-2	1	1	1	2,5-Furandione, 3,4-dimethyl-		7.1
3715.	3552-33-8	1	1	1	2,5-Furandione, 3-ethyl-4-methyl-		7.1
3716.	616-02-4	1	1	1	2,5-Furandione, 3-methyl-		7.1
3717.	72693-16-4	1	0	0	2,5-Furandione, 3-methyl-4-(phenylmethyl)-		7.1
3718.	16493-20-2	1	0	0	2,5-Furandione, 3-methyl-4-propyl-		7.1
3719.	61679-89-8	1	0	0	2,5-Furandione, 3-propyl-		7.1
3720.	98-02-2	0	1	0	2-Furanmethanethiol		10.2, 18.1
3721.	40795-25-3	1	0	0	Furanmethanol		2.5, 10.2
3722.	98-00-0	1	1	1	2-Furanmethanol {furfuryl alcohol}		0.4, 2.5, 10.2

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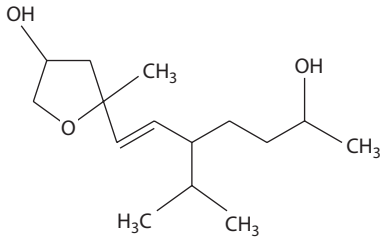
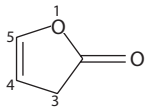
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3723.	623-17-6	1	1	1	2-Furanmethanol, acetate		5.3, 10.2
3724.		1	0	0	2-Furanmethanol, 2,3-dihydro-5-methoxy-		2.5, 10.2
3725.	60047-17-8	0	1	0	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-		2.5, 10.2
3726.	5989-33-3	0	1	0	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*Z*)- {*cis*-linalool oxide}		2.5, 10.2, 24.3, 25.29
3727.	23007-29-6	0	1	0	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*E*)- {*trans*-linalool oxide}		2.5, 10.2
3728.	13493-97-5	0	1	0	2-Furanmethanol, formate		5.3, 10.2
3729.	55664-77-2	0	1	0	2-Furanmethanol, methyl-		2.5, 10.2
3730.	3857-25-8	1	1	1	2-Furanmethanol, 5-methyl-		2.5, 10.2
3731.	54774-28-6	0	1	0	2-Furanmethanol, 5-methyltetrahydro-		2.5, 10.2
3732.	61481-02-5	1	0	0	2-Furanmethanol, 5-(1-pyrrolidinylmethyl)-		2.5, 10.2, 17.4
3733.	97-99-4	1	1	1	2-Furanmethanol, tetrahydro-		2.5, 10.2
3734.	4412-91-3	1	0	0	3-Furanmethanol		2.5, 10.2
3735.	29848-46-2	1	0	0	3-Furanol, tetrahydro-5,5-dimethyl-		2.5, 10.2
3736.	66607-70-3	0	1	0	3-Furanol, tetrahydro-5-[6-hydroxy-3-(1-methylethyl)-1-heptenyl]-5-methyl-		2.5, 10.2
3737.	20825-71-2	1	1	1	2(3*H*)-Furanone {butenolide}		6.3
3738.		1	0	0	2(3*H*)-Furanone, acetyl-		3.13, 6.3
3739.	517-23-7	1	0	0	2(3*H*)-Furanone, 3-acetyldihydro-		3.13, 6.3
3740.	7400-67-1	1	0	0	2(3*H*)-Furanone, 4-acetyldihydro-		3.13, 6.3
3741.	29393-32-6	1	1	1	2(3*H*)-Furanone, 5-acetyldihydro-		3.13, 6.3
3742.	19405-99-3	1	0	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-		5.3, 6.3
3743.	19405-98-2	1	0	0	2(3*H*)-Furanone, 4-(acetyloxy)dihydro-		5.3, 6.3
3744.		1	0	0	2(3*H*)-Furanone, 4-(acetyloxy)dihydro-5-hydroxy-		2.5, 5.3, 6.3
3745.	26817-24-3	1	0	0	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-		5.3, 6.3
3746.	61892-43-1	1	0	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-4-hydroxy-		2.5, 5.3, 6.3
3747.	61892-44-2	1	0	0	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-4-hydroxy-		2.5, 5.3, 6.3
3748.	160115-54-8	0	1	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1*E*,3S*)]]-		3.13, 5.3, 6.3
3749.	160224-93-1	0	1	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5α(1*E*,3S*)]]-		3.13, 5.3, 6.3
3750.	1192-20-7	1	0	0	2(3*H*)-Furanone, 3-aminodihydro-		6.3, 12.2
3751.		0	1	0	2(3*H*)-Furanone, 3-(3-butenyl)-dihydro-		6.3

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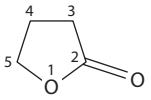
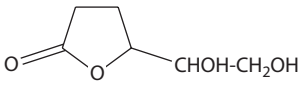
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3752.	104-50-7	0	1	0	2(3*H*)-Furanone, 5-butyldihydro- {γ-octalactone}		6.3, 24.3, 25.29
3753.	39212-23-2	0	1	0	2(3*H*)-Furanone, 5-butyldihydro-4-methyl-		6.3
3754.		1	0	0	2(3*H*)-Furanone, 5-butylidene-		6.3
3755.	96-48-0	1	0	0	2(3*H*)-Furanone, dihydro- {butyrolactone}		6.3, 24.3
3756.	72902-81-9	1	0	0	2(3*H*)-Furanone, dihydro-3, 3-dimethyl-4-hydroxy-		2.5, 6.3
3757.	38273-97-1	0	1	0	2(3*H*)-Furanone, dihydro-3,3-dimethyl-5-(2-oxopropyl)-		3.13, 6.3
3758.	13092-55-2	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-		2.5, 6.3
3759.	17675-99-9	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-, (*Z*)-		2.5, 6.3
3760.	25596-90-1	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy- (3R,4S)		2.5, 6.3
3761.		1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-		2.5, 6.3
3762.	61892-57-7	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-4-methyl-		2.5, 6.3
3763.	63700-30-1	1	0	0	2(3*H*)-Furanone, dihydro-3, 4-dihydroxy-3-methyl-		2.5, 6.3
3764.	18465-71-9	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-, (3R-*Z*)-		2.5, 6.3
3765.		1	0	0	2(3*H*)-Furanone, dihydro-3, 4-dihydroxy-4-methyl-		2.5, 6.3
3766.		1	0	0	2(3*H*)-Furanone, dihydro-3, 4-dihydroxy-5-methyl-		2.5, 6.3
3767.	61989-58-0	1	0	0	2(3*H*)-Furanone, dihydro-5- (1,2-dihydroxyethyl)-		2.5, 6.3
3768.	72693-07-3	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dimethyl-		6.3
3769.	5145-01-7	1	1	1	2(3*H*)-Furanone, dihydro-3,5-dimethyl-		6.3
3770.	13861-97-7	0	1	0	2(3*H*)-Furanone, dihydro-4,4-dimethyl-		6.3
3771.		1	0	0	2(3*H*)-Furanone, dihydro-4,4-dimethyl-5-hydroxymethyl-		2.5, 6.3
3772.	6971-63-7	1	1	1	2(3*H*)-Furanone, dihydro-4,5-dimethyl-		6.3
3773.	90026-55-4	1	1	1	2(3*H*)-Furanone, dihydro-4, 5-dimethyl-, (4*R*-Z)-		6.3
3774.	110171-22-7	1	0	0	2(3*H*)-Furanone, dihydro-4, 5-dimethyl-, (4R-*E*)-		6.3
3775.	3123-97-5	0	1	0	2(3*H*)-Furanone, dihydro-5,5-dimethyl-		6.3
3776.		0	1	0	2(3*H*)-Furanone, dihydro-5- (1,4-dimethyl-1-pentenyl)-		6.3
3777.	1073-11-6	0	1	0	2(3*H*)-Furanone, dihydro-5-ethenyl-5-methyl-		6.3
3778.	16496-51-8	1	1	1	2(3*H*)-Furanone, dihydro-4-ethyl-		6.3
3779.	695-06-7	1	1	1	2(3*H*)-Furanone, dihydro-5-ethyl- {γ-hexalactone}		6.3, 24.3, 25.29
3780.	2610-98-2	0	1	0	2(3*H*)-Furanone, dihydro-5-ethyl-3-methyl-		6.3
3781.	2865-82-9	0	1	0	2(3*H*)-Furanone, dihydro-5-ethyl-5-methyl-		6.3
3782.	158815-74-8	0	1	0	2(3*H*)-Furanone, dihydro-5- (3-ethyl-4-methyl-1-pentenyl)-3-hydroxy-5-methyl-		2.5, 6.3

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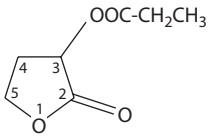
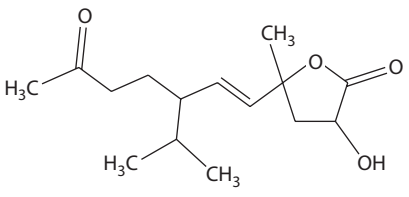
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3783.	61892-46-4	1	0	0	2(3*H*)-Furanone, dihydro-4-ethynyl-5-hydroxy-3-methyl-		2.5, 6.3
3784.		0	1	0	2(3*H*)-Furanone, dihydro-5-(5-heptenyl)-		6.3
3785.	104-67-6	0	1	0	2(3*H*)-Furanone, dihydro-5-heptyl- {γ-undecalactone}		6.3
3786.	706-14-9	0	1	0	2(3*H*)-Furanone, dihydro-5-hexyl- {γ-decalactone}		6.3, 24.3, 25.29
3787.		1	0	0	2(3*H*)-Furanone, dihydro(hydroxy)-		2.5, 6.3
3788.		1	0	0	2(3*H*)-Furanone, dihydro(hydroxymethyl)-		2.5, 6.3
3789.	18132-98-4	1	0	0	2(3*H*)-Furanone, dihydro-3-(hydroxymethyl)-		2.5, 6.3
3790.	1608-63-5	0	1	0	2(3*H*)-Furanone, dihydro-3-(1-methylethyl)-		6.3
3791.	60016-73-1	1	1	1	2(3*H*)-Furanone, dihydro-(2-oxopropyl)-		3.13, 6.3
3792.	25600-22-0	1	0	0	2(3*H*)-Furanone, dihydro-3-(1-oxopropoxy)-		5.3, 6.3
3793.	71385-84-7	1	1	1	2(3*H*)-Furanone, dihydro-3-(2-oxopropyl)-		3.13, 6.3
3794.	65331-00-2	1	0	0	2(3*H*)-Furanone, dihydro-4-(2-oxopropyl)-		3.13, 6.3
3795.	61892-49-7	1	0	0	2(3*H*)-Furanone, dihydro-5-(1-oxopropyl)-		3.13, 6.3
3796.	85564-78-9	1	0	0	2(3*H*)-Furanone, dihydro-3,4,5-trimethyl-		6.3
3797.	53155-68-3	0	1	0	2(3*H*)-Furanone, dihydro-3,4,5-trimethyl-, (3α,4α,5α)-		6.3
3798.	19444-84-9	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-		2.5, 6.3
3799.	25600-22-0	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-, propanoate		5.3, 6.3
3800.	19444-86-1	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-3-(hydroxymethyl)-		2.5, 6.3
3801.	1192-42-3	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-3-methyl-		2.5, 6.3
3802.	6969-43-3	0	1	0	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4,5-trimethyl-		2.5, 6.3
3803.	52126-90-6	1	1	1	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-		2.5, 6.3
3804.	599-04-2	1	1	1	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (R)-		2.5, 6.3
3805.		1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(1-hydroxyethyl)-		2.5, 6.3
3806.		1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(1-hydroxyethyl)- {isomer}		2.5, 6.3
3807.	61892-52-2	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-		2.5, 6.3
3808.	61892-50-0	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-5-methyl-		2.5, 6.3
3809.	53561-62-9	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-		2.5, 6.3
3810.		1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl- {isomer}		2.5, 6.3
3811.	158815-71-5	0	1	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1*E*,3S*)]]-		2.5, 3.13, 6.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3812.		1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-3,4,4-trimethyl-		2.5, 6.3
3813.	5469-16-9	1	1	1	2(3*H*)-Furanone, dihydro-4-hydroxy-		2.5, 6.3
3814.	3285-47-0	1	0	0	2(3*H*)-Furanone, dihydro-4-hydroxy-3,3-dimethyl-		2.5, 6.3
3815.	61892-45-3	1	0	0	2(3*H*)-Furanone, dihydro-4-hydroxy-3-(hydroxymethyl)-		2.5, 6.3
3816.	36679-81-9	1	1	1	2(3*H*)-Furanone, dihydro-4-(hydroxymethyl)-		2.5, 6.3
3817.	34945-05-6	1	0	0	2(3*H*)-Furanone, dihydro-4-hydroxy-4-methyl-		2.5, 6.3
3818.		0	1	0	2(3*H*)-Furanone, dihydro-4-(2,5,6-trimethyl-5,6-epoxyoctanyl)-		6.3, 10.2
3819.	50768-69-9	1	0	0	2(3*H*)-Furanone, dihydro-5-hydroxy-		2.5, 6.3
3820.	27610-27-1	1	1	1	2(3*H*)-Furanone, dihydro-5-(1-hydroxyethyl)-		2.5, 6.3
3821.	61892-47-5	1	0	0	2(3*H*)-Furanone, dihydro-5-hydroxy-4-methyl-		2.5, 6.3
3822.	10374-51-3	1	1	1	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-		2.5, 6.3
3823.	1679-47-6	0	1	0	2(3*H*)-Furanone, dihydro-3-methyl-		6.3
3824.	1679-49-8	1	1	1	2(3*H*)-Furanone, dihydro-4-methyl-		6.3
3825.	108-29-2	1	1	1	2(3*H*)-Furanone, dihydro-5-methyl- {α-angelica lactone, γ-valerolactone}		6.3, 24.3, 25.29, 26.9
3826.		0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-(3-oxobutyl)-		3.13, 6.3
3827.		0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-(3-methyl-1-butenyl)-		6.3
3828.		0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-		6.3
3829.	80797-69-9	0	1	0	2(3*H*)-Furanone, dihydro-5-(3-methyl-1-butenyl)-		6.3
3830.	2429-94-9	0	1	0	2(3*H*)-Furanone,dihydro-5-(3-methylbutyl)-		6.3
3831.	10547-88-3 150669-60-6	0	1	0	2(3*H*)-Furanone,dihydro-4-(1-methylethyl)-		6.3
3832.	38624-29-2	0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-		6.3
3833.		0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-methyl-1,2-butadienyl)-		6.3
3834.	129742-48-9	0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-, (*E*)-(+)-		3.13, 6.3
3835.	133561-47-4	0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-		3.13, 6.3
3836.	2305-05-7	0	1	0	2(*3H*)-Furanone, dihydro-5-octyl- {γ-dodecalactone}		6.3
3837.	23938-71-8	1	0	0	2(3*H*)-Furanone,dihydro-3-(1-oxopropyl)-		6.3
3838.	76710-90-2	0	1	0	2(3*H*)-Furanone, dihydro-5-(2-pentenyl)-, (*Z*)-		6.3
3839.	104-61-0	1	1	1	2(3*H*)-Furanone, dihydro-5-pentyl- {γ-nonalactone}		6.3, 24.3, 25.29
3840.	105-21-5	1	1	1	2(3*H*)-Furanone, dihydro-5-propyl- {γ-heptalactone}		6.3, 24.3, 25.29
3841.	20971-79-3	1	0	0	2(3*H*)-Furanone, dihydro-5-(3-pyridinyl)-		6.3, 17.7

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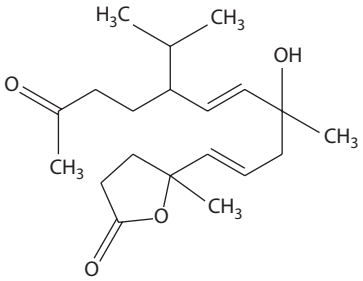
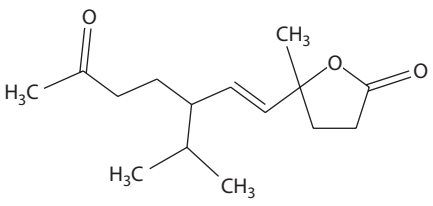
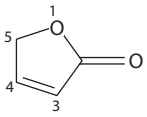
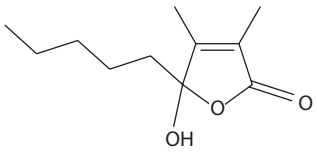
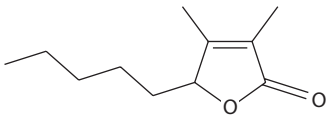
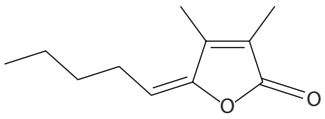
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
3842.	61892-55-5	1	0	0	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-4-methyl-		2.5, 6.3
3843.	72507-34-7	0	1	0	2(3*H*)-Furanone, dihydro-5-[1-methyl-4-(1-methylethyl)-7-oxo-2-octenyl]-		3.13, 6.3
3844.	102734-52-1	0	1	0	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-, [5S-[5R*(1*E*,4R*,5*E*,7R*)]]-		2.5, 3.13, 6.3
3845.	102734-53-2	0	1	0	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1, 5-undecadienyl]-5-methyl-, [5S-[5R*(1*E*,4S*,5*E*,7R*)]]-		2.5, 3.13, 6.3
3846.	102734-54-3	0	1	0	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1, 5-undecadienyl]-5-methyl-, [5R-[5R*(1*E*,4S*,5*E*,7S*)]]-		2.5, 3.13, 6.3
3847.	102734-55-4	0	1	0	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1, 5-undecadienyl]-5-methyl-, [5R-[5R*(1*E*,4R*,5*E*,7S*)]]-		2.5, 3.13, 6.3
3848.	80744-25-8	0	1	0	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-		2.5, 3.13, 6.3
3849.		0	1	0	2(3*H*)-Furanone,dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1, 5-undecadienyl]-5-methyl- {stereoisomer}		2.5, 3.13, 6.3
3850.		0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-(5-methyl-2-furanyl)-		6.3, 10.2
3851.	60646-31-3	1	0	0	2(3*H*)-Furanone, dihydro-5-methyl-5-(1-methylethyl)-, (S)-		6.3
3852.	57213-51-1	0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-		3.13, 6.3
3853.	3284-93-3	0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-propyl-		6.3
3854.	10008-73-8	1	0	0	2(3*H*)-Furanone, dihydro-5-methylene-		6.3
3855.		0	1	0	2(3*H*)-Furanone, dihydro-5-(1,1,3-trimethyl-2-butenyl)-		6.3
3856.	2981-96-6	1	0	0	2(3*H*)-Furanone, dihydro-4,5,5-trimethyl-		6.3
3857.	64291-81-2	0	1	0	2(3*H*)-Furanone, dihydrodimethyl-		6.3
3858.		0	1	0	2(3*H*)-Furanone, 3,3-dimethyl-		6.3
3859.		1	1	1	2(3*H*)-Furanone, 3,4-dimethyl-		6.3
3860.	61892-58-8	1	0	0	2(3*H*)-Furanone, 3-(hydroxymethyl)-5-methyl-		2.5, 6.3

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3861.	591-12-8	1	1	1	2(3*H*)-Furanone, 5-methyl- {4-hydroxy-3-pentenoic acid lactone, α-angelica lactone}		6.3, 24.3, 25.29
3862.	497-23-4	1	1	1	2(5*H*)-Furanone {crotonolactone}		6.3
3863.		1	0	0	2(5*H*)-Furanone, acetyl-		3.13, 6.3
3864.	80436-91-5	1	0	0	2(5*H*)-Furanone, 3-acetyl-		3.13, 6.3
3865.	61892-42-0	1	0	0	2(5*H*)-Furanone, 3-acetyl-4-methyl-		3.13, 6.3
3866.	38260-27-4	1	0	0	2(5*H*)-Furanone, 4-acetyl-		3.13, 6.3
3867.	61892-53-3	1	0	0	2(5*H*)-Furanone, 5-acetyl-		3.13, 6.3
3868.		1	0	0	2(5*H*)-Furanone, 5-butylidene-		6.3
3869.	14668-67-8	1	0	0	2(5*H*)-Furanone, 3,5-diethyl-		6.3
3870.		1	0	0	2(5*H*)-Furanone, 3,4-dihydroxy-		6.3
3871.	1575-46-8	1	0	0	2(5*H*)-Furanone, 3,4-dimethyl-		6.3
3872.	5584-69-0	1	1	1	2(5*H*)-Furanone, 3,5-dimethyl-		6.3
3873.	10547-85-0	1	1	1	2(5*H*)-Furanone, 4,5-dimethyl-		6.3
3874.	20019-64-1	0	1	0	2(5*H*)-Furanone, 5,5-dimethyl-		6.3
3875.	150669-55-9	0	1	0	2(5*H*)-Furanone, 5,5-dimethyl-4-ethyl-		6.3
3876.	6067-11-4	0	1	0	2(5*H*)-Furanone, 3,4-dimethyl-5-hydroxy-5-pentyl-		2.5, 6.3
3877.	14300-74-4	1	0	0	2(5*H*)-Furanone, 3,4-dimethyl-5-methylene-		6.3
3878.	10547-84-9	1	1	1	2(5*H*)-Furanone, 3,4-dimethyl-5-pentyl- {dihydrobovolide}		6.3
3879.	774-64-1	1	1	1	2(5*H*)-Furanone, 3,4-dimethyl-5-pentylidene- {bovolide}		6.3
3880.	107935-59-1	0	1	0	2(5*H*)-Furanone, 3,4-dimethyl-5-pentylidene-, dihydro derivative		6.3
3881.	66309-74-8	1	0	0	2(5*H*)-Furanone, 3,4-dimethyl-5-(1-propenyl)-		6.3
3882.	66309-75-9	1	0	0	2(5*H*)-Furanone, 5-ethenyl-		6.3
3883.		0	1	0	2(5*H*)-Furanone, 5-ethenyl-3-methyl-		6.3
3884.		0	1	0	2(5*H*)-Furanone, 4-ethyl-		6.3
3885.	2407-43-4	1	1	1	2(5*H*)-Furanone, 5-ethyl-		6.3
3886.	698-10-2	0	1	0	2(5*H*)-Furanone, 5-ethyl-3-hydroxy-4-methyl-		6.3
3887.	14668-66-7	1	0	0	2(5*H*)-Furanone, 3-ethyl-5-methyl-		6.3
3888.	54467-53-7	0	1	0	2(5*H*)-Furanone, 4-ethyl-5-methyl-		6.3
3889.	26329-68-0	1	0	0	2(5*H*)-Furanone, 5-ethyl-3-methyl-		6.3
3890.	52945-87-6	1	0	0	2(5*H*)-Furanone, 5-ethyl-4-methyl-		6.3
3891.	6066-62-2	1	0	0	2(5*H*)-Furanone, 5-ethylidene-3,4-dimethyl-		6.3
3892.	71126-48-2	1	0	0	2(5*H*)-Furanone, 5-ethylidene-3-methyl-, (*Z*)-		6.3
3893.	28664-35-9	0	1	0	2(5*H*)-Furanone, 3-hydroxy-4,5-dimethyl-		2.5, 6.3

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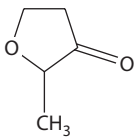
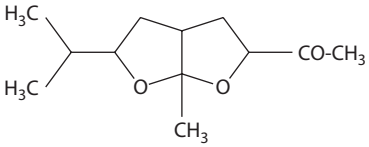
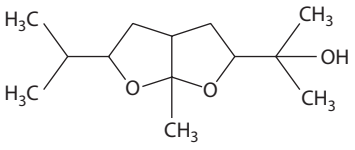
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
3894.		1	0	0	2(5*H*)-Furanone, 3-hydroxy-5-(1-hydroxyethyl)-		2.5, 6.3
3895.	54621-96-4	1	0	0	2(5*H*)-Furanone, 5-(1-hydroxyethyl)-, [R-(R*,S*)]-		2.5, 6.3
3896.		1	0	0	2(5*H*)-Furanone, 3-(hydroxymethyl)-		2.5, 6.3
3897.	80904-75-2	1	0	0	2(5*H*)-Furanone, 4-(hydroxymethyl)-		2.5, 6.3
3898.	22122-36-7	1	1	1	2(5*H*)-Furanone, 3-methyl-		6.3
3899.	6124-79-4	1	1	1	2(5*H*)-Furanone, 4-methyl-		6.3
3900.	591-11-7	1	1	1	2(5*H*)-Furanone, 5-methyl- {β-angelica lactone}		6.3
3901.	108-28-1	1	1	1	2(5H)-Furanone, 5-methylene- {protoanemonin}		6.3
3902.	7754-93-0	0	1	0	2(5*H*)-Furanone, 3-(1-methylethyl)-		6.3
3903.	10547-89-4	1	1	1	2(5*H*)-Furanone, 4-(1-methylethyl)-		6.3
3904.	61892-54-4	1	1	1	2(5*H*)-Furanone, 3-methyl-5-methylene-		6.3
3905.	150669-54-8	0	1	0	2(5*H*)-Furanone, 5-methyl-5-(1-methylethyl)-		6.3
3906.	150669-57-1	0	1	0	2(5*H*)-Furanone, 4-methyl-5-(3-oxobutyl)		3.13, 6.3
3907.		0	1	0	2(5*H*)-Furanone, 5-methyl-4-(3-oxo-4-methylpentyl)-		3.13, 6.3
3908.	150669-53-7	0	1	0	2(5*H*)-Furanone, 4-(4-methyl-1-pentyl)-		6.3
3909.	77267-30-2	0	1	0	2(5*H*)-Furanone, 5-(2-pentenyl)-, (*Z*)-		6.3
3910.	21963-26-8	0	1	0	2(5*H*)-Furanone, 5-pentyl-		6.3
3911.	33488-51-6	1	1	1	2(5*H*)-Furanone, 3,4,5-trimethyl-		6.3
3912.	50598-50-0	0	1	0	2(5*H*)-Furanone, 3,5,5-trimethyl-		6.3
3913.	4182-41-6	0	1	0	2(5*H*)-Furanone, 4,5,5-trimethyl-		6.3
3914.	3511-31-7	1	1	1	3(2*H*)-Furanone		3.13, 10.2
3915.	22929-52-8	1	1	1	3(2*H*)-Furanone, dihydro-		3.13, 10.2
3916.	33909-95-4	1	0	0	3(2*H*)-Furanone, dihydro-2,5-dimethyl-,(*E*)-		3.13, 10.2
3917.	33794-61-5	1	0	0	3(2*H*)-Furanone, dihydro-2,5-dimethyl-,(*Z*)-		3.13, 10.2
3918.	3188-00-9	1	1	1	3(2*H*)-Furanone, dihydro-2-methyl- {2-methyltetrahydrofuran-3-one}		3.13, 10.2, 24.3, 25.29
3919.	89364-27-2	1	1	1	3(2*H*)-Furanone, dihydro-4-methyl-		3.13, 10.2
3920.		0	1	0	3(2*H*)-Furanone, dihydro-5-methyl-5-propyl-		3.13, 10.2
3921.	14400-67-0	1	0	0	3(2*H*)-Furanone, 2,5-dimethyl-		3.13, 10.2
3922.	27538-09-6	0	1	0	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl-		2.5, 3.13, 10.2
3923.	17678-20-5	1	0	0	3(2*H*)-Furanone, 4-hydroxy-2-(hydroxymethyl)-5-methyl-		2.5, 3.13, 10.2
3924.	3658-77-3	1	1	1	3(2*H*)-Furanone, 4-hydroxy-2,5-dimethyl- {furaneol}		2.5, 3.13, 10.2
3925.	484-20-8	0	1	0	7*H*-Furo[3,2-*g*][1]benzopyran-7-one, 4-methoxy-		3.13, 6.3, 10.2
3926.		0	1	0	Furo[3,2-*b*]furan, tetrahydro-2-acetyl-3a-methyl-5-(1-methylethyl)-		3.13, 10.2
3927.		0	1	0	Furo[3,2-*b*]furan-2(3*H*)-methanol, tetrahydro-α,α,3a-trimethyl-5-(1-methylethyl)-		2.5, 10.2

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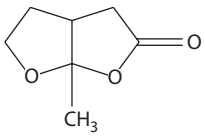
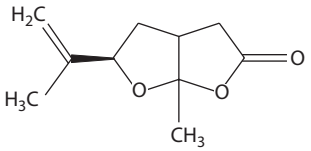
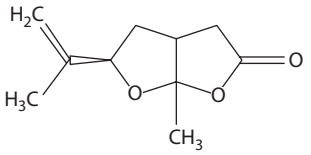
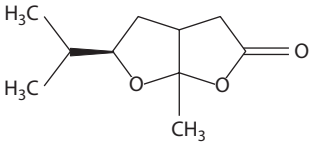
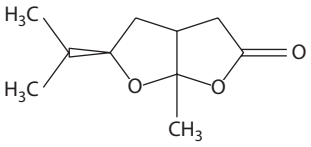
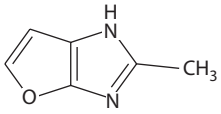
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3928.	60026-27-9	0	1	0	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-		6.3, 10.2
3929.		0	1	0	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethenyl)-		6.3, 10.2
3930.		0	1	0	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethenyl)-		6.3, 10.2
3931.		0	1	0	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethyl)-		6.3, 10.2
3932.		0	1	0	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-5-(1-methylethyl)-		6.3, 10.2
3933.	61893-05-8	1	0	0	1*H*-Furo[2,3-*d*]imidazole, 2-methyl-		10.2, 17.4
3934.	72686-97-6	0	1	0	2*H*-Furo[3,2-*c*] isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, (2α,3aα,5aβ,8β,9aS*)-		2.5, 10.2
3935.	72747-21-8	0	1	0	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, [2R-(2α,3aβ,5aα,8α,9aR*)]-		2.5, 10.2
3936.	37209-50-0	0	1	0	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, acetate, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberin}		5.3, 10.2
3937.	56857-64-8	0	1	0	3a*H*-Furo[3,2-*c*] isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberol}		2.5, 10.2
3938.	7440-54-2	1	1	1	Gadolinium	Gd	20.5
3939.	9037-55-2	0	1	0	*D*-Galactan		2.5, 8.3
3940.	9051-94-9	0	1	0	β-(1→ 4)-*D*-Galactan		2.5, 8.3
3941.	526-99-8	0	1	0	Galactaric acid	$HOOC\text{-}(CHOH)_4\text{-}COOH$	0.4, 2.5, 4.3, 8.3
3942.		0	1	0	Galactitol, 2,3-di-*O*-methyl-	$HOH_2C\text{-}[CH(OCH_3)]_2\text{-}(CHOH)_2\text{-}CH_2OH$	2.5, 10.2

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3943.		0	1	0	Galactitol, 2,4-di-*O*-methyl-		2.5, 10.2
3944.		0	1	0	Galactitol, 2,6-di-*O*-methyl-	$HOH_2C\text{-}CH(OCH_3)\text{-}(CHOH)_3\text{-}CH_2OCH_3$	2.5, 8.3, 10.2
3945.		0	1	0	Galactitol, 2-*O*-methyl-		2.5, 8.3, 10.2
3946.		0	1	0	Galactitol, 3-*O*-methyl-		2.5, 8.3, 10.2
3947.		0	1	0	Galactitol, 2,3,4,6-tetra-*O*-methyl-		2.5, 8.3, 10.2
3948.		0	1	0	Galactitol, 2,3,4-tri-*O*-methyl-		2.5, 8.3, 10.2
3949.		0	1	0	Galactitol, 2,3,6-tri-*O*-methyl-		2.5, 8.3, 10.2
3950.		0	1	0	Galactitol, 2,4,6-tri-*O*-methyl-		2.5, 8.3, 10.2
3951.	9036-66-2	1	1	1	*D*-Galacto-*L*-arabinan		2.5, 8.3, 10.2
3952.	33818-21-2	1	0	0	α-*D*-Galactofuranose, 1,6-anhydro-		2.5, 8.3, 10.2
3953.	107389-81-1	0	1	0	Galactoglucomannan		2.5, 8.3, 10.2
3954.	9040-29-3	0	1	0	*D*-Galacto-*D*-gluco-*D*-mannan		2.5, 8.3, 10.2
3955.	644-76-8	1	0	0	β-*D*-Galactopyranose, 1,6-anhydro-		2.5, 8.3, 10.2
3956.	26656-33-7	0	1	0	*D*-Galactopyranuronic acid, homopolymer		2.5, 8.3, 10.2
3957.	6118-79-2	0	1	0	2-*0*-α-*D*-Galactopyranuronosyl-*L*-mannose, 6-deoxy-		2.5, 8.3, 10.2
3958.	1948-54-5	0	1	0	Galactose, 2-amino-2-deoxy-		2.5, 10.2, 12.2
3959.	35381-83-0	0	1	0	Galactose, diether with 1,2,3-propanetriol (1:2)		2.5, 8.3, 10.2
3960.	59-23-4	1	1	1	*D*-Galactose		0.4, 2.5, 8.3, 10.2, 24.3, 25.29
3961.	7535-00-4	0	1	0	*D*-Galactose, 2-amino-2-deoxy- {galactosamine}		2.5, 8.3, 10.2, 12.2
3962.	1949-89-9	0	1	0	*D*-Galactose, 2-deoxy-		2.5, 8.3, 10.2
3963.	9001-34-7	0	1	0	Galactosidase		22.2
3964.	97234-09-8	0	1	0	*D*-Galactoside, [(1-oxohexadecatrienyl)oxy][(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		2.5, 8.3, 10.2
3965.	97234-10-1	0	1	0	*D*-Galactoside, [(1-oxohexadecyl)oxy][(1-oxooctadecatrienyl)oxy]propyl, (*Z,Z,Z*)-		2.5, 8.3, 10.2
3966.	97276-55-6	0	1	0	*D*-Galactoside, [(1-oxooctadecadienyl)oxy][(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		2.5, 8.3, 10.2
3967.	97232-94-5	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl *O*-*D*-galactosyl-, (all-*Z*)-		2.5, 8.3, 10.2
3968.	97170-15-5	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl, (all-*Z*)-		2.5, 8.3, 10.2
3969.	97233-43-7	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl *O*-*D*-galactosyl-, (all-*Z*)-		2.5, 8.3, 10.2
3970.	97170-14-4	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-		2.5, 8.3, 10.2
3971.	97275-71-3	0	1	0	*D*-Galactoside, 2,3-dihydroxypropyl, 2′(or 3′)-hexadecanoate 3′(or 2′)-octadecadienoate, (*Z,Z*)-		2.5, 8.3, 10.2
3972.	100092-00-0	0	1	0	Galactoxyloglucan {amyloid}		2.5, 8.3, 10.2

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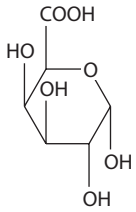
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
3973.	14982-50-4	1	1	1	Galacturonic acid		0.4, 2.5, 4.3, 8.3, 10.2
3974.	25990-10-7	0	1	0	Galacturonic acid, homopolymer		0.4, 2.5, 4.3, 8.3, 10.2
3975.	685-73-4	1	1	1	*D*-Galacturonic acid		2.5, 4.3, 8.3, 10.2
3976.	34150-36-2	0	1	0	*D*-Galacturonic acid, anhydro-		2.5, 4.3, 7.1, 10.2
3977.	25249-06-3	0	1	0	*D*-Galacturonic acid, homopolymer		2.5, 4.3, 7.1, 10.2
3978.	7440-55-3	1	1	1	Gallium		20.5
3979.	152347-17-6	0	1	0	GenBank D16204		22.2
3980.	152347-18-7	0	1	0	GenBank D16205		22.2
3981.	152347-16-5	0	1	0	GenBank D16206		22.2
3982.	143787-54-6	0	1	0	GenBank L02124		22.2
3983.	150472-46-1	0	1	0	GenBank L13439		22.2
3984.	150472-47-2	0	1	0	GenBank L13440		22.2
3985.	150472-48-3	0	1	0	GenBank L13441		22.2
3986.	150472-49-4	0	1	0	GenBank L13442		22.2
3987.	150472-50-7	0	1	0	GenBank L13443		22.2
3988.	149241-78-1	0	1	0	GenBank L14953		22.2
3989.		0	1	0	GenBank M73791		22.2
3990.	144680-39-7	0	1	0	GenBank M74102		22.2
3991.	144680-37-5	0	1	0	GenBank M74103		22.2
3992.	142693-30-9	0	1	0	GenBank M84650		22.2
3993.	145767-36-8	0	1	0	GenBank M87838		22.2
3994.	145767-40-4	0	1	0	GenBank M87839		22.2
3995.	141683-31-0	0	1	0	GenBank M94135		22.2
3996.		0	1	0	GenBank X58527		22.2
3997.	139854-77-6	0	1	0	GenBank X60057		22.2
3998.	140352-16-5	0	1	0	GenBank X61113		22.2
3999.	140352-17-6	0	1	0	GenBank X61114		22.2
4000.	139857-64-0	0	1	0	GenBank X61750		22.2
4001.		0	1	0	GenBank X61826		22.2
4002.	140360-05-0	0	1	0	GenBank X62339		22.2
4003.	141005-27-8	0	1	0	GenBank X62368		22.2
4004.	140104-46-7	0	1	0	GenBank X62395		22.2
4005.		0	1	0	GenBank X62500		22.2
4006.	142965-21-7	0	1	0	GenBank X63078		22.2
4007.	145905-43-7	0	1	0	GenBank X63607		22.2
4008.	139867-08-6	0	1	0	GenBank X64398		22.2
4009.	139869-01-5	0	1	0	GenBank X64399		22.2
4010.	140830-68-8	0	1	0	GenBank X64423		22.2
4011.		0	1	0	GenBank X64621		22.2
4012.	141164-37-6	0	1	0	GenBank X65117		22.2
4013.	141164-36-5	0	1	0	GenBank X65118		22.2
4014.	147904-32-3	0	1	0	GenBank X65982		22.2

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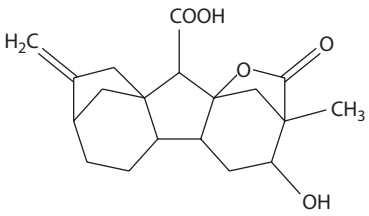
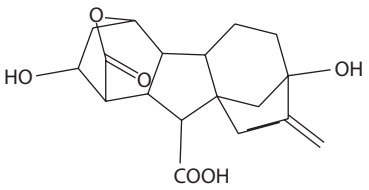
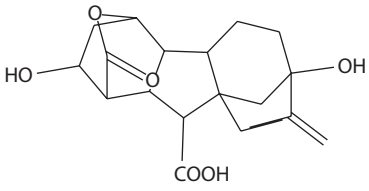
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4015.	144031-18-5	0	1	0	GenBank X66145		22.2
4016.	143341-50-8	0	1	0	GenBank X67158		22.2
4017.	151468-68-7	0	1	0	GenBank X69971		22.2
4018.	148757-17-9	0	1	0	GenBank X71015		22.2
4019.		0	1	0	GenBank Z11803		22.2
4020.	142914-46-3	0	1	0	GenBank Z12619		22.2
4021.	142914-45-2	0	1	0	GenBank Z12623		22.2
4022.	152651-60-0	0	1	0	GenBank Z14079		22.2
4023.	152651-59-7	0	1	0	GenBank Z14080		22.2
4024.	152651-58-6	0	1	0	GenBank Z14081		22.2
4025.	152651-57-5	0	1	0	GenBank Z14082		22.2
4026.	152651-61-1	0	1	0	GenBank Z14085		22.2
4027.	148544-79-0	0	1	0	GenBank Z16403		22.2
4028.	148544-80-3	0	1	0	GenBank Z16404		22.2
4029.	554-91-6	0	1	0	Gentiobiose		0.4, 2.5, 10.2
4030.	7440-56-4	1	1	1	Germanium	Ge	20.5
4031.	19147-78-5	0	1	0	Gibbane-1,10-dicarboxylic acid, 2,3-epoxy-4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,3β,4aα,4bβ,10β)-		2.5, 4.3, 6.3
4032.	545-97-1	0	1	0	Gibbane-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		2.5, 4.3, 6.3
4033.	468-44-0	0	1	0	Gibbane-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-,1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		2.5, 4.3, 6.3
4034.	561-56-8	0	1	0	Gibb-2-ene-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,4aα,4bβ,10β)-		2.5, 4.3, 6.3
4035.	77-06-5	0	1	0	Gibb-3-ene-1,10-dicarboxylicacid,2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)- {gibberellic acid}		2.5, 4.3, 6.3
4036.	125-67-7	0	1	0	Gibb-3-ene-1,10-dicarboxylic acid, 2, 4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, potassium salt {gibberellic acid, potassium salt}		2.5, 6.3, 20.6, 21.3
4037.	510-75-8	0	1	0	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-		2.5, 4.3, 6.3
4038.	9007-83-4	0	1	0	Globulins, γ-		20.6, 22.2

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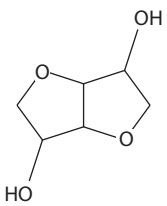
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4039.	9037-91-6	0	1	0	Glucan		2.5, 8.3
4040.	9012-72-0	0	1	0	β-(1,3)-*D*-Glucan {glucan}		2.5, 8.3
4041.	9051-97-2	0	1	0	β-*D*-Glucan, (1→3)-		2.5, 8.3
4042.	9044-93-3	0	1	0	β-1,3-Glucanase		22.2
4043.	9025-37-0	0	1	0	Glucanase, endo-1,3-β-		22.2
4044.	128512-83-4	0	1	0	Glucanase, endo-1,3-β-(tobacco clone pGL31 isoenzyme)		22.2
4045.	128512-84-5	0	1	0	Glucanase, endo-1,3-β- (tobacco clone pGL36 isoenzyme)		22.2
4046.	128512-85-6	0	1	0	Glucanase, endo-1,3-β- (tobacco clone pGL43 isoenzyme)		22.2
4047.	128512-86-7	0	1	0	Glucanase, endo-1,3-β- (tobacco isoenzyme)		22.2
4048.	62213-14-3	0	1	0	Glucanase, endo-1,3(4)-β-		22.2
4049.	117277-96-0	0	1	0	Glucanase, preproendo-1,3-β-		22.2
4050.	128475-00-3	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme signal peptide)		22.2
4051.	128475-01-4	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme signal peptide) 26-*L*-threonine-28-*L*-glutamic acid		22.2
4052.	128512-87-8	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme protein moiety)		22.2
4053.	128512-88-9	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGluc39.3 isoenzyme protein moiety)		22.2
4054.	128512-89-0	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pGL31 isoenzyme protein moiety)		22.2
4055.	128512-90-3	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pGL36 isoenzyme protein moiety)		22.2
4056.	128512-91-4	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pGL43 isoenzyme protein moiety)		22.2
4057.	128512-92-5	0	1	0	Glucanase, preproendo-1,3-β- (tobacco isoenzyme protein moiety)		22.2
4058.	117277-97-1	0	1	0	Glucanase, proendo-1,3-β-		22.2
4059.	652-67-5	1	0	0	*D*-Glucitol, 1,4:3,6-dianhydro-		2.5, 10.2
4060.	7425-74-3	1	1	1	β-*D*-Glucofuranose, 1,6-anhydro-		2.5, 8.3, 10.2
4061.	4451-30-3	1	1	1	β-*D*-Glucofuranose, 1,5:3,6-dianhydro-		2.5, 8.3, 10.2
4062.	66537-22-2	1	1	1	Glucometasaccharinic acid, γ-lactone		2.5, 6.3, 8.3, 10.2

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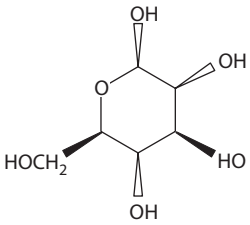
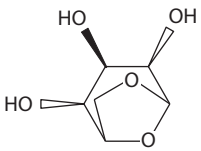
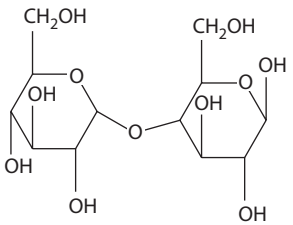
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4063.	492-62-6	0	1	0	α-*D*-Glucopyranose		2.5, 8.3, 10.2
4064.	492-61-5	1	1	1	β-*D*-Glucopyranose		2.5, 8.3, 10.2
4065.		0	1	0	α-*D*-Glucopyranose, 1-acetate 2,3,4,6-tetrakis((+)-3-methylbutanoate)		2.5, 5.3, 8.3, 10.2
4066.	28977-67-5	1	1	1	β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylvalerate) = β-*D*-glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylpentanoate)		2.5, 5.3, 8.3, 10.2
4067.	60517-74-0	0	1	0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)		2.5, 5.3, 8.3, 9.22, 10.2
4068.	25545-13-5	0	1	0	*D*-Glucopyranose, 4-(4-hydroxybenzoate)		2.5, 5.3, 8.3, 9.22, 10.2
4069.	23445-11-6	0	1	0	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)		2.5, 5.3, 8.3, 9.22, 10.2
4070.	41682-52-4	0	1	0	β-*D*-Glucopyranose, 1-(3-phenyl-2-propenoate)		2.5, 5.3, 8.3, 10.2
4071.	59-56-3	0	1	0	α-*D*-Glucopyranose, 1-(dihydrogen phosphate)		2.5, 5.3, 8.3, 10.2
4072.	498-07-7	1	1	1	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan}		0.4, 2.5, 8.3, 10.2, 25.29
4073.	61891-55-2	1	0	0	β-*D*-Glucopyranose, 1,6-anhydro-, monoacetate		2.5, 5.3, 8.3, 10.2
4074.	10139-18-1	0	1	0	α-*D*-Glucopyranose, 1,6-bis (dihydrogen phosphate)		2.5, 5.3, 8.3, 10.2
4075.	21056-52-0	0	1	0	β-*D*-Glucopyranose, 1-benzoate		2.5, 5.3, 8.3, 10.2
4076.	69-79-4 4482-75-1 9005-84-9	0	1	0	α-*D*-Glucopyranose,4-*O*-α-*D*-glucopyranosyl- {amylodextrin, α-maltose}		0.4, 2.5, 8.3, 10.2, 25.29
4077.		0	1	0	α-*D*-Glucopyranose, 1,2,3,4,5-penta((+)-3-methylbutanoate)		5.3, 8.3, 10.2
4078.		0	1	0	α-*D*-Glucopyranose, 1,3,4,6-tetrakis((+)-3-methylbutanoate)		5.3, 8.3, 10.2
4079.		0	1	0	α-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		5.3, 8.3, 10.2
4080.		0	1	0	β-*D*-Glucopyranose, 2,3,4,5-tetrakis((+)-3-methylbutanoate)		5.3, 8.3, 10.2
4081.	133-99-3	0	1	0	β-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {β-maltose}		2.5, 8.3, 10.2

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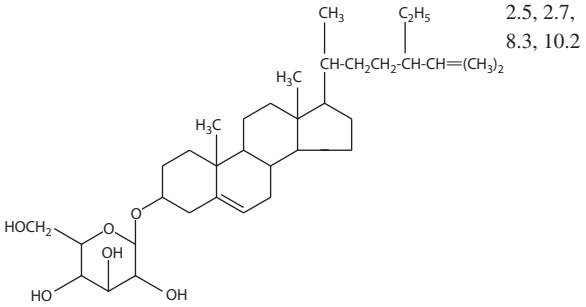
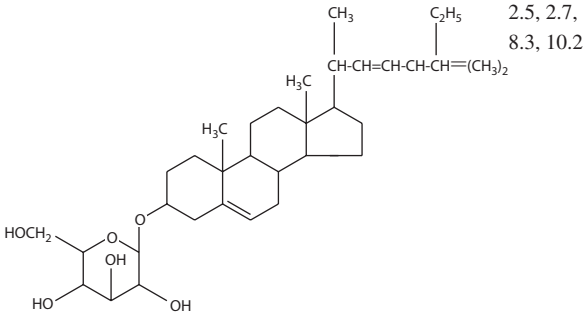
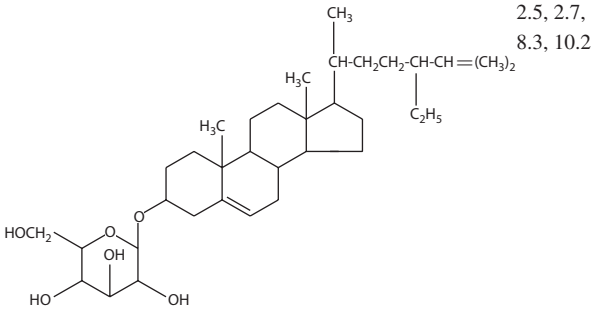
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4082.	64461-84-3	0	1	0	β-*D*-Glucopyranose, 6-(3-phenyl-2-propenoate)		5.3, 8.3, 10.2
4083.	7724-09-6	0	1	0	β-*D*-Glucopyranoside, (2-hydroxyphenyl)methyl-		2.5, 8.3, 9.22, 10.2
4084.	7073-61-2	1	1	1	β-*D*-Glucopyranoside, (3β)-cholest-5-en-3-yl- {cholesteryl glucoside}		2.5, 2.7, 8.3, 10.2
4085.	32214-82-7	1	1	1	β-*D*-Glucopyranoside, (3β)-ergost-5-en-3-yl- {campesteryl glucoside}		2.5, 2.7, 8.3, 10.2
4086.		0	1	0	β-*D*-Glucopyranoside, 3-hexen-1-yl- {3-hexen-1-yl glucoside, leaf acid glucoside}		2.5, 8.3, 10.2
4087.	474-58-8	1	1	1	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl- {β-sitosteryl glucoside}		2.5, 2.7, 8.3, 10.2
4088.	19716-26-8	1	1	1	β-*D*-Glucopyranoside, (3β,22*E*)-stigmasta-5,22-dien-3-yl- {stigmasteryl glucoside}		2.5, 2.7, 8.3, 10.2
4089.	51064-38-1	1	1	1	β-*D*-Glucopyranoside, (3β,24S)-stigmast-5-en-3-yl- {γ-sitosteryl glucoside}		2.5, 2.7, 8.3, 10.2

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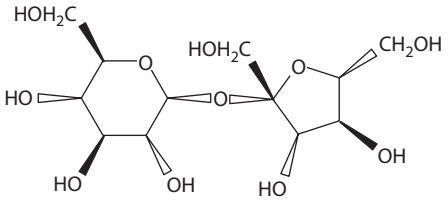
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4090.	57-50-1	1	1	1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose}		0.4, 2.5, 8.3, 10.2, 24.3, 25.29
4091.		0	1	0	^{14}C- α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose-^{14}C}		25.29
4092.	126-14-7	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate		2.5, 5.3, 8.3, 10.2
4093.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-		2.5, 5.3, 8.3, 10.2
4094.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-3′-acetyl-		2.5, 5.3, 8.3, 10.2
4095.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-*O*-acetyl-2,3,4-tri-*O*-acyl-4′-acetyl-		2.5, 5.3, 8.3, 10.2
4096.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-		2.5, 5.3, 8.3, 10.2
4097.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′-*O*-acetyl-		2.5, 5.3, 8.3, 10.2
4098.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-4′-*O*-acetyl-		2.5, 5.3, 8.3, 10.2
4099.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-3′,4′-*O*-diacetyl-		2.5, 5.3, 8.3, 10.2
4100.		0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 2,3,4-tri-*O*-acyl-1′,3′,4′-*O*-triacetyl-		2.5, 5.3, 8.3, 10.2
4101.	470-55-3	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→ 6)-*O*-α-*D*-galactopyranosyl-(1→6)-		2.5, 8.3, 10.2
4102.	512-69-6	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1→6)- {raffinose}		2.5, 8.3, 10.2
4103.	13101-54-7	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→4)- {erlose}		2.5, 8.3, 10.2
4104.	25954-44-3	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-β-*D*-glucopyranosyl-(1→6)-		2.5, 8.3, 10.2
4105.	98913-58-7	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 3-methylpentanoate		2.5, 5.3, 8.3, 10.2
4106.	154063-13-5	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(2-methylbutanoate)		2.5, 5.3, 8.3, 10.2
4107.	97614-61-4	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(3-methylpentanoate)		2.5, 5.3, 8.3, 10.2

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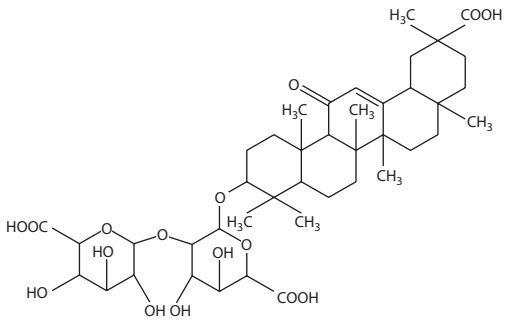
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4108.	106033-38-9	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(3-methylpentanoate), [2(S),3(S),4(S)]-		2.5, 5.3, 8.3, 10.2
4109.	41055-68-9	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, labeled with ^{13}C		2.5, 8.3, 10.2
4110.	21291-36-1	0	1	0	α-*D*-Glucopyranoside,β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→6)-		2.5, 8.3, 10.2
4111.	88848-61-7	0	1	0	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl 2-*O*-β-*D*-glucopyranosyl-, [1S-(1α,2β,3α,7β)]-		2.5, 8.3, 10.2
4112.	99499-89-5	0	1	0	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl *O*-6-deoxy-α-*L*-mannopyranosyl-(1→4)-*O*-β-*D*-glucopyranosyl-(1→4)-, [1S-(1α,2β,3α,7β)]-		2.5, 8.3, 10.2
4113.	138-52-3	0	1	0	β-*D*-Glucopyranoside, 2-(hydroxymethyl)phenyl-		2.5, 8.3, 10.2
4114.	136448-99-2	0	1	0	β-*D*-Glucopyranoside, 2-[5-(acetyloxy)-1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl]-2-hydroxypropyl-, 2,3,4,6-tetraacetate, [2R-[2α(S*),5α,8β,8aα]]-		2.5, 5.3, 8.3, 10.2
4115.	75039-16-6	0	1	0	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl-, mono (dihydrogen phosphate) (ester), (*E*)-		2.5, 5.3, 8.3, 10.2, 12.2, 17.23
4116.	62512-96-3	0	1	0	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)butyl-		2.5, 8.3, 10.2, 17.23
4117.	78081-83-1	0	1	0	β-*D*-Glucopyranoside, 3-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo [4.1.0]hept-1-yl)-1-methyl-2-propenyl-		2.5, 8.3, 10.2
4118.	63648-83-9	0	1	0	α-*D*-Glucopyranoside, 3-*O*-acetyl-β-*D*-fructofuranosyl-		2.5, 8.3, 10.2
4119.	470-57-5	0	1	0	α-*D*-Glucopyranoside, *O*-α-*D*-galactopyranosyl-(1→6)-β-*D*-fructofuranosyl- {theanderose}		2.5, 8.3, 10.2
4120.	1464-44-4	0	1	0	β-*D*-Glucopyranoside, phenyl-		2.5, 8.3, 10.2
4121.	1405-86-3	0	1	0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid, glycyrrhizin}		2.5, 3.13, 4.3, 8.3, 10.2

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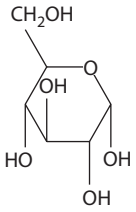
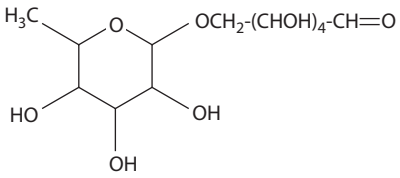
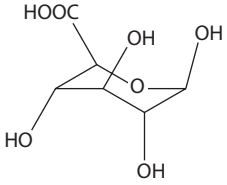
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4122.	53956-04-0	0	1	0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated, glycyrrhizin ammoniated}		2.5, 3.13, 8.3, 10.2
4123.	50-99-7 26655-34-5	1	1	1	α-*D*-Glucose		0.4, 2.5, 8.3, 10.2, 24.3, 25.29
4124.	110187-42-3	0	1	0	Glucose, labeled with ^{13}C {glucose-^{13}C}		2.5, 8.3, 10.2
4125.	9050-36-6	1	1	1	α-*D*-Glucose, labeled with ^{14}C {α-*D*-glucose-^{14}C}		2.5, 8.3, 10.2, 25.29
4126.	3416-24-8	0	1	0	*D*-Glucose, 2-deoxy-, 2-amino- {glucosamine}		2.5, 8.3, 10.2, 12.2
4127.	1398-61-4	0	1	0	*D*-Glucose,β-(1,4)-2-acetamido-2-deoxy-		2.5, 8.3, 10.2, 13.1
4128.	90-74-4	0	1	0	*D*-Glucose, *6-O*-(6-deoxy-α-*L*-mannopyranosyl)- {rutinose}		2.5, 3.12, 8.3, 10.2
4129.	28905-12-6	1	1	1	β-*D*-Glucose		2.5, 8.3, 10.2
4130.	9001-22-3	0	1	0	Glucosidase, β- {emulsin, amygdalase, synaptase}		22.2
4131.	9001-42-7	0	1	0	Glucosidase, α- {maltase}		22.2
4132.	9012-47-9	0	1	0	Glucosidase, amylo-1,6-		22.2
4133.	9031-48-5	0	1	0	Glucosyltransferase		22.2
4134.	9027-19-4	0	1	0	Glucosyltransferase, uridine diphosphoglucose-1,4-β-glucan		22.2
4135.	50812-18-5	0	1	0	β-*D*-Glucosyltransferase, uridine diphosphoglucose-flavonol 3-*O*-glucoside		22.2
4136.	9030-05-1	0	1	0	Glucosyltransferase, uridine diphosphoglucose-fructose		22.2
4137.	9030-06-2	0	1	0	Glucosyltransferase, uridine diphosphoglucose-fructose phosphate		22.2
4138.	146480-37-7 156859-11-9	0	1	0	Glucosyltransferase, uridine diphosphoglucose-salicylate 3-		22.2
4139.	37294-28-3	1	1	1	Glucoxylan		2.5, 8.3, 10.2
4140.	576-37-4	1	1	1	Glucuronic acid		0.4, 2.5, 4.3, 8.3, 10.2, 25.29
4141.	6556-12-3	0	1	0	*D*-Glucuronic acid		2.5, 4.3, 8.3, 10.2
4142.	14984-34-0	0	1	0	*D*-Glucuronic acid, monosodium salt		20.6

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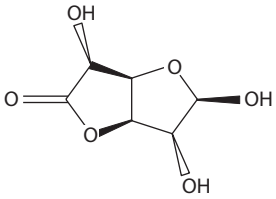
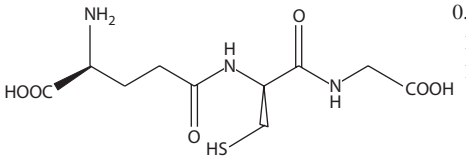
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4143.	28905-07-9	0	1	0	α-*D*-Glucuronic acid, methyl ester		2.5, 5.3, 8.3, 10.2
4144.	9001-45-0	0	1	0	Glucuronidase, β-		22.2
4145.	66369-21-9	0	1	0	Glucuronoarabinoxylan		2.5, 8.3, 10.2
4146.	32449-92-6	0	1	0	*D*-Glucurono-3,6-lactone		2.5, 6.3, 8.3, 10.2
4147.	62930-75-0	0	1	0	Glucuronomannan		2.5, 8.3, 10.2
4148.	77272-02-7	0	1	0	Glucuronomannoarabinan		2.5, 8.3, 10.2
4149.	37317-38-7	0	1	0	Glucuronoxylan		2.5, 8.3, 10.2
4150.	6899-05-4	1	1	1	Glutamic acid	$HOOC\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 24.3, 25.29
4151.	56-86-0	1	1	1	*L*-Glutamic acid		4.3, 4.10, 12.2
4152.	997-68-2	0	1	0	*L*-Glutamic acid, *N*-(5-amino-5-carboxypentyl)-, (S)-		4.3, 4.10, 12.2
4153.	58-05-9	0	1	0	*L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-		3.13, 4.3, 4.10, 12.2
4154.	1116-22-9	0	1	0	*L*-Glutamic acid, *N*-*L*-γ-glutamyl-		4.3, 4.10, 12.2
4155.	3929-61-1	0	1	0	*L*-Glutamic acid, *N*-*L*-α-glutamyl-		4.3, 4.10, 12.2
4156.	6899-04-3	0	1	0	Glutamine	$H_2N\text{-}OC\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 12.2, 13.1
4157.	56-85-9	1	1	1	*L*-Glutamine		0.4, 4.3, 4.10, 12.2, 13.1, 24.3
4158.	9046-27-9	0	1	0	Glutamyltransferase, γ-		22.2
4159.	9061-41-0	0	1	0	Glutenin		22..2
4160.	56-40-6	1	1	1	Glycine	$H_2N\text{-}CH_2\text{-}COOH$	0.4, 4.3, 4.10, 12.2, 25.29
4161.	18875-39-3	0	1	0	Glycine, labeled with ^{14}C {glycine-^{14}C}		4.3, 4.10, 12.2
4162.	4429-05-4	0	1	0	Glycine, *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 10.2, 12.2
4163.	88476-94-2	0	1	0	Glycine, *N*-(1-nitroso-*L*-prolyl)-		4.3, 4.10, 12.2, 13.1, 15.8, 17.4
4164.	70-18-8	0	1	0	Glycine, *N*-(*N*-*L*-γ-glutamyl-*L*-cysteinyl)- {glutathione}		0.4, 4.3, 4.10, 12.2, 13.1, 18.1
4165.	1071-83-6	0	1	0	Glycine, *N*-(phosphonomethyl)-		4.3, 4.10, 12.2
4166.	1118-68-9	0	1	0	Glycine, *N,N*-dimethyl-	$(H_3C)_2{=}N\text{-}CH_2\text{-}COOH$	4.3, 4.10, 12.2
4167.	73360-07-3	0	1	0	Glycine, *N*-[2-(2-aminoethoxy)ethenyl]-		4.3, 4.10, 10.2, 12.2
4168.	19246-18-5	0	1	0	Glycine, *N*-*L*-cysteinyl-		4.3, 4.10, 12.2, 18.1

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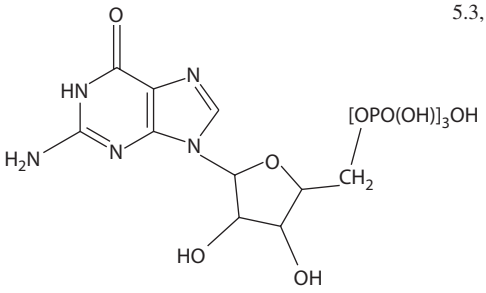
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4169.	20661-60-3	0	1	0	Glycine, *N*-methyl-*N*-nitro-		4.3, 4.10, 12.2, 16.1
4170.	13256-22-9	1	1	1	Glycine, *N*-methyl-*N*-nitroso- {NSAR}	H_3C-N(NO)-CH_2-COOH	4.3, 4.10, 12.2, 15.8, 23.5
4171.		1	1	1	Glycine, *N*-methyl-*N*-nitroso-, methyl ester	H_3C-N(NO)-CH_2-COO CH_3	5.3, 12.2, 15.8
4172.		0	1	0	Glycolase		0.4, 22.2
4173.	83534-39-8	0	1	0	Glycosidase		22.2
4174.	9001-97-2	0	1	0	Glycosyltransferase, α-glucan-branching		22.2
4175.	37347-76-5	0	1	0	Glyoxalase		22.2
4176.	7440-57-5	1	1	1	Gold	Au	20.5
4177.	306-60-5	0	1	0	Guanidine, (4-aminobutyl)-		12.2
4178.	86-01-1	0	1	0	Guanosine 5′-(tetrahydrogen triphosphate)		5.3, 12.2, 17.23
4179.	7440-58-6	1	1	1	Hafnium	Hf	20.5
4180.	9034-32-6	0	1	0	Hemicellulose		0.4, 2.5, 8.3, 10.2, 25.29
4181.	63100-39-0	0	1	0	Hemicellulose A		2.5, 8.3, 10.2
4182.	63100-40-3	0	1	0	Hemicellulose B		2.5, 8.3, 10.2
4183.	65058-12-0	0	1	0	Hemicellulose C		2.5, 8.3, 10.2
4184.	629-94-7	1	1	1	Heneicosane	H_3C-$(CH_2)_{19}$-CH_3	1.10
4185.	1560-82-3	1	1	1	Heneicosane, 2-methyl-	H_3C-$CH(CH_3)$-$(CH_2)_{18}$-CH_3	1.10
4186.	6418-47-9	1	0	0	Heneicosane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{17}$-CH_3	1.10
4187.	2363-71-5	1	1	1	Heneicosanoic acid	H_3C-$(CH_2)_{19}$-COOH	4.3
4188.	42233-02-3	1	1	1	Heneicosanoic acid, docosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{21}$-CH_3	5.3
4189.	42232-93-9	1	1	1	Heneicosanoic acid, dodecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{11}$-CH_3	5.3
4190.	42233-00-1	1	1	1	Heneicosanoic acid, eicosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{19}$-CH_3	5.3
4191.	42233-01-2	1	1	1	Heneicosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{20}$-CH_3	5.3
4192.		1	1	1	Heneicosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{26}$-CH_3	5.3
4193.	42232-98-4	1	1	1	Heneicosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{16}$-CH_3	5.3
4194.		1	0	0	Heneicosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{25}$-CH_3	5.3
4195.	42232-97-3	1	1	1	Heneicosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{15}$-CH_3	5.3
4196.	42232-99-5	1	1	1	Heneicosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{18}$-CH_3	5.3
4197.	121878-00-0	1	1	1	Heneicosanoic acid, octacosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{27}$-CH_3	5.3
4198.		1	0	0	Heneicosanoic acid, octadecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{17}$-CH_3	5.3
4199.		1	1	1	Heneicosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{24}$-CH_3	5.3
4200.	42232-96-2	1	1	1	Heneicosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{14}$-CH_3	5.3
4201.	42233-04-5	1	1	1	Heneicosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{23}$-CH_3	5.3
4202.	42232-95-1	1	1	1	Heneicosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{13}$-CH_3	5.3
4203.	42233-03-4	1	1	1	Heneicosanoic acid, tricosyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{22}$-CH_3	5.3
4204.	42232-94-0	1	1	1	Heneicosanoic acid, tridecyl ester	H_3C-$(CH_2)_{19}$-COO-$(CH_2)_{12}$-CH_3	5.3
4205.	36332-94-2	1	1	1	Heneicosanoic acid, 19-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{17}$-COOH	4.3
4206.	121877-70-1	1	1	1	Heneicosanoic acid, 19-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{17}$-COO-$(CH_2)_{21}$-CH_3	5.3
4207.	121877-61-0	1	1	1	Heneicosanoic acid, 19-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{17}$-COO-$(CH_2)_{20}$-CH_3	5.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4208.	6704-01-4	1	1	1	Heneicosanoic acid, 20-methyl-	$(H_3C)_2$═CH-$(CH_2)_{18}$-COOH	4.3
4209.	71278-17-6	1	0	0	Heneicosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester		5.3
4210.	15594-90-8	1	1	1	1-Heneicosanol	H_3C-$(CH_2)_{19}$-CH_2OH	2.5
4211.	27400-79-9	1	0	0	Heneicosene		1.11
4212.	1599-68-4	1	0	0	1-Heneicosene	H_3C-$(CH_2)_{18}$-CH═CH_2	1.11
4213.		1	0	0	1-Heneicosene, 2-methyl-	H_2C═$C(CH_3)$-$(CH_2)_{18}$-CH_3	1.11
4214.		1	0	0	2-Heneicosene, (*Z*)-	H_3C-CH═CH-$(CH_2)_{17}$-CH_3	1.11
4215.		1	0	0	2-Heneicosene, (*E*)-		1.11
4216.		1	0	0	2-Heneicosene, 2-methyl-	H_3C-$C(CH_3)$H═CH-$(CH_2)_{17}$-CH_3	1.11
4217.		1	0	0	2-Heneicosene, 19-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{15}$-$CH(CH_3)$-CH_2-CH_3	1.11
4218.		1	0	0	2-Heneicosene, 19-methyl-, (*E*)-		1.11
4219.		1	0	0	2-Heneicosene, 20-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{16}$-$CH(CH_3)_2$	1.11
4220.		1	0	0	2-Heneicosene, 20-methyl-, (*E*)-		1.11
4221.	28984-67-0	1	1	1	Heneicosenoic acid		4.3
4222.	66288-40-2	1	0	0	Heneicosenoic acid, 19-methyl-		4.3
4223.	66288-41-3	1	0	0	Heneicosenoic acid, 20-methyl-		4.3
4224.	7194-87-8	1	0	0	Hentetracontane	H_3C-$(CH_2)_{39}$-CH_3	1.10
4225.	6704-02-5	1	0	0	5,9,13,17,21,25,29-Hentriacontaheptaen-2-one, 6,10,14,18,22,26,30-heptamethyl-		3.13
4226.	630-04-6	1	1	1	Hentriacontane	H_3C-$(CH_2)_{29}$-CH_3	0.4, 1.10, 25.29, 26.9
4227.	1720-12-3	1	1	1	Hentriacontane, 2-methyl-	$(H_3C)_2$═CH-$(CH_2)_{28}$-CH_3	1.10
4228.	4981-99-1	1	1	1	Hentriacontane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{27}$-CH_3	1.10
4229.	38232-01-8	1	0	0	Hentriacontanoic acid	H_3C-$(CH_2)_{29}$-COOH	4.3
4230.	71278-18-7	1	0	0	Hentriacontanoic acid, hentriacontyl ester	H_3C-$(CH_2)_{29}$-COO-$(CH_2)_{30}$-CH_3	5.3
4231.	502-73-8	1	1	1	16-Hentriacontanone	H_3C-$(CH_2)_{14}$-CO-$(CH_2)_{14}$-CH_3	0.4, 3.13
4232.	77046-64-1	1	1	1	Hentriacontene		1.11
4233.	18435-54-6	1	0	0	1-Hentriacontene	H_3C-$(CH_2)_{28}$-CH═CH_2	1.11
4234.		1	0	0	1-Hentriacontene, 2-methyl-	H_2C═$C(CH_3)$-$(CH_2)_{28}$-CH_3	1.11
4235.		1	0	0	2-Hentriacontene, (*Z*)-	H_3C-CH═CH-$(CH_2)_{27}$-CH_3	1.11
4236.		1	0	0	2-Hentriacontene, (*E*)-		1.11
4237.		1	1	1	2-Hentriacontene, 2-methyl-	H_3C-$C(CH_3)$═CH-$(CH_2)_{27}$-CH_3	1.11
4238.		1	0	0	2-Hentriacontene, 29-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{25}$-$CH(CH_3)$-CH_2-CH_3	1.11
4239.		1	0	0	2-Hentriacontene, 29-methyl-, (*E*)-		1.11
4240.		1	0	0	2-Hentriacontene, 30-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{26}$-$CH(CH_3)_2$	1.11
4241.		1	0	0	2-Hentriacontene, 30-methyl-, (*E*)-		1.11
4242.	7719-93-9	1	1	1	Heptacontane	H_3C-$(CH_2)_{35}$-CH_3	1.10
4243.	32304-17-9	1	1	1	5,9,13,17,21,25-Heptacosahexaen-2-one, 6,10,14,18,22,26-hexamethyl-, (all-*E*)-		3.13
4244.	593-49-7	1	1	1	Heptacosane	H_3C-$(CH_2)_{25}$-CH_3	0.4, 1.10
4245.	1561-00-8	1	1	1	Heptacosane, 2-methyl-	$(H_3C)_2$═CH-$(CH_2)_{24}$-CH_3	1.10
4246.	14167-66-9	1	1	1	Heptacosane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{23}$-CH_3	1.10
4247.	7138-40-1	1	0	0	Heptacosanoic acid	H_3C-$(CH_2)_{25}$-COOH	4.3
4248.	121877-96-1	1	1	1	Heptacosanoic acid, docosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{21}$-CH_3	5.3
4249.		1	1	1	Heptacosanoic acid, dodecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{11}$-CH_3	5.3
4250.	117063-83-9	1	1	1	Heptacosanoic acid, eicosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{19}$-CH_3	5.3
4251.		1	1	1	Heptacosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{20}$-CH_3	5.3
4252.		1	1	1	Heptacosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{26}$-CH_3	5.3
4253.		1	1	1	Heptacosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{16}$-CH_3	5.3
4254.		1	1	1	Heptacosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{25}$-CH_3	5.3
4255.		1	1	1	Heptacosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{15}$-CH_3	5.3

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4256.		1	1	1	Heptacosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{18}$-CH_3	5.3
4257.		1	1	1	Heptacosanoic acid, octadecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{17}$-CH_3	5.3
4258.		1	1	1	Heptacosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{24}$-CH_3	5.3
4259.		1	1	1	Heptacosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{14}$-CH_3	5.3
4260.		1	1	1	Heptacosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{231}$-CH_3	5.3
4261.		1	1	1	Heptacosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{13}$-CH_3	5.3
4262.		1	1	1	Heptacosanoic acid, tricosyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{22}$-CH_3	5.3
4263.		1	1	1	Heptacosanoic acid, tridecyl ester	H_3C-$(CH_2)_{25}$-COO-$(CH_2)_{12}$-CH_3	5.3
4264.	121878-01-1	1	1	1	Heptacosanoic acid, 25-methyl-, docosyl ester	H_3C-$CH_2CH(CH_3)$-$(CH_2)_{23}$-COO-$(CH_2)_{21}$-CH_3	5.3
4265.	121877-93-8	1	1	1	Heptacosanoic acid, 25-methyl-, heneicosyl ester	H_3C-$CH_2CH(CH_3)$-$(CH_2)_{23}$-COO-$(CH_2)_{20}$-CH_3	5.3
4266.	2004-39-9	0	1	0	1-Heptacosanol	H_3C-$(CH_2)_{25}$-CH_2OH	2.5
4267.	63785-26-2	0	1	0	1-Heptacosanol, 26-methyl-	$(H_3C)_2$═CH-$(CH_2)_{24}$-CH_2OH	2.5
4268.	542-50-7	0	1	0	14-Heptacosanone	H_3C-$(CH_2)_{12}$-CO-$(CH_2)_{12}$-CH_3	3.13
4269.	67537-80-8	1	0	0	Heptacosene		1.11
4270.	15306-27-1	1	0	0	1-Heptacosene	H_3C-$(CH_2)_{24}$-CH═CH_2	1.11
4271.		1	0	0	2-Heptacosene, (*Z*)-	H_3C-CH═CH-$(CH_2)_{23}$-CH_3	1.11
4272.		1	0	0	2-Heptacosene, (*E*)-		1.11
4273.		1	0	0	2-Heptacosene, 2-methyl-	H_3C-$C(CH_3)$═CH-$(CH_2)_{23}$-CH_3	1.11
4274.		1	0	0	2-Heptacosene, 25-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{21}$-$CH(CH_3)$-CH_2-CH_3	1.11
4275.		1	0	0	2-Heptacosene, 25-methyl-, (*E*)-		1.11
4276.		1	0	0	2-Heptacosene, 26-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{22}$-$CH(CH_3)_2$	1.11
4277.		1	0	0	2-Heptacosene, 26-methyl-, (*E*)-		1.11
4278.	56797-42-3	0	1	0	8,11-Heptadecadienal, (*Z,Z*)-		3.12
4279.	37822-80-3	0	1	0	Heptadecadienoic acid, methyl ester		5.3
4280.	629-90-3	0	1	0	Heptadecanal	H_3C-$(CH_2)_{15}$-CH═O	3.12
4281.	629-78-7	1	1	1	Heptadecane	H_3C-$(CH_2)_{15}$-CH_3	1.10
4282.	1560-89-0	1	1	1	Heptadecane, 2-methyl-	H_3C-$(CH_2)_{14}$-CH═$(CH_3)_2$	1.10
4283.	6418-44-6	0	1	0	Heptadecane, 3-methyl-	H_3C-$(CH_2)_{13}$-$CH(CH_3)$-CH_2-CH_3	1.10
4284.	13287-23-5	1	0	0	Heptadecane, 8-methyl-	H_3C-$(CH_2)_6$-$CH(CH_3)$-$(CH_2)_8$-CH_3	1.10
4285.	506-12-7	1	1	1	Heptadecanoic acid	H_3C-$(CH_2)_{15}$-COOH	4.3
4286.	42218-25-7	1	1	1	Heptadecanoic acid, docosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{21}$-CH_3	5.3
4287.	42232-43-9	1	1	1	Heptadecanoic acid, dodecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{11}$-CH_3	5.3
4288.	36617-53-5	1	1	1	Heptadecanoic acid, eicosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{19}$-CH_3	5.3
4289.	42232-52-0	1	1	1	Heptadecanoic acid, heneicosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{20}$-CH_3	5.3
4290.		1	1	1	Heptadecanoic acid, heptacosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{26}$-CH_3	5.3
4291.	36617-50-2	1	1	1	Heptadecanoic acid, heptadecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{16}$-CH_3	5.3
4292.	121877-64-3	1	1	1	Heptadecanoic acid, hexacosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{25}$-CH_3	5.3
4293.	36617-49-9	1	1	1	Heptadecanoic acid, hexadecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{15}$-CH_3	5.3
4294.	1731-92-6	1	1	1	Heptadecanoic acid, methyl ester	H_3C-$(CH_2)_{15}$-COO-CH_3	5.3
4295.	36617-52-4	1	1	1	Heptadecanoic acid, nonadecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{18}$-CH_3	5.3
4296.	36617-51-3	1	1	1	Heptadecanoic acid, octadecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{17}$-CH_3	5.3
4297.		1	1	1	Heptadecanoic acid, pentacosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{24}$-CH_3	5.3
4298.	36617-48-8	1	1	1	Heptadecanoic acid, pentadecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{14}$-CH_3	5.3
4299.	42232-54-2	1	1	1	Heptadecanoic acid, tetracosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{23}$-CH_3	5.3
4300.	36617-47-7	1	1	1	Heptadecanoic acid, tetradecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{13}$-CH_3	5.3
4301.	42232-53-1	1	1	1	Heptadecanoic acid, tricosyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{22}$-CH_3	5.3
4302.	36617-46-6	1	1	1	Heptadecanoic acid, tridecyl ester	H_3C-$(CH_2)_{15}$-COO-$(CH_2)_{12}$-CH_3	5.3
4303.	29709-08-8	1	1	1	Heptadecanoic acid, 15-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COOH	4.3
4304.	121877-42-7	1	1	1	Heptadecanoic acid, 15-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{20}$-CH_3	5.3
4305.	121877-68-7	1	1	1	Heptadecanoic acid, 15-methyl-, hexacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{25}$-CH_3	5.3

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	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
4306.	121877-81-4	1	1	1	Heptadecanoic acid, 15-methyl-, octacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{27}$-CH_3	5.3
4307.	121877-52-9	1	1	1	Heptadecanoic acid, 15-methyl-, tricosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{13}$-COO-$(CH_2)_{22}$-CH_3	5.3
4308.	2724-58-5	1	1	1	Heptadecanoic acid, 16-methyl-	$(H_3C)_2$=CH-$(CH_2)_{14}$-COOH	4.3
4309.	150462-99-0	0	1	0	Heptadecanoic acid, 16-methyl-, 2-(acetyloxy)-1-(hydroxymethyl)ethyl ester		2.5, 5.3
4310.	150462-98-9	0	1	0	Heptadecanoic acid, 16-methyl-, 3-(acetyloxy)-2-hydroxypropyl ester		2.5, 5.3
4311.	121877-46-1	1	1	1	Heptadecanoic acid, 16-methyl-, docosyl ester	$(H_3C)_2$=CH-$(CH_2)_{14}$-COO-$(CH_2)_{21}$-CH_3	5.3
4312.	52458-35-2	0	1	0	Heptadecanoic acid, 16-methyl-, ethyl ester	$(H_3C)_2$=CH-$(CH_2)_{14}$-COO-C_2H_5	5.3
4313.	121877-36-9	1	1	1	Heptadecanoic acid, 16-methyl-, heneicosyl ester	$(H_3C)_2$=CH-$(CH_2)_{14}$-COO-$(CH_2)_{20}$-CH_3	5.3
4314.	5129-61-3	0	1	0	Heptadecanoic acid, 16-methyl-, methyl ester	$(H_3C)_2$=CH-$(CH_2)_{14}$-COO-CH_3	5.3
4315.	121877-50-7	1	1	1	Heptadecanoic acid, 16-methyl-, tricosyl ester	$(H_3C)_2$=CH-$(CH_2)_{14}$-COO-$(CH_2)_{22}$-CH_3	5.3
4316.		0	1	0	Heptadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl heptadecanoate}		5.3
4317.	71278-19-8	1	0	0	Heptadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester		5.3
4318.	1454-85-9	1	1	1	1-Heptadecanol	H_3C-$(CH_2)_{15}$-CH_2OH	2.5
4319.	41744-75-6	1	0	0	1-Heptadecanol, 16-methyl-	$(H_3C)_2$=CH-$(CH_2)_{14}$-CH_2OH	2.5
4320.	56797-44-5	0	1	0	8,11,14-Heptadecatrienal, (*Z,Z,Z*)-		3.12
4321.	37822-82-5	0	1	0	Heptadecatrienoic acid, methyl ester		5.3
4322.	26266-05-7	1	1	1	Heptadecene	H-$(CH_2)_{15-n}$-CH=CH-$(CH_2)_n$-H	1.11
4323.	6765-39-5	1	0	0	1-Heptadecene	H_3C-$(CH_2)_{14}$-CH=CH_2	1.11
4324.		1	0	0	1-Heptadecene, 2-methyl-	H_2C=$C(CH_3)$-$(CH_2)_{14}$-CH_3	1.11
4325.		1	0	0	2-Heptadecene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{13}$-CH_3	1.11
4326.		1	0	0	2-Heptadecene, (*E*)-		1.11
4327.	13287-12-2	1	0	0	2-Heptadecene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{13}$-CH_3	1.11
4328.		1	0	0	2-Heptadecene, 15-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{11}$-$CH(CH_3)$-CH_2-CH_3	1.11
4329.		1	0	0	2-Heptadecene, 15-methyl-, (*E*)-		1.11
4330.		1	0	0	2-Heptadecene, 16-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{12}$-$CH(CH_3)_2$	1.11
4331.		1	0	0	2-Heptadecene, 16-methyl-, (*E*)-		1.11
4332.	36232-39-0	1	0	0	2-Heptadecene, 4-methylene-8,12,16-trimethyl-	H_3C-CH=CH-C(=CH_2)-CH_2-{$(CH_2)_2$-$CH(CH_3)$-CH_2}$_3$-H	1.11
4333.	26265-99-6	1	1	1	Heptadecenoic acid	H-$(CH_2)_{14-n}$-CH=CH-$(CH_2)_n$-COOH	4.3
4334.	31424-16-5	0	1	0	Heptadecenoic acid, methyl ester	H-$(CH_2)_{14-n}$-CH=CH-$(CH_2)_n$-COO-CH_3	5.3
4335.	4313-03-5 5910-85-0	0	1	0	2,4-Heptadienal	O=CH-CH=CH-CH=CH-CH_2-CH=O	3.12, 24.3, 25.29
4336.	51945-98-3	0	1	0	1,5-Heptadiene-3,4-diol	H_3C-CH=CH-CHOH-CHOH-CH=CH_2	2.5
4337.	74630-29-8	0	1	0	1,5-Heptadiene, 3,3,5-trimethyl-	H_3C-CH=$C(CH_3)$-CH_2-$C(CH_3)_2$-CH=CH_2	1.11
4338.	74421-05-9	1	0	0	2,4-Heptadiene, 2,4-dimethyl-		1.11
4339.	4634-87-1	1	0	0	2,4-Heptadiene, 2,6-dimethyl-		1.11
4340.	72693-11-9	0	1	0	2,5-Heptadienoic acid, 2,3-dimethyl-		4.3
4341.	54557-55-0	0	1	0	4,6-Heptadienoic acid, 6-methyl-3-(1-methylethyl)-, (*E*)-		4.3

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4342.	54557-57-2 80114-59-6	0	1	0	4,6-Heptadienoic acid, 6-methyl-3-(1-methylethyl)-, methyl ester, (*E*)-		5.3
4343.		1	0	0	1,6-Heptadien-4-ol		2.5
4344.	77411-76-8	0	1	0	3,5-Heptadien-2-ol, 2,6-dimethyl-		2.5
4345.	57935-33-8	0	1	0	4,6-Heptadien-1-ol, 6-methyl-3-(1-methylethyl)-, (*E*)-		2.5
4346.	79-78-7	0	1	0	1,6-Heptadien-3-one,1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {allylionone}		3.13
4347.	504-20-1	0	1	0	2,5-Heptadien-4-one, 2.6-dimethyl- {phorone}		3.13
4348.		0	1	0	3,5-Heptadien-2-one, 6-methyl-, (*Z*)-		3.13
4349.	1604-28-0	1	1	1	3,5-Heptadien-2-one, 6-methyl-, (*E*)-	$(H_3C)_2$═C═CH-CH═CH-CO-CH_3	3.13, 24.3, 25.29
4350.		0	1	0	4,6-Heptadien-2-one		3.13
4351.		0	1	0	4,6-Heptadien-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methylfuranyl)-		3.13, 10.2
4352.	3511-27-1	1	0	0	1,5-Heptadien-3-yne	H_3C-CH═CH-C≡C-CH═CH_2	1.11
4353.	111-71-7	1	0	0	Heptanal	H_3C-$(CH_2)_5$-CH═O	3.12
4354.	2363-85-1	1	0	0	Heptanal, 2-oxo-	H_3C-$(CH_2)_4$-CO-CH═O	3.12, 3.13
4355.	111-68-2	1	1	1	1-Heptanamine	H_3C-$(CH_2)_6$-NH_2	12.2
4356.	142-82-5	1	0	0	Heptane	H_3C-$(CH_2)_5$-CH_3	1.10
4357.	629-06-1	1	0	0	Heptane, 1-chloro-	H_3C-$(CH_2)_5$-CH_2Cl	18.4
4358.		1	0	0	Heptane, dimethyl-		1.10
4359.	2213-23-2	0	1	0	Heptane, 2,4-dimethyl-		1.10
4360.	592-27-8	1	0	0	Heptane, 2-methyl-	H_3C-$(CH_2)_4$-CH═$(CH_3)_2$	1.10
4361.	15869-80-4	1	0	0	Heptane, 3-ethyl-	H_3C-$(CH_2)_3$-CH═$(C_2H_5)_2$	1.10
4362.	589-81-1	1	0	0	Heptane, 3-methyl-	H_3C-$(CH_2)_3$-CH(CH_3)-CH_2-CH_3	1.10
4363.	1632-16-2	0	1	0	Heptane, 3-methylene-	H_3C-$(CH_2)_3$-C(═CH_2)-CH_2-CH_3	1.11
4364.	646-20-8	1	0	0	Heptanedinitrile	NC-$(CH_2)_5$-CN	11.2
4365.	111-16-0	1	0	0	Heptanedioic acid {pimelic acid}	HOOC-$(CH_2)_5$-COOH	4.3
4366.	535-24-0	0	1	0	Heptanedioic acid, 2,6-diamino-3-hydroxy-		2.5, 4.3, 12.2
4367.	96-04-8	1	0	0	2,3-Heptanedione	H_3C-$(CH_2)_3$-CO-CO-CH_3	3.13
4368.	7307-02-0	1	0	0	2,4-Heptanedione	H_3C-$(CH_2)_2$-CO-CH_2-CO-CH_3	3.13
4369.	3002-23-1	0	1	0	2,4-Heptanedione, 6-methyl-	$(H_3C)_2$═CH-CH_2-CO-CH_2-CO-CH_3	3.13
4370.	1703-51-1	1	1	1	2,5-Heptanedione	H_3C-CH_2-CO-$(CH_2)_2$-CO-CH_3	3.13
4371.		0	1	0	2,5-Heptanedione, 4-(1-methylethyl)-		3.13
4372.	13901-85-4	1	1	1	2,5-Heptanedione, 6-methyl-	$(H_3C)_2$═CH-CO-$(CH_2)_2$-CO-CH_3	3.13
4373.	13505-34-5	1	1	1	2,6-Heptanedione	H_3C-CO-$(CH_2)_3$-CO-CH_3	3.13
4374.		0	1	0	2,6-Heptanedione, 3-methyl-	H_3C-CO-CH(CH_3)-$(CH_2)_2$-CO-CH_3	3.13
4375.	629-08-3	1	0	0	Heptanenitrile		11.2
4376.	111-14-8	1	1	1	Heptanoic acid {enanthic acid}	H_3C-$(CH_2)_5$-COOH	4.3, 24.3, 25.29
4377.	97259-93-3	0	1	0	Heptanoic acid, dimethyl-		4.3
4378.	106-30-9	0	1	0	Heptanoic acid, ethyl ester	H_3C-$(CH_2)_5$-COO-C_2H_5	5.3
4379.	106-73-0	0	1	0	Heptanoic acid, methyl ester	H_3C-$(CH_2)_5$-COO-CH_3	5.3
4380.	3274-29-1	0	1	0	Heptanoic acid, 2-ethyl-		4.3
4381.	1188-02-9	0	1	0	Heptanoic acid, 2-methyl-		4.3
4382.	59262-53-2	0	1	0	Heptanoic acid, 3-(1-methylethyl)-6-oxo-, (S)-		3.13, 4.3
4383.	39815-78-6	0	1	0	Heptanoic acid, 3-oxo-, methyl ester	H_3C-$(CH_2)_3$-CO-CH_2-COO-CH_3	3.13, 5.3
4384.	1070-68-4	0	1	0	Heptanoic acid, 5-methyl-		4.3
4385.	42330-36-9	0	1	0	Heptanoic acid, 5-methyl-, (S)-		4.3
4386.	929-10-2	0	1	0	Heptanoic acid, 6-methyl-		4.3
4387.	3128-07-2	1	0	0	Heptanoic acid, 6-oxo-	H_3C-CO-$(CH_2)_4$-COOH	3.13, 4.3

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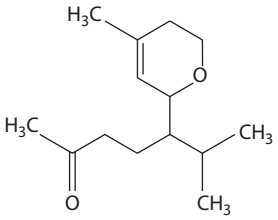
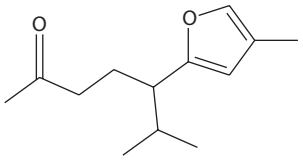
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4388.	98188-02-4	0	1	0	Heptanoic acid, 7-(2-furanyl)-, methyl ester		5.3, 10.2
4389.	53535-33-4	0	1	0	Heptanol		2.5
4390.	111-70-6	1	1	1	1-Heptanol	H_3C-$(CH_2)_5$-CH_2OH	2.5
4391.	1653-40-3	0	1	0	1-Heptanol, 6-methyl-		2.5
4392.	543-49-7	0	1	0	2-Heptanol	H_3C-$(CH_2)_4$-$CHOH$-CH_3	2.5
4393.	4730-22-7	0	1	0	2-Heptanol, 6-methyl-		2.5
4394.	110-43-0	1	1	1	2-Heptanone {methyl pentyl ketone}	H_3C-$(CH_2)_4$-CO-CH_3	3.13, 24.3, 25.29
4395.	52812-44-9	1	0	0	2-Heptanone, 5-(3-acetyloxiranyl)-6-methyl-		3.13
4396.	52812-43-8	0	1	0	2-Heptanone, 5-[3-(1-hydroxy-1-methylethyl)oxiranyl]-6-methyl-		2.5, 3.13, 10.2
4397.		0	1	0	2-Heptanone, 5-(2,3-dihydro-4-methyl-6-pyranyl)-6-methyl-		3.13, 10.2
4398.		0	1	0	2-Heptanone, 5-(5,6-dihydro-4-methyl-2-pyranyl)-6-methyl-		3.13, 10.2
4399.	541-85-5	0	1	0	2-Heptanone, 5-methyl-		3.13
4400.	121269-00-9	0	1	0	2-Heptanone, 6-(5-methyl-2-furanyl)-		3.13, 10.2
4401.	72693-12-0	1	0	0	2-Heptanone, 6-hydroxy-	H_3C-$CHOH$-$(CH_2)_3$-CO-CH_3	2.5, 3.13
4402.	928-68-7	1	1	1	2-Heptanone, 6-methyl-		3.13
4403.	41059-93-2	0	1	0	2-Heptanone, 6-methyl-5-(4-methyl-2-furanyl)- {solanofuran}		3.13, 10.2
4404.	106-35-4	1	0	0	3-Heptanone {ethyl butyl ketone}	H_3C-CH_2-CO-$(CH_2)_3$-CH_3	3.13
4405.	19549-83-8	1	0	0	3-Heptanone, 2,6-dimethyl-		3.13
4406.	123-19-3	1	1	1	4-Heptanone {butyrone, dipropyl ketone}	H_3C-$(CH_2)_2$-CO-$(CH_2)_2$-CH_3	0.4, 3.13
4407.	108-83-8	1	0	0	4-Heptanone, 2,6-dimethyl-		3.13
4408.		1	0	0	4-Heptanone, 5-hydroxy-		2.5, 3.13
4409.	7194-84-5	1	1	1	Heptatriacontane	H_3C-$(CH_2)_{35}$-CH_3	1.10
4410.	24587-25-5	1	0	0	1,3,5-Heptatriene	H_3C-$(CH{=}CH)_2$-$CH{=}CH_2$	1.11
4411.		1	0	0	1,3,5-Heptatriene, 1.6-dimethyl-		1.11
4412.		1	0	0	1,3,5-Heptatriene, 1.6-dimethyl- {isomer}		1.11
4413.		1	0	0	1,3,6-Heptatriene, 2.5.6-trimethyl-		1.11
4414.	2463-63-0	0	1	0	2-Heptenal	H_3C-$(CH_2)_3$-$CH{=}CH$-$CH{=}O$	3.12, 24.3
4415.	30567-26-1	1	0	0	2-Heptenal, 2-methyl-	H_3C-$(CH_2)_3$-$CH{=}C(CH_3)$-$CH{=}O$	3.12
4416.	6728-31-0	0	1	0	4-Heptenal	H_3C-CH_2-$CH{=}CH$-$(CH_2)_2$-$CH{=}O$	3.12
4417.	34098-52-7	0	1	0	*D*-xylo-Hept-2-enaric acid, 2,6-anhydro-3-deoxy- {2*H*-pyran-2,4-dicarboxylic acid, 3,4-dihydro-3,4-dihydroxy-}		2.5, 4.3, 10.2
4418.		1	0	0	Heptene		1.11
4419.	592-76-7	1	0	0	1-Heptene	$H_2C{=}CH$-$(CH_2)_4$-CH_3	1.11
4420.		1	0	0	1-Heptene, 2-methyl-		1.11

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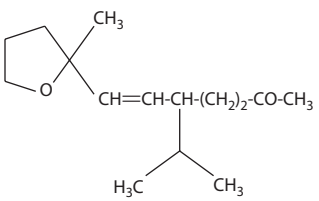
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
4421.	592-77-8	1	0	0	2-Heptene	H_3C-CH═CH-$(CH_2)_3$-CH_3	1.11
4422.	14686-13-6	1	0	0	2-Heptene, (*E*)-		1.11
4423.	77288-93-8	0	1	0	2-Heptene-1,6-diol,3-(1-methylethyl)-,(*E*)-	H_3C-CHOH-$(CH_2)_2$-C[$CH(CH_3)_2$]═CH-CH_2OH	2.5
4424.	21504-51-8	1	1	1	3-Heptene-2,5-dione, 6-methyl-		3.13
4425.	25377-46-2	1	1	1	Heptenoic acid		4.3
4426.	18999-28-5	1	1	1	2-Heptenoic acid	H_3C-$(CH_2)_3$-CH═CH-COOH	4.3
4427.	10352-88-2	0	1	0	2-Heptenoic acid, (*E*)-		4.3
4428.	499-84-3	0	1	0	2-Heptenoicacid,3-(1-methylethyl)-6-oxo-	H_3C-CO-$(CH_2)_2$-C[$CH(CH_3)_2$]═CH-COOH	3.13, 4.3
4429.	41654-06-2	0	1	0	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)-		3.13, 4.3
4430.	63892-03-5	0	1	0	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (Z)-		3.13, 4.3
4431.	35194-37-7	1	1	1	4-Heptenoic acid	H_3C-CH_2-CH═CH-$(CH_2)_2$-COOH	4.3
4432.	41653-95-6	0	1	0	4-Heptenoic acid, (*Z*)-		4.3
4433.	105728-84-5	0	1	0	4-Heptenoic acid, 6-hydroxy-		2.5, 4.3
4434.	41654-07-3	0	1	0	4-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)-	H_3C-CO-CH═CH-CH[$CH(CH_3)_2$]-CH_2-COOH	3.13, 4.3
4435.	1119-60-4	0	1	0	6-Heptenoic acid	H_2C═CH-$(CH_2)_4$-COOH	4.3
4436.		0	1	0	6-Heptenoic acid, 5-methyl-	H_2C═CH-CH(CH_3)-$(CH_2)_3$-COOH	4.3
4437.	30414-57-4	0	1	0	6-Heptenoic acid, 3-oxo-, methyl ester	H_2C═CH-$(CH_2)_2$-CO-CH_2-COO-CH_3	5.3
4438.	1335-09-7	0	1	0	Heptenol, methyl-		2.5
4439.	33467-76-4	0	1	0	2-Hepten-1-ol (*E*)	H_3C-$(CH_2)_3$-CH═CH-CH_2OH	2.5
4440.	55454-22-3	0	1	0	2-Hepten-1-ol (*Z*)		2.5
4441.	70898-26-9	0	1	0	3-Hepten-2-ol, 5-ethyl-2,6-dimethyl-		2.5
4442.		0	1	0	3-Hepten-2-ol, 5-(1-methylethy)-2-methyl-		2.5
4443.	58927-84-7	0	1	0	4-Hepten-2-ol, 6-methyl-, (*E*)-		2.5
4444.	1569-60-4	0	1	0	5-Hepten-2-ol, 6-methyl-		2.5
4445.	42201-30-9	0	1	0	6-Hepten-2-ol, 4-methylene-		2.5
4446.	57782-61-3	0	1	0	6-Hepten-2-ol, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)-		2.5, 10.2
4447.	409-02-9	0	1	0	Heptenone, methyl-		3.13
4448.	1119-44-4	0	1	0	3-Hepten-2-one	H_3C-$(CH_2)_2$-CH═CH-CO-CH_3	3.13
4449.	133561-46-3	0	1	0	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-		2.5, 3.13
4450.	129742-47-8	0	1	0	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-, [R-(*E*)]-		2.5, 3.13
4451.	57283-79-1	0	1	0	3-Hepten-2-one, 5-ethyl-6-methyl-		3.13
4452.	50767-76-5	0	1	0	3-Hepten-2-one, 5-ethyl-6-methyl-, (*E*)-		3.13
4453.	57283-79-1	0	1	0	3-Hepten-2-one, 5-(1-methylethyl)-		3.13
4454.	2009-74-7	1	1	1	3-Hepten-2-one, 6-methyl-		3.13
4455.	152209-54-6	0	1	0	3-Hepten-2-one, 5-(1-methylethyl)-7-[2-methyl-3-(3-methyl-5-oxo-3-hexenyl) oxiranyl]-, [2S-[2α(3*E*,5R*),3β(*E*)]]-		3.13, 10.2
4456.	110-93-0	1	1	1	5-Hepten-2-one, 6-methyl-		3.13, 24.3, 25.29
4457.	57782-60-2	0	1	0	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)-		3.13, 10.2
4458.	104669-35-4	0	1	0	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-4-hydroxy-2-methyl-2-furanyl)-		2.5, 3.13, 10.2

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	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
4459.	160115-55-9	0	1	0	6-Hepten-2-one, 7-[4-(acetyloxy) tetrahydro-5-hydroxy-2-methyl-2-furanyl]-5-(1-methylethyl)-		2.5, 3.13, 5.3, 10.2
4460.	117210-48-7	0	1	0	6-Hepten-2-one, 7-[tetrahydro-2-methyl-5-(1-methylethyl)-2-furanyl]-		3.13, 10.2
4461.		0	1	0	Heptose		2.5, 8.3
4462.		1	0	0	Heptoxyl radical	$O(CH_2)_6CH_3$	27.1
4463.	628-71-7	1	0	0	1-Heptyne	H_3C-$(CH_2)_4$-C≡CH	1.11
4464.	2586-89-2	1	0	0	3-Heptyne	H_3C-$(CH_2)_2$-C≡C-CH_2-CH_3	1.11
4465.	630-01-3	1	1	1	Hexacosane	H_3C-$(CH_2)_{24}$-CH_3	1.10
4466.	1561-02-0	1	1	1	Hexacosane, 2-methyl-	$(H_3C)_2$=CH-$(CH_2)_{23}$-CH_3	1.10
4467.	65820-56-6	0	1	0	Hexacosane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{22}$-CH_3	1.10
4468.	506-46-7	1	1	1	Hexacosanoic acid {cerotinic acid}	H_3C-$(CH_2)_{24}$-COOH	4.3
4469.	108657-23-4	1	1	1	Hexacosanoic acid, docosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{21}$-CH_3	5.3
4470.		1	1	1	Hexacosanoic acid, dodecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{11}$-CH_3	5.3
4471.	121877-83-6	1	1	1	Hexacosanoic acid, eicosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{19}$-CH_3	5.3
4472.		1	1	1	Hexacosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl hexacosanoate}		2.7, 5.3
4473.	121877-89-2	1	1	1	Hexacosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{20}$-CH_3	5.3
4474.	75696-56-9	1	1	1	Hexacosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{26}$-CH_3	5.3
4475.		1	1	1	Hexacosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{16}$-CH_3	5.3
4476.	10210-18-1	1	1	1	Hexacosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{25}$-CH_3	5.3
4477.		1	1	1	Hexacosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{15}$-CH_3	5.3
4478.		1	1	1	Hexacosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{18}$-CH_3	5.3
4479.		1	1	1	Hexacosanoic acid, octadecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{17}$-CH_3	5.3
4480.		1	1	1	Hexacosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{24}$-CH_3	5.3
4481.		1	1	1	Hexacosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{14}$-CH_3	5.3
4482.		1	1	1	Hexacosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{23}$-CH_3	5.3
4483.		1	1	1	Hexacosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{193}$-CH_3	5.3
4484.	121877-97-2	1	1	1	Hexacosanoic acid, tricosyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{22}$-CH_3	5.3
4485.		1	1	1	Hexacosanoic acid, tridecyl ester	H_3C-$(CH_2)_{24}$-COO-$(CH_2)_{12}$-CH_3	5.3
4486.		1	0	0	Hexacosanoic acid, 24-methyl-		4.3
4487.	121877-92-7	1	1	1	Hexacosanoic acid, 24-methyl-, docosyl ester		5.3
4488.	121877-90-5	1	1	1	Hexacosanoic acid, 24-methyl-, heneicosyl ester		5.3
4489.	506-52-5	0	1	0	1-Hexacosanol	H_3C-$(CH_2)_{24}$-CH_2OH	2.5
4490.	63785-25-1	0	1	0	1-Hexacosanol, 24-methyl-		2.5
4491.		0	1	0	1-Hexacosanol, 25-methyl-		2.5
4492.	64808-91-9	1	0	0	Hexacosene		1.11
4493.	18835-33-1	1	0	0	1-Hexacosene	H_2C=CH-$(CH_2)_{23}$-CH_3	1.11
4494.		1	0	0	1-Hexacosene, 2-methyl-	H_2C=$C(CH_3)$-$(CH_2)_{23}$-CH_3	1.11
4495.		1	0	0	2-Hexacosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{22}$-CH_3	1.11
4496.		1	0	0	2-Hexacosene, (*E*)-		1.11
4497.		1	0	0	2-Hexacosene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{22}$-CH_3	1.11
4498.		1	0	0	2-Hexacosene, 24-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{20}$-$CH(CH_3)$-CH_2-CH_3	1.11
4499.		1	0	0	2-Hexacosene, 24-methyl-, (*E*)-		1.11
4500.		1	0	0	2-Hexacosene, 25-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{21}$-$CH(CH_3)_2$	1.11
4501.		1	0	0	2-Hexacosene, 25-methyl-, (*E*)-		1.11
4502.	30917-33-0	1	0	0	1,3-Hexadecadiene, 2,6,10,14-tetramethyl-	$H[CH_2CH_2CH(CH_3)CH_2]_3$-CH=CH-$C(CH_3)$=$CH_2$	1.11

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4503.	21980-71-2	1	0	0	1,3-Hexadecadiene, 3,7,11,15-tetramethyl- {phytadiene}	$H[CH_2CH(CH_3)CH_2CH_2]_3$-CH=CH-C($CH_3$)=$CH_2$	1.11
4504.		1	0	0	1,3-Hexadecadiene, 2,6,10-trimethyl-		1.11
4505.		0	1	0	2,4-Hexadecadiene,3,7,11,15-tetramethyl-		1.11
4506.	25377-52-0	1	1	1	Hexadecadienoic acid {palmitolenic acid}		4.3
4507.	29961-54-4	0	1	0	Hexadecadienoic acid, methyl ester		5.3
4508.	629-80-1	0	1	0	Hexadecanal	H_3C-$(CH_2)_{14}$-CH=O	3.12
4509.	544-76-3	1	1	1	Hexadecane	H_3C-$(CH_2)_{14}$-CH_3	1.10
4510.	1560-92-5	1	1	1	Hexadecane, 2-methyl-	H_3C-$(CH_2)_{13}$-CH=$(CH_3)_2$	1.10
4511.	6418-43-5	0	1	0	Hexadecane, 3-methyl-	H_3C-$(CH_2)_{12}$-CH(CH_3)-CH_2-CH_3	1.10
4512.	638-36-8	1	1	1	Hexadecane, 2,6,10,14-tetramethyl- {phytane}		1.10
4513.	36232-38-9	1	0	0	Hexadecane,2,6,10-trimethyl-14-methylene-		1.11
4514.	60922-91-0	1	0	0	Hexadecane, mixture with pentane		1.10
4515.	505-54-4	0	1	0	Hexadecanedioic acid	HOOC-$(CH_2)_{14}$-COOH	4.3
4516.	57-10-3	1	1	1	Hexadecanoic acid {palmitic acid}	H_3C-$(CH_2)_{14}$-COOH	0.4, 4.3, 24.3, 25.29, 26.9
4517.	111-06-8	1	0	0	Hexadecanoic acid, butyl ester		5.3
4518.	42232-33-7	1	1	1	Hexadecanoic acid, docosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{21}$-CH_3	5.3
4519.	42232-29-1	1	1	1	Hexadecanoic acid, dodecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{11}$-CH_3	5.3
4520.	80252-38-6	1	1	1	Hexadecanoic acid, dotriacontyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{31}$-CH_3	5.3
4521.	22413-01-0	1	1	1	Hexadecanoic acid, eicosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{19}$-CH_3	5.3
4522.	628-97-7	1	1	1	Hexadecanoic acid, ethyl ester {ethyl palmitate}	H_3C-$(CH_2)_{14}$-COO-CH_2-CH_3	5.3, 24.3, 25.29
4523.	42232-32-6	1	1	1	Hexadecanoic acid, heneicosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{20}$-CH_3	5.3
4524.	94632-82-3	1	1	1	Hexadecanoic acid, heptacosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{26}$-CH_3	5.3
4525.	18466-06-3	1	1	1	Hexadecanoic acid, heptadecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{16}$-CH_3	5.3
4526.	60007-87-6	1	1	1	Hexadecanoic acid, hexacosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{25}$-CH_3	5.3
4527.	540-10-3	1	1	1	Hexadecanoic acid, hexadecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{15}$-CH_3	5.3
4528.	23470-00-0	1	0	0	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester {glyceryl 2-hexadecanoate}	H_3C-$(CH_2)_{14}$-COO-CH=$(CH_2OH)_2$	2.5, 5.3
4529.	28801-93-6	1	1	1	Hexadecanoic acid, methyl-		4.3
4530.	112-39-0	1	1	1	Hexadecanoic acid, methyl ester	H_3C-$(CH_2)_{14}$-COO-CH_3	5.3
4531.	142-91-6	1	1	1	Hexadecanoic acid, (1-methylethyl) ester		5.3
4532.	36617-44-4	1	1	1	Hexadecanoic acid, nonadecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{18}$-CH_3	5.3
4533.	78509-52-1	1	1	1	Hexadecanoic acid, octacosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{27}$-CH_3	5.3
4534.	2598-99-4	1	1	1	Hexadecanoic acid, octadecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{17}$-CH_3	5.3
4535.	94632-81-2	1	1	1	Hexadecanoic acid, pentacosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{24}$-CH_3	5.3
4536.	18299-77-9	1	1	1	Hexadecanoic acid, pentadecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{14}$-CH_3	5.3
4537.	42232-35-9	1	1	1	Hexadecanoic acid, tetracosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{33}$-CH_3	5.3
4538.	4536-26-9	1	1	1	Hexadecanoic acid, tetradecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{13}$-CH_3	5.3
4539.	84461-48-3	1	1	1	Hexadecanoic acid, tetratriacontyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{33}$-CH_3	5.3
4540.	6027-71-0	1	1	1	Hexadecanoic acid, triacontyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{29}$-CH_3	5.3
4541.	42232-34-8	1	1	1	Hexadecanoic acid, tricosyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{22}$-CH_3	5.3
4542.	36617-38-6	1	1	1	Hexadecanoic acid, tridecyl ester	H_3C-$(CH_2)_{14}$-COO-$(CH_2)_{13}$-CH_3	5.3
4543.	3233-90-7	0	1	0	Hexadecanoic acid, 10,16-dihydroxy-		2.5, 4.3
4544.	5918-29-6	1	1	1	Hexadecanoic acid, 14-methyl-	H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COOH	4.3
4545.	121877-41-6	1	1	1	Hexadecanoic acid, 14-methyl-, docosyl ester	H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{21}$-CH_3	5.3
4546.	121877-33-6	1	1	1	Hexadecanoic acid, 14-methyl-, heneicosyl ester	H_3C-CH_2-CH(CH_3)-$(CH_2)_{12}$-COO-$(CH_2)_{20}$-CH_3	5.3

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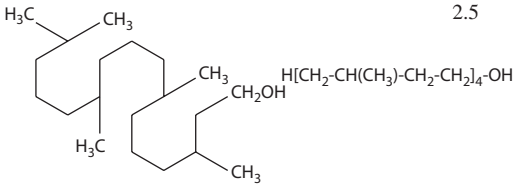
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4547.	121877-67-6	1	1	1	Hexadecanoic acid, 14-methyl-, heptacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{12}$-COO-$(CH_2)_{26}$-CH_3	5.3
4548.	121877-58-5	1	1	1	Hexadecanoic acid, 14-methyl-, hexacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{12}$-COO-$(CH_2)_{25}$-CH_3	5.3
4549.	2490-49-5	1	1	1	Hexadecanoic acid, 14-methyl-, methyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{12}$-COO-CH_3	5.3
4550.	121877-74-5	1	1	1	Hexadecanoic acid, 14-methyl-, octacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{12}$-COO-$(CH_2)_{27}$-CH_3	5.3
4551.	1603-03-8	1	1	1	Hexadecanoic acid, 15-methyl-	$(H_3C)_2$═CH-$(CH_2)_{13}$-COOH	4.3
4552.	121877-39-2	1	1	1	Hexadecanoic acid, 15-methyl-, docosyl ester	$(H_3C)_2$═CH-$(CH_2)_{13}$-COO-$(CH_2)_{21}$-CH_3	5.3
4553.	6929-04-0	0	1	0	Hexadecanoic acid, 15-methyl-, methyl ester	$(H_3C)_2$═CH-$(CH_2)_{13}$-COO-CH_3	5.3
4554.	506-13-8	0	1	0	Hexadecanoic acid, 16-hydroxy-	$HOCH_2$-$(CH_2)_{14}$-COOH	2.5, 4.3
4555.	27147-71-3	0	1	0	Hexadecanoic acid, 2-methyl-	H_3C-$(CH_2)_{13}$-$CH(CH_3)$-COOH	4.3
4556.	42172-35-0	0	1	0	Hexadecanoic acid, 3-methyl-	H_3C-$(CH_2)_{12}$-$CH(CH_3)$-CH_2-COOH	4.3
4557.	11017-44-0 71607-94-8	1	1	1	Hexadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester {solanesyl hexadecanoate}		5.3
4558.	1118-77-0	0	1	0	Hexadecanoic acid, 3,7,11,15-tetramethyl-, methyl ester		5.3
4559.	53950-58-6	1	1	1	Hexadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
4560.	124-29-8 36653-82-4	1	1	1	1-Hexadecanol {cetyl alcohol}	H_3C-$(CH_2)_{14}$-CH_2OH	2.5
4561.	2490-43-9	0	1	0	1-Hexadecanol, 14-methyl-		2.5
4562.	645-72-7	1	1	1	1-Hexadecanol, 3,7,11,15-tetramethyl- {dihydrophytol}		2.5
4563.	60054-55-9	0	1	0	1-Hexadecanol, 7,11,15-trimethyl-3-methylene-		2.5
4564.	18787-63-8	1	1	1	2-Hexadecanone	H_3C-$(CH_2)_{13}$-CO-CH_3	3.13
4565.	34083-18-6	1	0	0	2,6,10,14-Hexadecatetraene, 2,6,10,14-tetramethyl-	H-$[CH_2$-$C(CH_3)$═CH-$CH_2]_4$-H	1.11
4566.	7481-01-8	0	1	0	2,6,10,14-Hexadecatetraene, 2,6,10,14-tetramethyl-, (*E,E*)-		1.11
4567.	70901-63-2	0	1	0	1,6,10,14-Hexadecatetraene, 7,11,15-trimethyl-3-methylene-, (*E,E*)-		1.11
4568.	76540-54-0	0	1	0	1,6,10,14-Hexadecatetraene-3,9-diol, 3,7,11,15-tetramethyl-		2.5
4569.	76540-55-1	0	1	0	2,6,10,15-Hexadecatetraene-1,14-diol, 2,6,10,14-tetramethyl-, [S-(*Z,E,E*)]-		2.5
4570.	25377-56-4	1	1	1	Hexadecatrienoic acid		4.3
4571.	32839-24-0	0	1	0	Hexadecatrienoic acid, (*Z,Z,Z*)-		4.3
4572.	37822-81-4	0	1	0	Hexadecatrienoic acid, methyl ester		5.3
4573.	*63871-00-1*	1	0	0	Hexadecatrien-1-ol,3,7,11,15-tetramethyl-		2.5
4574.	26952-14-7	0	1	0	Hexadecene		1.11
4575.	629-73-2	1	0	0	1-Hexadecene {1-cetene}	H_2C═CH-$(CH_2)_{13}$-CH_3	1.11

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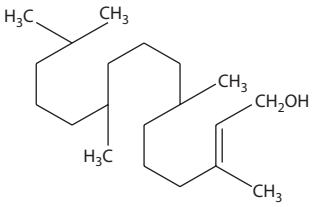
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4576.	61868-19-7	1	0	0	1-Hexadecene, 2-methyl-	$H_2C{=}C(CH_3)\text{-}(CH_2)_{13}\text{-}CH_3$	1.11
4577.	71278-20-1	1	0	0	1-Hexadecene, 2,6,10-trimethyl-		1.11
4578.	504-96-1	1	1	1	1-Hexadecene, 3-methylene-7,11,15-trimethyl- {neophytadiene}	$H_2C{=}CH\text{-}C(=CH_2)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)CH_2\}_3\text{-}H$	1.11, 25.29
4579.	30221-44-4	0	1	0	1-Hexadecene, 3,7,11,15-tetramethyl- {phytene 1}		1.11
4580.		1	0	0	2-Hexadecene, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{12}\text{-}CH_3$	1.11
4581.	26741-29-7	1	0	0	2-Hexadecene, (*E*)-		1.11
4582.	73120-40-8	1	0	0	2-Hexadecene, 2-methyl-	$H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{12}\text{-}CH_3$	1.11
4583.		1	0	0	2-Hexadecene, 14-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{10}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1.11
4584.		1	0	0	2-Hexadecene, 14-methyl-, (*E*)-		1.11
4585.		1	0	0	2-Hexadecene, 15-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{11}\text{-}CH(CH_3)_2$	1.11
4586.		1	0	0	2-Hexadecene, 15-methyl-, (*E*)-		1.11
4587.	51806-25-8	0	1	0	4-Hexadecene, 3-methylene-7,11,15-trimethyl-	$H_3C\text{-}CH_2\text{-}C(=CH_2)\text{-}CH{=}CH\text{-}CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\}_2\text{-}H$	1.11
4588.	25447-95-4	1	1	1	Hexadecenoic acid		4.3
4589.	29960-49-4	0	1	0	Hexadecenoic acid, methyl ester		5.3
4590.	28039-99-8	0	1	0	Hexadecenoic acid, (Z)-		4.3
4591.	1686-10-8	0	1	0	3-Hexadecenoic acid, (*E*)-		4.3
4592.	373-49-9	1	1	1	9-Hexadecenoic acid, (*Z*)- {palmitoleic acid}	$H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_5\text{-}COOH$	4.3
4593.	10030-73-6 2091-29-4	1	1	1	9-Hexadecenoic acid, (*E*)- {palmitelaidic acid}	$H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_5\text{-}COOH$	4.3
4594.	1120-25-8	0	1	0	9-Hexadecenoic acid, methyl ester, (Z)-	$H_3C\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_5\text{-}COO\text{-}CH_3$	5.3
4595.	505-32-8 60046-87-9	1	1	1	1-Hexadecen-3-ol, 3,7,11,15-tetramethyl- {isophytol}		2.5
4596.	22104-83-2	0	1	0	2-Hexadecen-1-ol	$H_3C\text{-}(CH_2)_{12}\text{-}CH{=}CH\text{-}CH_2OH$	2.5
4597.	102608-53-7	0	1	0	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-		2.5
4598.	150-86-7	1	1	1	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(*E*)]]- {phytol}		2.5, 25.29
4599.	60026-26-8	0	1	0	7-Hexadecen-6-one,3,7,11,15-tetramethyl-		3.13
4600.	80466-34-8	0	1	0	2,4-Hexadienal	$H_3C\text{-}(CH{=}CH)_2\text{-}CH{=}O$	3.12
4601.	142-83-6	1	1	1	2,4-Hexadienal, (*E,E*)-		3.12
4602.	54612-24-7	1	0	0	Hexadiene, dimethyl-		1.11
4603.		1	0	0	Hexadiene, methyl-		1.11
4604.	592-48-3	1	0	0	1,3-Hexadiene		1.11
4605.	62338-07-2	1	0	0	1,3-Hexadiene, 2,5-dimethyl-3-ethyl-		1.11
4606.	592-45-0	1	0	0	1,4-Hexadiene		1.11
4607.	927-97-9	1	0	0	1,4-Hexadiene, 2,5-dimethyl-	$H_2C{=}C(CH_3)\text{-}CH_2\text{-}CH{=}C(CH_3)\text{-}CH_3$	1.11
4608.	592-42-7	1	0	0	1,5-Hexadiene		1.11
4609.	592-46-1	1	0	0	2,4-Hexadiene		1.11
4610.		1	0	0	2,4-Hexadiene {isomer}		1.11
4611.	764-13-6	1	0	0	2,4-Hexadiene, 2,5-dimethyl-	$H_3C\text{-}C(CH_3){=}CH\text{-}CH{=}C(CH_3)\text{-}CH_3$	1.11
4612.	21293-01-6	1	0	0	2,4-Hexadiene, 3,4-dimethyl-		1.11
4613.	110-44-1 22500-92-1	1	1	1	2,4-Hexadienoic acid, (*E,E*)- {sorbic acid}	$H_3C\text{-}(CH{=}CH)_2\text{-}COOH$	4.3, 24.3, 25.29

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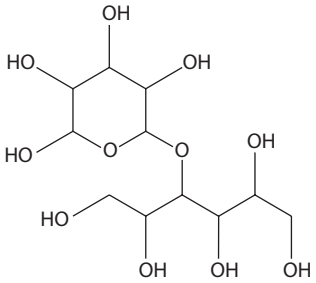
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4614.	590-00-1 24624-61-5	0	1	0	2,4-Hexadienoic acid, potassium salt	H_3C-$(CH{=}CH)_2$-COOK	20.2
4615.	90-65-3	1	1	1	2,5-Hexadienoic acid, 3-methoxy-5-methyl-4-oxo-		3.13, 4.3, 10.2
4616.	94806-37-8	1	0	0	1,5-Hexadien-3-ol, 5-methyl-		2.5
4617.	10420-90-3	1	0	0	1,3-Hexadien-5-yne	$HC{\equiv}C$-$CH{=}CH$-$CH{=}CH_2$	1.11
4618.	821-08-9	1	0	0	1,5-Hexadien-3-yne {divinylacetylene}	$H_2C{=}CH$-$C{\equiv}C$-$CH{=}CH_2$	1.11
4619.		1	0	0	Hexadiyne		1.11
4620.	66-25-1	1	1	1	Hexanal {caproic aldehyde}	H_3C-$(CH_2)_4$-$CH{=}O$	3.12, 24.3, 25.29
4621.	15303-46-5	0	1	0	Hexanal, 2-(1-methylethyl)-5-oxo-		3.12, 3.13
4622.	2363-84-0	1	0	0	Hexanal, 2-oxo-	H_3C-$(CH_2)_3$-CO-$CH{=}O$	3.12, 3.13
4623.	25346-59-2	0	1	0	Hexanal, 4-oxo-	H_3C-CH_2-CO-$(CH_2)_2$-$CH{=}O$	3.12, 3.13
4624.	628-02-4	1	0	0	Hexanamide	H_3C-$(CH_2)_4$-CO-NH_2	13.1
4625.	111-26-2	1	1	1	1-Hexanamine	H_3C-$(CH_2)_5$-NH_2	12.2
4626.	28056-87-3	1	0	0	1-Hexanamine, 2-ethyl-*N,N*-dimethyl-		12.2
4627.	110-54-3	1	1	1	Hexane	H_3C-$(CH_2)_4$-CH_3	1.10, 25.29
4628.	33240-56-1	1	0	0	Hexane, 1-chloro-5-methyl-		18.4
4629.	28777-67-5	1	0	0	Hexane, dimethyl-		1.10
4630.	589-43-5, 116502-44-4	1	0	0	Hexane, 2,4-dimethyl-		1.10
4631.	592-13-2	1	0	0	Hexane, 2,5-dimethyl-		1.10
4632.	50-70-4	1	1	1	Hexane, hexahydroxy- {sorbitol, glucitol}	$HOCH_2$-$(CHOH)_4$-CH_2OH	0.4, 2.5, 8.3, 24.3, 25.29
4633.	585-88-6	0	1	0	Hexane, hexahydroxy-, 4-*O*-β-*D*-glucopyranosyl- {maltitol, 4-*O*-β-*D*-glucopyranosyl-*D*-glucitol}		2.5, 8.3, 10.2
4634.		0	1	0	Hexane, hexahydroxy-, 2,6-di-*O*-methyl-		2.5, 8.3, 10.2
4635.		0	1	0	Hexane, hexahydroxy-, 2,3,6-tri-*O*-methyl-		2.5, 8.3, 10.2
4636.		0	1	0	Hexane, hexahydroxy-, 2,3,4,6-tetra-*O*-methyl-		2.5, 8.3, 10.2
4637.	591-76-4	1	0	0	Hexane, 2-methyl-		1.10
4638.	589-34-4	1	0	0	Hexane, 3-methyl-		1.10
4639.	1071-81-4	1	0	0	Hexane, 2,2,5,5-tetramethyl-	$(H_3C)_3{\equiv}C$-$(CH_2)_2$-$C{\equiv}(CH_3)_3$	1.10
4640.	124-04-9	1	1	1	Hexanedioic acid {adipic acid}	HOOC-$(CH_2)_4$-COOH	4.3
4641.	542-32-5	0	1	0	Hexanedioic acid, 2-amino-		4.3, 12.2
4642.	123-79-5	1	0	0	Hexanedioic acid, dioctyl ester		5.3
4643.	103-23-1	1	0	0	Hexanedioic acid, bis(2-ethylhexyl) ester		5.3
4644.	3184-35-8	1	1	1	Hexanedioic acid, 2-oxo-		3.13, 4.3
4645.	102488-05-1	0	1	0	1,5-Hexanediol, 2-(1-methylethyl)-		2.5
4646.	77289-00-0	0	1	0	1,5-Hexanediol, 2-(1-methylethyl)-, [S-(R*,R*)]-		2.5
4647.	1462-11-9	1	0	0	1,5-Hexanediol, 5-methyl-		2.5
4648.	2935-44-6	1	1	1	2,5-Hexanediol	H_3C-$CHOH$ $(CH_2)_2$-$CHOH$-CH_3	2.5
4649.	29044-06-2	0	1	0	2,5-Hexanediol, 2-methyl-		2.5
4650.	3848-24-6	1	0	0	2,3-Hexanedione	H_3C-CO-CO-$(CH_2)_3$-CH_3	3.13
4651.	110-13-4	1	1	1	2,5-Hexanedione {acetonylacetone}		3.13

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
4652.	61892-85-1	1	0	0	2,5-Hexanedione, 3-hydroxy-		2.5, 3.13
4653.	4437-50-7	1	0	0	2,5-Hexanedione, 3-methyl-		3.13
4654.	4437-51-8	1	0	0	3,4-Hexanedione	H_3C-CH_2-CO-CO-CH_2-CH_3	3.13
4655.		1	0	0	3,4-Hexanedione, 2-methyl-		3.13
4656.	628-73-9	1	0	0	Hexanenitrile {capronitrile}	H_3C-$(CH_2)_4$-CN	11.2
4657.	64350-07-8	1	0	0	Hexanenitrile, 2-hydroxy-		2.5, 11.2
4658.	111-31-9	1	0	0	1-Hexanethiol	H_3C-$(CH_2)_5$-SH	18.1
4659.	106-69-4	1	0	0	1,2,6-Hexanetriol		2.5
4660.	18990-98-2	1	0	0	1,3,6-Hexanetriol		2.5
4661.	142-62-1	1	1	1	Hexanoic acid {caproic acid}	H_3C-$(CH_2)_4$-COOH	0.4, 4.3, 21.3, 24.3, 25.29
4662.	626-82-4	0	1	0	Hexanoic acid, butyl ester		5.3
4663.	60308-81-8	0	1	0	Hexanoic acid, 4,5-dimethyl-		4.3
4664.	123-66-0	1	1	1	Hexanoic acid, ethyl ester {ethyl caproate}	H_3C-$(CH_2)_4$-COO-C_2H_5	5.3, 24.3, 25.29
4665.		1	1	1	Hexanoic acid, 2,6-di-(methylnitrosoamino)-	R-$(CH_2)_4$-CH(R)-COOH where R═H_3C-N(NO)-	4.3, 12.2, 15.8
4666.	149-57-5	1	1	1	Hexanoic acid, 2-ethyl-		4.3
4667.	2983-37-1	0	1	0	Hexanoic acid, 2-ethyl-, ethyl ester		5.3
4668.		1	0	0	Hexanoic acid, hydroxy-		2.5, 4.3
4669.	6064-63-7	0	1	0	Hexanoic acid, 2-hydroxy-		2.5, 4.3
4670.	6946-90-3	0	1	0	Hexanoic acid, 2-hydroxy-, ethyl ester		2.5, 5.3
4671.	2305-25-1	0	1	0	Hexanoic acid, 3-hydroxy-, ethyl ester		2.5, 5.3
4672.	1191-25-9	1	0	0	Hexanoic acid, 6-hydroxy-		2.5, 4.3
4673.	40309-49-7	0	1	0	Hexanoic acid, 3-hydroxy-5-methyl-		2.5, 4.3
4674.	31501-11-8	0	1	0	Hexanoic acid, *cis*-3-hexenyl ester		5.3
4675.	106-70-7	0	1	0	Hexanoic acid, methyl ester	H_3C-$(CH_2)_4$-COO-CH_3	5.3
4676.	4536-23-6	1	1	1	Hexanoic acid, 2-methyl- {2-methylhexanoic acid}		4.3, 24.3, 25.29
4677.	3780-58-3	0	1	0	Hexanoic acid, 3-methyl-		4.3
4678.	2198-61-0	0	1	0	Hexanoic acid, 3-methylbutyl ester		5.3
4679.	1561-11-1	0	1	0	Hexanoic acid, 4-methyl-		4.3
4680.	6818-07-1	1	0	0	Hexanoic acid, 4-methyl-5-oxo-		3.13, 4.3
4681.	628-46-6	0	1	0	Hexanoic acid, 5-methyl-		4.3
4682.	2177-83-5	0	1	0	Hexanoic acid, 5-methyl-, methyl ester		5.3
4683.	30414-55-2	0	1	0	Hexanoic acid, 5-methyl-3-oxo-, methyl ester		3.13, 5.3
4684.	41654-04-0	0	1	0	Hexanoic acid, 5-methyl-4-oxo-		3.13, 4.3
4685.	2543-54-6	0	1	0	Hexanoic acid, 2-(1-methylethyl)-5-oxo-		3.13, 4.3
4686.	16825-90-4	1	1	1	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, (S)-		3.13, 4.3
4687.	1842-56-4	0	1	0	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, methyl ester		3.13, 5.3
4688.	3249-68-1	1	0	0	Hexanoic acid, 3-oxo-, ethyl ester		3.13, 5.3
4689.	1117-74-4	1	1	1	Hexanoic acid, 4-oxo-		3.13, 4.3
4690.	3128-06-1	1	0	0	Hexanoic acid, 5-oxo-		3.13, 4.3
4691.	13984-57-1	1	0	0	Hexanoic acid, 5-oxo-, ethyl ester		3.13, 5.3
4692.	540-07-8	0	1	0	Hexanoic acid, pentyl ester	H_3C-$(CH_2)_4$-COO-$(CH_2)_4$-CH_3	5.3
4693.	6290-37-5	0	1	0	Hexanoic acid, 2-phenylethyl ester		5.3
4694.	6938-45-0	0	1	0	Hexanoic acid, phenylmethyl ester		5.3
4695.	123-68-2	1	1	1	Hexanoic acid, 2-propenyl ester		5.3
4696.	626-77-7	0	1	0	Hexanoic acid, propyl ester		5.3
4697.	2051-49-2	0	1	0	Hexanoic anhydride		7.1
4698.	25917-35-5	1	1	1	Hexanol		2.5

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4699.	111-27-3	1	1	1	1-Hexanol {caproyl alcohol}	H_3C-$(CH_2)_4$-CH_2OH	2.5, 21.3, 24.3, 25.29
4700.	104-76-7	1	1	1	1-Hexanol, 2-ethyl-	H_3C-$(CH_2)_3$-$CH(C_2H_5)$-CH_2OH	2.5, 24.3
4701.	61949-26-6	1	0	0	1-Hexanol, methyl-		2.5
4702.	818-49-5	0	1	0	1-Hexanol, 4-methyl-		2.5
4703.	627-98-5	0	1	0	1-Hexanol, 5-methyl-	$(H_3C)_2$═CH-$(CH_2)_3$-CH_2OH	2.5
4704.	3452-97-9	0	1	0	1-Hexanol, 3,5,5-trimethyl-		2.5
4705.	626-93-7	1	1	1	2-Hexanol	H_3C-$(CH_2)_3$-CHOH-CH_3	2.5
4706.		0	1	0	2-Hexanol, 2-cyclohexanyl-		2.5
4707.	625-23-0	1	1	1	2-Hexanol, 2-methyl-		2.5
4708.	627-59-8	1	1	1	2-Hexanol, 5-methyl-		2.5
4709.	623-37-0	1	1	1	3-Hexanol		2.5
4710.	2180-43-0	1	0	0	3-Hexanol, 1-phenyl-		2.5
4711.		1	0	0	4-Hexanol, 1-phenyl-		2.5
4712.		1	0	0	Hexanone		3.13
4713.	14360-50-0	1	0	0	1-Hexanone, 1-(2-furanyl)-		3.13, 10.2
4714.	591-78-6	1	1	1	2-Hexanone {butyl methyl ketone}	H_3C-$(CH_2)_3$-CO-CH_3	3.13
4715.	72693-13-1	1	0	0	2-Hexanone, 5,6-dihydroxy-		2.5, 3.13
4716.	56745-61-0	1	0	0	2-Hexanone, 5-hydroxy-		2.5, 3.13
4717.	68208-73-1	1	0	0	2-Hexanone, 6-hydroxy-5-methyl-		2.5, 3.13
4718.	2550-21-2	0	1	0	2-Hexanone, 3-methyl-		3.13
4719.	105-42-0	1	0	0	2-Hexanone, 4-methyl-		3.13
4720.	110-12-3	1	0	0	2-Hexanone, 5-methyl-		3.13
4721.	589-38-8	1	1	1	3-Hexanone {ethyl propyl ketone}		3.13
4722.	623-56-3	1	0	0	3-Hexanone, 5-methyl-		3.13
4723.	70322-25-7 71278-21-2	1	1	1	1,3,6,10,14,18,22,26,30,34-Hexatriacontadecaene, 3,7,11,15,19,23,27,31, 35-nonamethyl- {solanesene}		1.11
4724.	630-06-8	1	1	1	Hexatriacontane	H_3C-$(CH_2)_{34}$-CH_3	1.10
4725.	71278-22-3	1	0	0	1,6,10,14,18,22,26,30, 34-Hexatriacontanonaene, 7,11,15,19,23,27,31, 35-octamethyl-3-methylene-		1.11
4726.	66327-99-9	1	0	0	2,6,10,14,18,22,26,30, 34-Hexatriacontanonaene, 2,6,10,14,18,22,26,30, 34-nonamethyl-, (all-*E*)-		1.11
4727.	60924-87-0	0	1	0	2,6,10,14,18,22,26,30, 35-Hexatriacontanonaene-1,34-diol, 3,7,11,15,19,23, 27,31,35-nonamethyl-, (all-*E*)-		2.5
4728.	60924-86-9	0	1	0	2,6,10,14,18,22,26,30, 33-Hexatriacontanonaene-1,35-diol, 3,7,11,15,19,23, 27,31,35-nonamethyl-, (all-*E*)-		2.5
4729.	101330-76-1	0	1	0	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27, 31,35-nonamethyl-, labeled with ^{14}C, (*Z,Z,Z*)- {solanesol-^{14}C}		2.5

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4730.	13190-97-1	1	1	1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)- {solanesol}	H-[CH_2-C(CH_3)=CH-CH_2]$_9$-OH	2.5, 25.29
4731.	29144-38-5 58000-93-4	1	1	1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, acetate, {solanesyl acetate}		5.3
4732.	2235-12-3	1	0	0	1,3,5-Hexatriene	H_2C=CH-CH=CH-CH=CH_2	1.11
4733.	41233-72-1	1	0	0	1,3,5-Hexatriene, 2-methyl-		1.11
4734.	24587-26-6	1	0	0	1,3,5-Hexatriene, 3-methyl-		1.11
4735.	1335-39-3	0	1	0	Hexenal		3.12
4736.	505-57-7	1	1	1	2-Hexenal	H_3C-(CH_2)$_2$-CH=CH-CH=O	3.12
4737.	6728-26-3	1	1	1	2-Hexenal, (*E*)-		3.12, 24.3, 25.29
4738.	16635-54-4	1	1	1	2-Hexenal, (*Z*)-		3.12
4739.		1	0	0	2-Hexenal, 2,5-dimethyl-		3.12
4740.	28467-88-1	1	0	0	2-Hexenal, 2-methyl-	H_3C-(CH_2)$_2$-CH=C(CH_3)-CH=O	3.12
4741.		1	0	0	2-Hexenal, 5-methyl-		3.12
4742.	21834-92-4	0	1	0	2-Hexenal, 5-methyl-2-phenyl-		3.12
4743.	25264-93-1	1	0	0	Hexene	H-(CH_2)$_n$-CH=CH-(CH_2)$_{(4-n)}$-H	1.11
4744.		1	0	0	Hexene, diamino		12.2
4745.		1	0	0	1-Hexen-1-aminocarbonyl- (1*E*)- {[(1*E*)-1-hex-1-en-1-yl]aminocarbonyl-}	CH_3(CH_2)$_3$-CH=CH-NH-C=O	27.1
4746.	592-41-6	1	0	0	1-Hexene	H_3C-(CH_2)$_3$-CH=CH_2	1.11
4747.	6094-02-6	1	0	0	1-Hexene, 2-methyl-		1.11
4748.	3404-61-3	1	0	0	1-Hexene, 3-methyl-		1.11
4749.	3769-23-1	1	0	0	1-Hexene, 4-methyl-		1.11
4750.	3524-73-0	1	0	0	1-Hexene, 5-methyl-	(H_3C)$_2$=CH-(CH_2)$_2$-CH=CH_2	1.11
4751.	592-43-8	1	0	0	2-Hexene	H_3C-(CH_2)$_2$-CH=CH-CH_3	1.11
4752.	4050-45-7	1	0	0	2-Hexene, (*E*)-		1.11
4753.	7688-21-3	1	0	0	2-Hexene, (*Z*)-		1.11
4754.	3404-78-2	1	0	0	2-Hexene, 2,5-dimethyl-	H_3C-CH(CH_3)-CH_2-CH=C(CH_3)-CH_3	1.11
4755.	2738-19-4	1	0	0	2-Hexene, 2-methyl-	H_3C-(CH_2)$_2$-CH=C(CH_3)-CH_3	1.11
4756.	3404-62-4	1	0	0	2-Hexene, 5-methyl-	H_3C-CH(CH_3)-CH_2-CH=CH-CH_3	1.11
4757.	592-47-2	1	0	0	3-Hexene	H_3C-CH_2-CH=CH-CH_2-CH_3	1.11
4758.	13269-52-8	1	1	1	3-Hexene, (*E*)-		1.11
4759.	7642-09-3	1	0	0	3-Hexene, (*Z*)-		1.11
4760.	4436-75-3	0	1	0	3-Hexene-2,5-dione		3.13
4761.	1289-40-3	1	0	0	Hexenoic acid		4.3
4762.	1191-04-4	0	1	0	2-Hexenoic acid	H_3C-(CH_2)$_2$-CH=CH-COOH	4.3
4763.	13419-69-7	0	1	0	2-Hexenoic acid, (*E*)-		4.3
4764.	5309-52-4	0	1	0	2-Hexenoic acid, 2-ethyl-		4.3
4765.	41653-96-7	0	1	0	2-Hexenoic acid, 5-methyl-	(H_3C)$_2$=CH-CH_2-CH=CH-COOH	4.3
4766.	51424-01-2	0	1	0	2-Hexenoic acid, 5-methyl-, (*E*)-		4.3
4767.	4219-24-3	1	1	1	3-Hexenoic acid {hydrosorbic acid}	H_3C-CH_2-CH=CH-CH_2-COOH	4.3, 24.3, 25.29
4768.	1775-43-5	0	1	0	3-Hexenoic acid, (*Z*)-		4.3
4769.	2396-78-3	0	1	0	3-Hexenoic acid, methyl ester	H_3C-CH_2-CH=CH-CH_2-COO-CH_3	5.3
4770.	35194-36-6	1	1	1	4-Hexenoic acid	H_3C-CH=CH-(CH_2)$_2$-COOH	4.3
4771.	1577-20-4	1	1	1	4-Hexenoic acid, (*E*)-		4.3
4772.	5636-65-7	0	1	0	4-Hexenoic acid, 5-methyl-		4.3
4773.	1577-22-6	0	1	0	5-Hexenoic acid		4.3
4774.	28261-03-2	0	1	0	Hexenol		2.5

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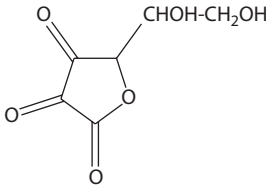
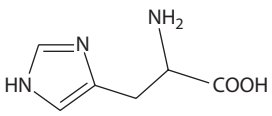
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4775.	928-95-0	0	1	0	2-Hexen-1-ol	H_3C-$(CH_2)_2$-CH═CH-CH_2OH	2.5, 24.3, 25.29
4776.	2305-21-7	0	1	0	2-Hexen-1-ol, (*E*)-		2.5
4777.	2497-18-9	0	1	0	2-Hexen-1-ol, acetate, (*E*)-		5.3, 24.3, 25.29
4778.	544-12-7	0	1	0	3-Hexen-1-ol		2.5
4779.	928-97-2	0	1	0	3-Hexen-1-ol, (*E*)-		2.5, 24.3
4780.	928-96-1	1	1	1	3-Hexen-1-ol, (*Z*)- {leaf alcohol}		2.5, 24.3, 25.29
4781.		1	1	1	3-Hexen-1-ol, (*Z*)-, labeled with ^{14}C {leaf alcohol-^{14}C}		2.5, 25.29
4782.	1708-82-3	0	1	0	3-Hexen-1-ol, acetate		5.3
4783.	3681-71-8	0	1	0	3-Hexen-1-ol, acetate, (*Z*)-		5.3
4784.	25152-85-6	0	1	0	3-Hexen-1-ol, benzoate, (*Z*)-		5.3
4785.	2315-09-5	0	1	0	3-Hexen-1-ol, formate		5.3
4786.	33467-73-1	0	1	0	3-Hexen-1-ol, formate, (*Z*)-		5.3
4787.	58461-27-1	1	0	0	4-Hexen-1-ol,5-methyl-2-(1-methylethyl)-		2.5
4788.	821-41-0	1	0	0	5-Hexen-1-ol		2.5
4789.	763-93-9	1	0	0	3-Hexen-2-one		3.13
4790.	5166-53-0	1	1	1	3-Hexen-2-one, 5-methyl-		3.13, 24.3
4791.	1821-29-0	0	1	0	3-Hexen-2-one, 5-methyl-, (*E*)-		3.13
4792.	25659-22-7	1	0	0	4-Hexen-3-one		3.13
4793.	17325-90-5	0	1	0	4-Hexen-3-one, 4,5-dimethyl-		3.13
4794.	109-49-9	1	1	1	5-Hexen-2-one	H_2C═CH-$(CH_2)_2$-CO-CH_3	3.13
4795.	55615-04-8	0	1	0	5-Hexen-2-one, 4,5-dimethyl-		3.13
4796.	121197-12-4	1	1	1	5-Hexen-3-one, 4,5-dihydroxy-		2.5, 3.13
4797.	33124-69-5	0	1	0	threo-2,3-Hexodiulosonic acid, γ-lactone {2,3-diketogulonic acid, γ-lactone}		2.5, 3.13, 6.3
4798.	490-83-5	0	1	0	*L*-threo-2,3-Hexodiulosonic acid, γ-lactone {*L*-2,3-diketogulonic acid, γ-lactone}		2.5, 3.13, 6.3
4799.	61989-59-1	1	0	0	Hexonic acid, 2,3-dideoxy-, γ-lactone, monoacetate		5.3, 6.3
4800.	61892-51-1	1	0	0	Hexonic acid, 3,6-dideoxy-, γ-lactone		6.3
4801.	61653-41-6	0	1	0	*D*-lyxo-Hexonic acid, 2-deoxy-, γ-lactone		6.3
4802.	45009-62-9	0	1	0	Hexoses		2.5, 8.3
4803.		1	0	0	Hexoxyl radical	$O(CH_2)_5CH_3$	27.1
4804.	62446-36-0	0	1	0	Hexuronic acid		4.3
4805.	26856-30-4	1	0	0	Hexyne	H-$(CH_2)_n$-C≡C-$(CH_2)_{(4-n)}$-H	1.11
4806.	693-02-7	1	0	0	1-Hexyne	HC≡C-$(CH_2)_3$-CH_3	1.11
4807.	2203-80-7	1	0	0	1-Hexyne, 5-methyl-	HC≡C-$(CH_2)_2$-$CH(CH_3)_2$	1.11
4808.	764-35-2	1	0	0	2-Hexyne	H_3C-C≡C-$(CH_2)_2$-CH_3	1.11
4809.	53566-37-3	1	0	0	2-Hexyne, 5-methyl-	H_3C-C≡C-CH_2-$CH(CH_3)_2$	1.11
4810.	928-49-4	1	0	0	3-Hexyne	H_3C-CH_2-C≡C-CH_2-CH_3	1.11
4811.	7006-35-1	0	1	0	Histidine		4.3, 4.10, 12.2, 17.4
4812.	71-00-1	1	0	0	*L*-Histidine		0.4, 4.3, 4.10, 12.2, 17.4, 24.3, 25.29

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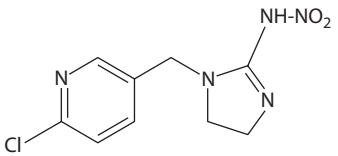
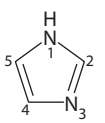
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4813.	332-80-9	1	1	1	*L*-Histidine, 1-methyl-		4.3, 4.10, 12.2, 17.4
4814.	368-16-1	1	1	1	*L*-Histidine, 3-methyl-		4.3, 4.10, 12.2, 17.4, 25.29
4815.	62504-27-2	0	1	0	*L*-Histidine, *N*-(1-carboxyethyl)-, (R)-		4.3, 4.10, 12.2, 17.4
4816.	7440-60-0	1	1	1	Holmium	Ho	20.5
4817.	8064-26-4	0	1	0	Holocellulose		2.5, 8.3, 25.29
4818.	454-29-5	0	1	0	*DL*-Homocysteine	$HS\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 12.2, 18.1, 25.29
4819.	498-19-1 672-15-1	1	1	1	Homoserine {2-amino-4-hydroxybutanoic acid}	$HO\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	2.5, 4.3, 4.10, 12.2
4820.	1415-93-6	0	1	0	Humic acids		2.5, 3.13, 4.3, 9.22
4821.	9024-25-3	0	1	0	Hydratase, aconitate		22.2
4822.	9032-88-6	0	1	0	Hydratase, fumarate		22.2
4823.	9014-08-8	0	1	0	Hydratase, phosphopyruvate		22.2
4824.	302-01-2	1	1	1	Hydrazine	$H_2N\text{-}NH_2$	12.2, 19.5, 23.5, 25.29
4825.	57-14-7	1	1	1	Hydrazine, 1,1-dimethyl-	$H_2N\text{-}N(CH_3)_2$	12.2, 23.5
4826.	624-80-6	1	0	0	Hydrazine, ethyl-	$H_2N\text{-}NH\text{-}CH_2\text{-}CH_3$	12.2
4827.	60-34-4	1	0	0	Hydrazine, methyl-	$H_2N\text{-}NH\text{-}CH_3$	12.2
4828.	74-90-8	1	1	1	Hydrocyanic acid {hydrogen cyanide}	HCN	0.4, 11.2, 19.5, 21.3, 23.5
4829.	1333-74-0	1	0	0	Hydrogen	H_2	0.4, 19.5
4830.	7722-84-1	1	0	0	Hydrogen peroxide	H_2O_2	27.1
4831.		1	0	0	Hydrogen peroxyl radical	OOH	27.1
4832.	7783-06-4	1	0	0	Hydrogen sulfide	H_2S	0.4, 18.1, 19.5
4833.	9027-05-8	0	1	0	Hydrogenase		22.2
4834.	9027-41-2	0	1	0	Hydrolase		22.2
4835.		0	1	0	Hydropectin		0.4, 8.3
4836.		1	0	0	Hydroquinone/semiquinone/ quinone radical		27.1
4837.	3352-57-6	1	0	0	Hydroxide radical		27.1
4838.	120598-69-8	0	1	0	Hydroxycinnamoyltransferase, putrescine		22.2
4839.	73904-44-6	0	1	0	Hydroxycinnamoyltransferase, shikimate		22.2
4840.	128909-19-3	0	1	0	Hydroxycinnamoyltransferase, tyramine		22.2
4841.	60321-02-0	0	1	0	Hydroxycinnamyl-CoA, quinate {hydroxycinnamyl transferase, quinate}		22.2
4842.	7803-49-8	0	1	0	Hydroxylamine	$HO\text{-}NH_2$	12.2
4843.		0	1	0	Hydroxylase, glycine		22.2
4844.	9029-83-8	0	1	0	Hydroxymethyltransferase, serine		22.2
4845.		1	0	0	1*H*-Imidazo[2.1-*a*]isoquinoline		17.21
4846.	105827-78-9	0	1	0	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl)methyl)-4,5-dihydro-*N*-nitro- {Admire®}		12.2, 16.1, 17.9, 18.4, 21.3
4847.	288-32-4	1	1	1	1*H*-Imidazole {1,3-diazole}		17.4

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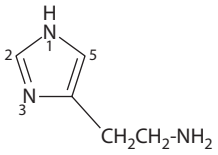
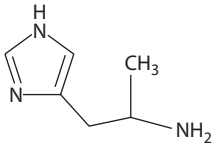
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4848.	2466-76-4	0	1	0	1*H*-Imidazole, 1-acetyl-		17.4
4849.		1	0	0	1*H*-Imidazole, C_3-alkyl- {three isomers detected}		17.4
4850.		1	0	0	1*H*-Imidazole, C_4-alkyl- {five isomers detected}		17.4
4851.		1	0	0	1*H*-Imidazole, C_5-alkyl- {four isomers detected}		17.4
4852.		1	0	0	1*H*-Imidazole, butyl-		17.4
4853.	50790-93-7	1	0	0	1*H*-Imidazole, 2-butyl-		17.4
4854.	931-35-1	0	1	0	1*H*-Imidazole, 4,5-dihydro-2-ethyl-4-methyl-		17.4
4855.	1739-84-0	1	0	0	1*H*-Imidazole, 1,2-dimethyl-		17.4
4856.	6338-45-0	1	0	0	1*H*-Imidazole, 1,4-dimethyl-		17.4
4857.	10447-93-5	1	0	0	1*H*-Imidazole, 1,5-dimethyl-		17.4
4858.	930-62-1	1	0	0	1*H*-Imidazole, 2,4-dimethyl-		17.4
4859.	2302-39-8	1	0	0	1*H*-Imidazole, 4,5-dimethyl-		17.4
4860.	37455-73-5	1	0	0	1*H*-Imidazole, 1,4-dimethyl-2-(1-methylethyl)-		17.4
4861.	40688-28-6	1	0	0	1*H*-Imidazole, 2,4-dimethyl-5-(1-methylethyl)-		17.4
4862.		1	0	0	1*H*-Imidazole, 2,5-dimethyl-4-(1-methylethyl)-		17.4
4863.		1	0	0	1*H*-Imidazole, 1,4-dimethyl-5-phenyl-		17.4
4864.	51-45-6	0	1	0	1*H*-Imidazole-4-ethanamine {histamine}		12.2, 17.4
4865.	75614-87-8	0	1	0	1*H*-Imidazole-4-ethanamine, α-methyl-		12.2, 17.4
4866.		1	0	0	1*H*-Imidazole, ethyl-		17.4
4867.	7098-07-9	1	0	0	1*H*-Imidazole, 1-ethyl-		17.4
4868.	1072-62-4	1	0	0	1*H*-Imidazole, 2-ethyl-		17.4
4869.	19141-85-6	1	0	0	1*H*-Imidazole, 4-ethyl-		17.4
4870.	21202-52-8	1	0	0	1*H*-Imidazole, 1-ethyl-2-methyl-		17.4
4871.	931-36-2	1	0	0	1*H*-Imidazole, 2-ethyl-4-methyl-		17.4
4872.		1	0	0	1*H*-Imidazole, 2-ethyl-4-(1-methylethyl)-		17.4
4873.	29239-89-2	1	0	0	1*H*-Imidazole, 4-ethyl-2-methyl-		17.4
4874.	37455-59-7	1	0	0	1*H*-Imidazole, 4-ethyl-2-(1-methylethyl)-		17.4
4875.	37455-56-4	1	0	0	1*H*-Imidazole, 4-ethyl-2-propyl-		17.4
4876.		1	0	0	1*H*-Imidazole, methyl-		17.4
4877.	616-47-7	1	0	0	1*H*-Imidazole, 1-methyl-		17.4
4878.	693-98-1	1	0	0	1*H*-Imidazole, 2-methyl-		17.4
4879.	822-36-6	1	0	0	1*H*-Imidazole, 4-methyl-		17.4
4880.	37455-55-3	1	0	0	1*H*-Imidazole, 4-methyl-2-propyl-		17.4
4881.	36947-68-9	1	0	0	1*H*-Imidazole, 2-(1-methylethyl)-		17.4
4882.	58650-48-9	1	0	0	1*H*-Imidazole, 4-(1-methylethyl)-		17.4
4883.	22509-02-0	1	0	0	1*H*-Imidazole, 1-methyl-2-(1-methylethyl)-		17.4
4884.	37455-52-0	1	0	0	1*H*-Imidazole, 2-methyl-4-(1-methylethyl)-		17.4

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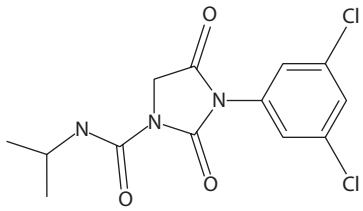
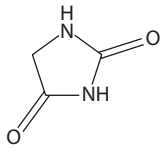
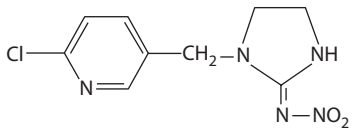
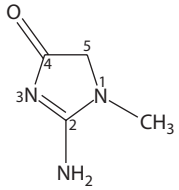
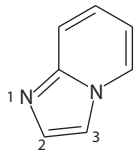
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4885.	37455-58-6	1	0	0	1*H*-Imidazole, 4-methyl-2-(1-methylethyl)-		17.4
4886.	61893-07-0	1	0	0	1*H*-Imidazole, 4-methyl-2-(1-methylpropyl)-		17.4
4887.	61893-06-9	1	0	0	1*H*-Imidazole, 2-(1-methylpropyl)-		17.4
4888.	61893-08-1	1	0	0	1*H*-Imidazole, 4-(2-methylpropyl)-		17.4
4889.		1	0	0	1*H*-Imidazole, pentyl-		17.4
4890.	91491-09-7	1	0	0	1*H*-Imidazole, propyl-		17.4
4891.	1842-63-3	1	0	0	1*H*-Imidazole, 1,2,4-trimethyl-		17.4
4892.	822-90-2	1	0	0	1*H*-Imidazole, 2,4,5-trimethyl-		17.4
4893.	20185-22-2	1	0	0	1*H*-Imidazole, 1,4,5-trimethyl-		17.4
4894.	10111-08-7	1	0	0	1*H*-Imidazole-2-carboxaldehyde		3.12, 17.4
4895.	36734-19-7	0	1	0	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®}		13.1, 14.1, 17.4, 18.4, 21.3, 25.29
4896.	461-72-3	1	0	0	2,4-Imidazolidinedione {hydantoin}		14.1, 17.4
4897.	61893-10-5	1	0	0	2,4-Imidazolidinedione, 1-(1-methylethyl)-		14.1, 17.4
4898.	17374-27-5	1	0	0	2,4-Imidazolidinedione, 1,5-dimethyl-		14.1, 17.4
4899.	61893-09-2	1	0	0	2,4-Imidazolidinedione, 1-ethyl-		14.1, 17.4
4900.	63637-90-1	1	0	0	2,4-Imidazolidinedione, 3-(1-methylethyl)-		14.1, 17.4
4901.	16935-34-5	1	0	0	2,4-Imidazolidinedione, 5-(1-methylethyl)-		14.1, 17.4
4902.	15414-82-1	1	0	0	2,4-Imidazolidinedione, 5-ethyl-		14.1, 17.4
4903.	616-04-6	1	0	0	2,4-Imidazolidinedione, 1-methyl-		14.1, 17.4
4904.		1	0	0	2,4-Imidazolidinedione, 3-methyl-		14.1, 17.4
4905.	616-03-5	1	1	1	2,4-Imidazolidinedione, 5-methyl-		14.1, 17.4
4906.	96-45-7	1	0	0	2-Imidazolidinethione {ethylenethiourea}		17.4, 18.1
4907.	138261-41-3	1	1	1	Imidazolidinimine, 1-((6-chloro-3-pyridinyl)methyl)-*N*-nitro- {Imidacloprid®}		16.1, 17.9, 18.4, 21.3
4908.	61892-75-9	1	0	0	4*H*-Imidazol-4-one, 1,5-dihydro-1-methyl-		17.4, 17.13
4909.	60-27-5	0	1	0	4*H*-Imidazol-4-one, 2-amino-1,5-dihydro-1-methyl- {creatinine}		12.2, 17.4, 17.13
4910.	274-76-0	1	0	0	Imidazo[1,2-*a*]pyridine		17.21
4911.		1	0	0	Imidazo[1,2-*a*]pyridine, C_2-alkyl-		17.21

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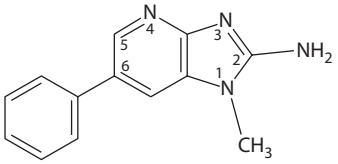
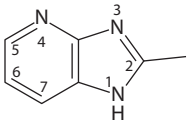
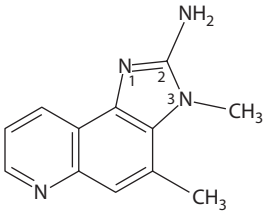
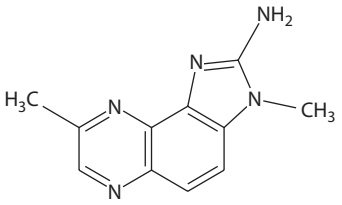
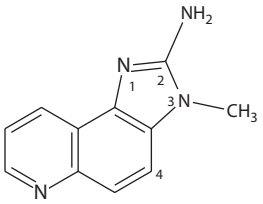
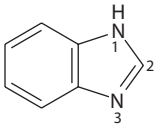
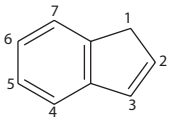
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4912.	875-80-9	1	0	0	Imidazo[1,2-*a*]pyridine, 2,3-dimethyl-		17.21
4913.	105650-23-5	1	0	0	1*H*-Imidazo[4,5-*b*]pyridin-2-amine, 1-methyl-6-phenyl- {PhIP}		12.2, 17.31, 23.5
4914.		1	0	0	1*H*-Imidazo[4,5-*b*]pyridine, methyl-		17.21
4915.	68175-07-5	1	0	0	1*H*-Imidazo[4,5-*b*]pyridine, 2-methyl-		17.21
4916.	27582-20-3	1	0	0	1*H*-Imidazo[4,5-*b*]pyridine, 7-methyl-		17.21
4917.	120293-52-9	0	1	0	1*H*-Imidazo[4,5-*c*]pyridine-4-propanoic acid, 4,6-dicarboxy-4,5,6,7-tetrahydro-, (4R-*cis*)-		4.3, 17.23
4918.	77094-11-2	1	0	0	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3,4-dimethyl- {MeIQ}		12.2, 17.31, 23.5
4919.	77500-04-0	1	0	0	3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 3,8-dimethyl-		12.2
4920.	76180-96-6	1	0	0	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3-methyl- {IQ}		12.2, 17.31, 23.5
4921.	95896-78-9	1	0	0	3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 3,4,8-trimethyl-		12.2
4922.	271-44-3	1	0	0	1*H*-Indazole		17.21
4923.	34879-87-3	0	1	0	1*H*-Indazole, 1,6-dimethyl-		17.21
4924.	95-13-6	1	0	0	1*H*-Indene		1.20, 25.29
4925.	71278-05-2	1	0	0	1*H*-Indene, diethyl-		1.20

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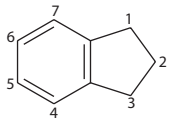
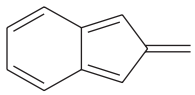
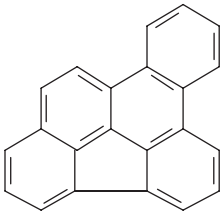
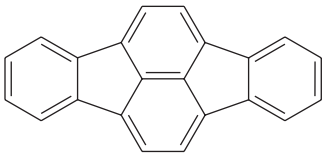
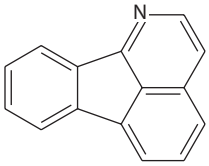
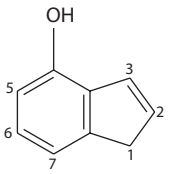
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4926.	496-11-7	1	1	1	1*H*-Indene, 2,3-dihydro- {indane}		1.20
4927.	53563-67-0	1	0	0	1*H*-Indene, 2,3-dihydrodimethyl- {four isomers detected}		1.20
4928.	17057-82-8	1	0	0	1*H*-Indene, 2,3-dihydro-1,2-dimethyl-		1.20
4929.	71278-02-9	1	0	0	1*H*-Indene, 2,3-dihydroethyl-		1.20
4930.	27133-93-3	1	0	0	1*H*-Indene, 2,3-dihydromethyl- {four isomers detected}		1.20
4931.	767-58-8	1	0	0	1*H*-Indene, 2,3-dihydro-1-methyl-		1.20
4932.	824-63-5	1	0	0	1*H*-Indene, 2,3-dihydro-2-methyl-		1.20
4933.	824-22-6	1	0	0	1*H*-Indene, 2,3-dihydro-4-methyl-		1.20
4934.	874-35-1	1	0	0	1*H*-Indene, 2,3-dihydro-5-methyl-		1.20
4935.	16204-57-2	0	1	0	1*H*-Indene, 2,3-dihydro-1,1,4, 5-tetramethyl-		1.20
4936.	942-43-8	0	1	0	1*H*-Indene, 2,3-dihydro-1,1,5,6- tetramethyl-		1.20
4937.	36541-18-1	1	0	0	1*H*-Indene, 2,3-dihydrotrimethyl-		1.20
4938.	29348-63-8	1	0	0	1*H*-Indene, dimethyl-		1.20
4939.	71278-06-3	1	0	0	1*H*-Indene, dimethylethyl-		1.20
4940.		1	0	0	1*H*-Indene, 5,6-dimethyl-2-phenyl-		1.20
4941.		1	0	0	1*H*-Indene, 2-(3′,4′-dimethylphenyl)-		1.20
4942.	58924-35-9	1	0	0	1*H*-Indene, ethyl-		1.20
4943.	77227-01-1	1	0	0	1*H*-Indene, ethylmethyl-		1.20
4944.	71278-07-4	1	0	0	1*H*-Indene, ethylpentamethyl-		1.20
4945.	77242-77-4 86901-30-6	1	0	0	1*H*-Indene, heptamethyl-		1.20
4946.	71278-08-5	1	0	0	1*H*-Indene, hexamethyl-		1.20
4947.	29036-25-7	1	0	0	1*H*-Indene, methyl- {at least three isomers are present in MSS}		1.20
4948.	767-59-9	1	0	0	1*H*-Indene, 1-methyl-		1.20
4949.	2177-47-1	1	0	0	1*H*-Indene, 2-methyl-		1.20
4950.	767-60-2	1	0	0	1*H*-Indene, 3-methyl-		1.20
4951.	2471-84-3	1	0	0	1*H*-Indene, 1-methylene-		1.20
4952.	6596-86-7	1	0	0	2*H*-Indene, 2-methylene- {benzofulvene}		1.20
4953.		1	0	0	1*H*-Indene, 4-methyl-2-(2′-methylphenyl)-		1.20
4954.		1	0	0	1*H*-Indene, 5-methyl-2-(4-methylphenyl)-		1.20
4955.		1	0	0	1*H*-Indene, 6-methyl-2-(4-methylphenyl)-		1.20
4956.		1	0	0	1*H*-Indene, 7-methyl-2-(2′-methylphenyl)-		1.20
4957.		1	0	0	1*H*-Indene, 7-(4′-methylphenyl)-		1.20
4958.	71278-09-6	1	0	0	1*H*-Indene, pentamethyl-		1.20
4959.	38638-41-4	1	0	0	1*H*-Indene, phenyl-		1.20
4960.		1	0	0	1*H*-Indene, 2-phenyl-		1.20
4961.		1	0	0	1*H*-Indene, phenyltrimethyl-		1.20
4962.	27135-78-0	1	0	0	1*H*-Indene, tetramethyl- {at least four isomers present in MSS}		1.20
4963.	60826-61-1	1	0	0	1*H*-Indene, trimethyl- {at least three isomers present in MSS}		1.20
4964.	37414-44-1	1	0	0	1*H*-Indene-2-carboxaldehyde, 2,3-dihydro-		3.12

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
4965.	30084-91-4	1	0	0	1*H*-Indene-5-carboxaldehyde, 2,3-dihydro-		3.12
4966.	606-23-5	1	0	0	1*H*-Indene-1,3(2*H*)-dione		3.13
4967.	668-30-4	1	0	0	Indeno[1,2,3,4-*defg*]chrysene {also known as indeno[3,2,1,7-*defg*] chrysene, dibenzo[*b,mno*]fluoranthene, naphtho[1,2,3,4-*ghi*]fluoranthene}		1.20
4968.	71277-94-6	1	0	0	Indeno[1,2,3,4-*defg*]chrysene, methyl- {indeno[3,2,1,7-*defg*]chrysene, methyl-; dibenzo[*b,mno*]fluoranthene, methyl-; naphtho[1,2,3,4-*ghi*]fluoranthene, methyl-}		1.20
4969.	193-43-1	1	0	0	Indeno[1,2,3-*cd*]fluoranthene		1.20
4970.	41699-07-4	1	0	0	Indeno[1,2,3-*cd*]fluoranthene, methyl-		1.20
4971.	98791-41-4	1	0	0	1*H*-Indeno[1,7-*ab*]fluorene		1.20
4972.	98791-42-5	1	0	0	1*H*-Indeno[1,7-*ab*]fluorene, 2,11-dihydro-		1.20
4973.	206-56-4	1	0	0	Indeno[1,2,3-*ij*]isoquinoline {1-azafluoranthene}		17.21
4974.		1	0	0	Indeno[1,2,3-*ij*]isoquinoline, dimethyl-		17.21
4975.		1	0	0	Indeno[1,2,3-*ij*]isoquinoline, methyl-		17.21
4976.	56631-57-3	1	0	0	1*H*-Indenol [1*H*-Inden-4-ol]		9.22
4977.	72692-86-5	1	0	0	1*H*-Indenol, 2,3-dihydromethyl- [1*H*-Inden-4-ol, 2,3-dihydromethyl-]		9.22
4978.	73850-11-0	1	0	0	1*H*-Indenol, dimethyl- [1*H*-Inden-4-ol, dimethyl-]		9.22
4979.	73850-20-1	1	0	0	1*H*-Indenol, ethylmethyl- [1*H*-Inden-4-ol, ethylmethyl-]		9.22
4980.	73850-12-1	1	0	0	1*H*-Indenol, methyl- [1*H*-Inden-4-ol, methyl-]		9.22
4981.	73850-09-6	1	0	0	1*H*-Indenol, tetramethyl- [1*H*-Inden-4-ol, tetramethyl-]		9.22
4982.	73850-10-9	1	0	0	1*H*-Indenol, trimethyl- [1*H*-Inden-4-ol, trimethyl-]		9.22
4983.	1641-41-4	1	0	0	1*H*-Indenol, 2,3-dihydro- [1*H*-Inden-4-ol, 2,3-dihydro-]		9.22
4984.	1470-94-6	1	0	0	1*H*-Inden-5-ol, 2,3-dihydro-		9.22
4985.	30286-23-8	1	0	0	Indenone, dihydro-		3.13
4986.	72692-87-6	1	0	0	Indenone, 1,3(or 2,3)-dihydrodimethyl-		3.13

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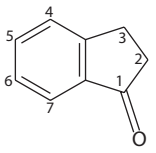
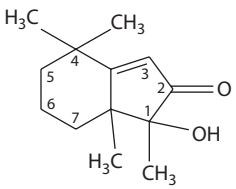
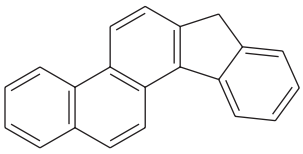
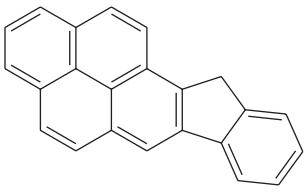
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
4987.	480-90-0	1	0	0	1*H*-Inden-1-one		3.13
4988.	83-33-0	1	0	0	1*H*-Inden-1-one, 2,3-dihydro- {1-indanone}		3.13
4989.	71278-03-0	1	0	0	1*H*-Inden-1-one, 2,3-dihydrodimethyl- {six isomers detected}		3.13
4990.	66309-83-9	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-2,6-dimethyl-		3.13
4991.	17714-57-7	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-3, 5-dimethyl-		3.13
4992.	5037-60-5	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-4, 7-dimethyl-		3.13
4993.	71278-04-1	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-ethyl-		3.13
4994.	57878-30-5	0	1	0	1*H*-Inden-1-one, 2,3-dihydro-5- hydroxy-3-methyl-		3.13
4995.	72692-69-4	1	0	0	1*H*-Inden-1-one, 2,3-dihydro- (methoxymethyl)-		3.13
4996.	65436-86-4	1	0	0	1*H*-Inden-1-one, 2,3-dihydromethyl- {four isomers detected}		3.13
4997.	17496-14-9	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-2-methyl-		3.13
4998.	6072-57-7	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-3-methyl-		3.13
4999.	24644-78-8	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-4-methyl-		3.13
5000.	4593-38-8	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-5-methyl-		3.13
5001.	24623-20-9	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-6-methyl-		3.13
5002.	66288-51-5	1	0	0	1*H*-Inden-1-one, 2,3-dihydrotrimethyl- {three isomers detected}		3.13
5003.	54789-23-0	1	1	1	1*H*-Inden-1-one, 2,3-dihydro-3,3,5,7- tetramethyl-		3.13
5004.	35322-84-0	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-3,4,7- trimethyl-		3.13
5005.	22303-81-7	1	0	0	1*H*-Inden-1-one, 3-methyl-		3.13
5006.	615-13-4	1	0	0	2*H*-Inden-2-one, 1,3-dihydro-		3.13
5007.		1	0	0	2*H*-Inden-2-one, dimethyl-		3.13
5008.		1	0	0	2*H*-Inden-2-one, methyl-		3.13
5009.	39815-71-9	0	1	0	2*H*-Inden-2-one,1,4,5,6,7,7a-hexahydro-1- hydroxy-1,4,4,7a-tetramethyl-		2.5, 3.13
5010.	220-97-3	1	0	0	11*H*-Indeno[2,1-*a*]phenanthrene {11*H*-naphtho[2,1-*a*]fluorene}		1.20
5011.	72254-06-9	1	0	0	Indenopyrene		1.20

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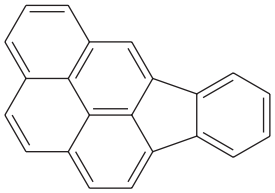
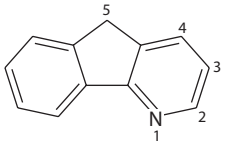
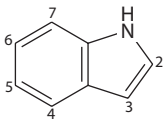
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5012.	193-39-5	1	1	1	Indeno[1,2,3-*cd*]pyrene {*o*-phenylenepyrene}		1.20, 23.5
5013.	64158-99-2	1	0	0	Indeno[1,2,3-*cd*]pyrene, dimethyl- {at least two isomers present in MSS}		1.20
5014.	64158-98-1	1	0	0	Indeno[1,2,3-*cd*]pyrene, methyl- {at least two isomers present in MSS}		1.20
5015.		1	0	0	Indeno[1,2,3-*cd*]pyrene, trimethyl- {at least two isomers present in MSS}		1.20
5016.	244-99-5	1	0	0	5*H*-Indeno[1,2-*b*]pyridine {4-azafluorene}		17.21
5017.		1	0	0	5*H*-Indeno[1,2-*b*]pyridine, dimethyl-		17.21
5018.		1	0	0	5*H*-Indeno[1,2-*b*]pyridine, methyl-		17.21
5019.	7440-74-6	1	1	1	Indium	In	20.5
5020.	120-72-9	1	1	1	1*H*-Indole {2,3-benzopyrrole}		17.21, 26.9
5021.		1	0	0	1*H*-Indole, alkyl-		17.21
5022.	5192-03-0	1	0	0	1*H*-Indole, 5-amino-		12.2
5023.	55191-12-3	1	0	0	1*H*-Indole, 1,3-dibutyl-		17.21
5024.	496-15-1	1	1	1	1*H*-Indole, 2,3-dihydro- {indoline}		17.21
5025.	6872-06-6	0	1	0	1*H*-Indole, 2,3-dihydro-2-methyl-		17.21
5026.		1	0	0	1*H*-Indole, 2,3-dihydro-3-(3-pyridinyl)-		17.9, 17.21
5027.	78210-52-3	1	0	0	1*H*-Indole, 2,3-dihydro-3-(3-pyridinylmethyl)-		17.9, 17.21
5028.	29930-57-2	1	0	0	1*H*-Indole, dimethyl-		17.21
5029.	875-79-6	1	0	0	1*H*-Indole, 1,2-dimethyl-		17.21
5030.	875-30-9	1	0	0	1*H*-Indole, 1,3-dimethyl-		17.21
5031.	27816-52-0	1	0	0	1*H*-Indole, 1,4-dimethyl-		17.21
5032.	27816-53-1	1	0	0	1*H*-Indole, 1,5-dimethyl-		17.21
5033.	5621-15-8	1	0	0	1*H*-Indole, 1,6-dimethyl-		17.21
5034.	5621-16-9	1	0	0	1*H*-Indole, 1,7-dimethyl-		17.21
5035.	91-55-4	1	0	0	1*H*-Indole, 2,3-dimethyl-		17.21
5036.	1196-79-8	1	0	0	1*H*-Indole, 2,5-dimethyl-		17.21
5037.		1	0	0	1*H*-Indole, 2,6-dimethyl-		17.21
5038.	3189-12-6	1	0	0	1*H*-Indole, 3,5-dimethyl-		17.21
5039.	5621-14-7	1	0	0	1*H*-Indole, 3,7-dimethyl-		17.21
5040.	54020-53-0	1	0	0	1*H*-Indole, 5,7-dimethyl-		17.21
5041.	64844-47-9	1	0	0	1*H*-Indole, dimethylethyl-		17.21
5042.	64844-49-1	1	0	0	1*H*-Indole, dimethylpropyl-		17.21
5043.	97542-81-9	1	0	0	1*H*-Indole, ethyl-		17.21
5044.	10604-59-8	1	0	0	1*H*-Indole, 1-ethyl-		17.21
5045.	3484-18-2	1	0	0	1*H*-Indole, 2-ethyl-		17.21
5046.	1484-19-1	1	0	0	1*H*-Indole, 3-ethyl-		17.21

(*continued*)

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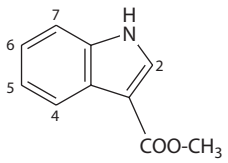
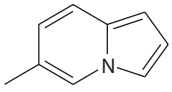
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5047.	68742-28-9	1	0	0	1*H*-Indole, 5-ethyl-		17.21
5048.	64844-45-7	1	0	0	1*H*-Indole, ethylmethyl-		17.21
5049.	64844-50-4	1	0	0	1*H*-Indole, ethylpropyl-		17.21
5050.	27323-28-0	1	1	1	1*H*-Indole, methyl-		17.21
5051.	603-76-9	1	0	0	1*H*-Indole, 1-methyl-		17.21
5052.	95-20-5	1	1	1	1*H*-Indole, 2-methyl-		17.21
5053.	83-34-1	1	1	1	1*H*-Indole, 3-methyl- {skatole}		17.21, 24.3
5054.	16096-32-5	1	0	0	1*H*-Indole, 4-methyl-		17.21
5055.	614-96-0	1	0	0	1*H*-Indole, 5-methyl-		17.21
5056.	3420-02-8	1	0	0	1*H*-Indole, 6-methyl-		17.21
5057.	933-67-5	1	0	0	1*H*-Indole, 7-methyl-		17.21
5058.		1	0	0	1*H*-Indole, (1-methylethyl)-		17.21
5059.	64844-52-6	1	0	0	1*H*-Indole, methylphenyl-		17.21
5060.	64844-46-8	1	0	0	1*H*-Indole, methylpropyl-		17.21
5061.		1	0	0	1*H*-Indole, 1-phenyl-		17.21
5062.	948-65-2	1	1	1	1*H*-Indole, 2-phenyl-		17.21
5063.	1504-16-1	1	0	0	1*H*-Indole, 3-phenyl-		17.21
5064.	64844-44-6	1	0	0	1*H*-Indole, propyl-		17.21
5065.	1859-92-3	1	0	0	1*H*-Indole, 3-propyl-		17.21
5066.	64844-48-0	1	0	0	1*H*-Indole, tetramethyl-		17.21
5067.	30642-36-5	1	0	0	1*H*-Indole, trimethyl-		17.21
5068.	1971-46-6	1	0	0	1*H*-Indole, 1,2,3-trimethyl-		17.21
5069.	10299-63-5	1	0	0	1*H*-Indole, 2,3,4-trimethyl-		17.21
5070.	21296-92-4	1	0	0	1*H*-Indole, 2,3,5-trimethyl-		17.21
5071.	22072-35-1	1	0	0	1*H*-indole, 2,3,6-trimethyl-		17.21
5072.	27505-78-8	1	0	0	1*H*-Indole, 2,3,7-trimethyl-		17.21
5073.		1	0	0	1*H*-Indole, 4,5,6-trimethyl-		17.21
5074.	54340-99-7	1	0	0	1*H*-Indole, 5,6,7-trimethyl-		17.21
5075.	31212-21-2	0	1	0	1*H*-Indoleacetamide		13.1
5076.	32536-43-9	0	1	0	1*H*-Indoleacetic acid		4.3
5077.		0	1	0	1*H*-Indole-2-acetonitrile, 1-methyl-		11.2
5078.	87-51-4	1	1	1	1*H*-Indole-3-acetic acid		4.3, 21.3
5079.	1912-33-0	0	1	0	1*H*-Indole-3-acetic acid, methyl ester		5.3
5080.	771-51-7	0	1	0	1*H*-Indole-3-acetonitrile		11.2, 26.9
5081.	133-32-4	0	1	0	1*H*-Indole-3-butanoic acid		4.3, 21.3
5082.		0	1	0	1*H*-Indole-3-butanoic acid, methyl ester		5.3
5083.	487-89-8	0	1	0	1*H*-Indole-3-carboxaldehyde		3.12
5084.	771-50-6	0	1	0	1*H*-Indole-3-carboxylic acid		4.3
5085.	942-24-5	0	1	0	1*H*-Indole-3-carboxylic acid, methyl ester		5.3
5086.	61-54-1	0	1	0	1*H*-Indole-3-ethanamine		12.2
5087.	526-55-6	0	1	0	1*H*-Indole-3-ethanol		2.5
5088.	830-96-6	0	1	0	1*H*-Indole-3-propanoic acid		4.3
5089.	5548-09-4	0	1	0	1*H*-Indole-3-propanoic acid, methyl ester		5.3
5090.	35656-49-6	0	1	0	1*H*-Indolepropanoic acid, α-oxo-		3.13, 4.3
5091.	392-12-1	0	1	0	1*H*-Indole-3-propanoic acid, α-oxo-		3.13, 4.3
5092.	1761-10-0	0	1	0	Indolizine, 3-methyl-		17.21
5093.	1761-11-1	1	0	0	Indolizine, 6-methyl-		17.21

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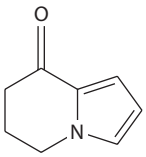
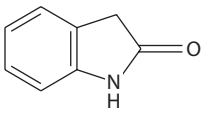
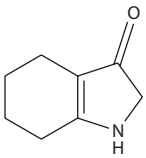
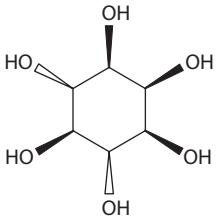
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5094.	54906-44-4	1	1	1	8(5*H*)-Indolizinone, 5,6,7,8-tetrahydro-{5-oxocyclohexa[*a*]pyrrole}		3.13
5095.	55041-88-8	0	1	0	8(5*H*)-Indolizinone, 6,7-dihydro-2-methyl-		3.13
5096.	50-67-9	1	1	1	1*H*-Indol-5-ol, 3-(2-aminoethyl)-		9.22, 12.2
5097.	59-48-3	1	0	0	2*H*-Indol-2-one, 1,3-dihydro-{phthalimidine, oxindole}		17.13
5098.	15379-45-0	1	0	0	2*H*-Indol-2-one, 1,3-dihydro-3-ethyl-		17.13
5099.	1504-06-9	1	0	0	2*H*-Indol-2-one, 1,3-dihydro-3-methyl-		17.13
5100.	20200-86-6	0	1	0	2*H*-Indol-2-one, 1,3-dihydro-1,3,3-trimethyl-		17.13
5101.	58074-25-2	0	1	0	3*H*-Indol-3-one, 2,3,4,5,6,7-hexahydro-{4,5,6,7-tetrahydro-3-indolinone}		3.13
5102.	6917-35-7	1	1	1	Inositol		0.4, 2.5, 8.3
5103.	87-89-8	1	1	1	myo-Inositol		2.5, 8.3
5104.	3615-82-5	0	1	0	myo-Inositol, hexakis(dihydrogen phosphate), calcium magnesium salt {phytin}		0.4, 2.5, 20.6
5105.	71608-14-5	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino] octadecyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5106.	71608-17-8	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-1-[(2-hydroxy-1-oxopentacosyl)amino] octadecyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5107.	71608-15-6	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino] octadecyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6

(*continued*)

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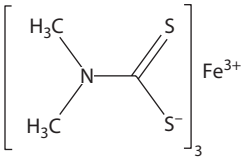
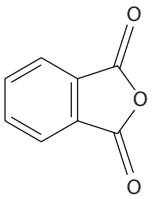
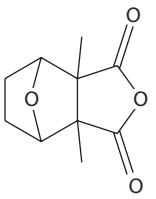
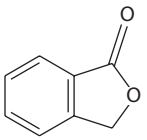
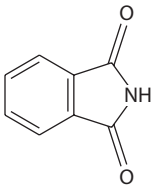
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5108.	71608-16-7	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl) amino]octadecyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5109.	71608-19-0	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl) amino]-8-octadecenyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5110.	71608-20-3	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5111.	71608-21-4	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5112.	71608-22-5	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxopentacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5113.	71608-23-6	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1→4)-*O*-alpha-*D*-glucopyranuronosyl-(1→2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxohexacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt		2.5, 8.3, 10.2, 20.6
5114.	89194-80-9	0	1	0	myo-Inositol, *O*-*D*-glucopyranosyl-		2.5, 8.3, 10.2, 20.6
5115.	49741-70-0	0	1	0	*D*-myo-Inositol, *O*-*D*-glucopyranosyl-		2.5, 8.3, 10.2
5116.		0	1	0	myo-Inositol, phosphatidyl-		2.5, 8.3
5117.	9025-67-6	0	1	0	Inulase		0.4, 22.2
5118.	20461-54-5	0	1	0	Iodide	I^{-1}	18.4, 20.5
5119.	7553-56-2	1	1	1	Iodine	I_2	0.4, 18.4, 19.5, 20.5
5120.	7439-88-5	1	1	1	Iridium	Ir	20.5
5121.	7439-89-6	1	1	1	Iron	Fe	0.4, 20.5
5122.	15438-31-0	1	1	1	Iron, ferrous ion	Fe^{+2}	20.5, 27.1
5123.		1	0	0	Iron, ferric ion	Fe^{+3}	20.5, 27.1
5124.	14596-12-4	1	1	1	Iron, isotope of mass 59	^{59}Fe	20.5
5125.	15281-98-8	1	0	0	Iron carbonyl	$Fe(CO)_4$	20.6

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5126.	7705-08-0	0	1	0	Iron chloride (ferric chloride)	$FeCl_3$	18.4, 20.6
5127.	1309-37-1 1332-37-2	0	1	0	Iron oxide (ferric oxide)	Fe_2O_3	20.6
5128.	13463-40-6	1	0	0	Iron pentacarbonyl	$Fe(CO)_5$	20.6
5129.	14484-64-1	0	1	0	Iron, tris(dimethylcarbamodithioato-S, S′)-, (OC-6-11)- {Ferbam®}		18.1, 20.6, 21.3
5130.	85-44-9	1	1	1	1,3-Isobenzofurandione {phthalic anhydride}		7.1
5131.	56-25-7	0	1	0	1,3-Isobenzofurandione, 3a,7a-dimethyl-4,7-epoxy-hexahydro- {cantharidin}		7.1, 10.2
5132.	87-41-2	0	1	0	1(3*H*)-Isobenzofuranone {phthalide}		6.3
5133.		1	0	0	1(3*H*)-Isobenzofuranone, methyl-		6.3
5134.	551-08-6	0	1	0	1(3*H*)-Isobenzofuranone, 3-butylidene-		6.3
5135.	13277-77-5	0	1	0	1(3*H*)-Isobenzofuranone, 3,7-dihydroxy-3,4,5,6-tetramethyl-		6.3
5136.	66309-76-0	1	0	0	1(3*H*)-Isobenzofuranone, 4,5,6,7-tetrahydro-		6.3
5137.	75-13-8	0	1	0	Isocyanic acid	H-N=C=O	19.5
5138.	52845-07-5	1	0	0	Isoeicosane		1.10
5139.	52655-10-4	0	1	0	Isoeicosanol		2.5
5140.	54365-40-1	1	1	1	Isoheptacosane		1.10
5141.	85-41-6	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione {phthalimide}		14.1
5142.	66309-86-2	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4,5-dimethyl-		14.1
5143.	17100-62-8	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4,6-dimethyl-		14.1
5144.	15540-88-2	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4,7-dimethyl-		14.1
5145.		1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, methyl-		14.1
5146.	7251-82-3	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4-methyl-		14.1
5147.	40314-06-5	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 5-methyl-		14.1
5148.	550-44-7	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, *N*-methyl-		14.1

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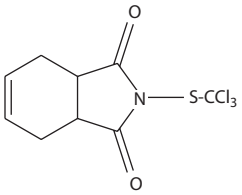
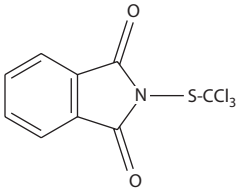
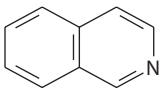
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5149.	133-06-2	1	1	1	1*H*-Isoindole-1,3(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]- {Captan®}		14.1, 18.1, 18.4, 21.3
5150.	133-07-3	0	1	0	1*H*-Isoindole-1,3(2*H*)-dione, 2-[(trichloromethyl)thio]- {Folpan®}		14.1, 18.1, 18.4, 21.3
5151.	480-91-1	1	0	0	1*H*-Isoindol-1-one, 2,3-dihydro- {phthalimidine}		14.1
5152.	6091-76-5	1	0	0	1*H*-Isoindol-1-one, 2,3-dihydro-3-methyl-		14.1
5153.	7004-09-3	0	1	0	Isoleucine	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 12.2
5154.	1509-34-8	0	1	0	Isoleucine, allo-		4.3, 4.10, 12.2
5155.	73-32-5	0	1	0	*L*-Isoleucine	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 12.2, 24.3, 25.29
5156.	139681-66-6	0	1	0	*L*-Isoleucine, *N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-valyl)-*L*-phenylalanyl]-*L*-leucyl]-		4.3, 4.10, 12.2, 18.1
5157.	80449-01-0	0	1	0	Isomerase, deoxyribonucleate topo-		22.2
5158.	9001-41-6	0	1	0	Isomerase, glucose phosphate		22.2
5159.	9055-95-2	0	1	0	Isomerase, pentose phosphate		22.2
5160.	9023-83-0	0	1	0	Isomerase, ribose phosphate		22.2
5161.	52701-70-9	0	1	0	Isopentacosane		1.10
5162.	27836-87-9	0	1	0	Isopentadecanoic acid		4.3
5163.		0	1	0	Isoperoxidase A_3		22.2
5164.		1	0	0	Isoquinolinamine		12.2
5165.	1532-84-9	1	0	0	1-Isoquinolinamine		12.2
5166.	119-65-3	1	1	1	Isoquinoline		17.21
5167.	64828-50-8	1	0	0	Isoquinoline, butyl-		17.21
5168.	7661-38-3	1	0	0	Isoquinoline, 1-butyl-		17.21
5169.	64973-79-1	1	0	0	Isoquinoline, dihydro-		17.21
5170.	65312-77-8	1	0	0	Isoquinoline, dihydroethyl-		17.21
5171.	65312-79-0	1	0	0	Isoquinoline, dihydromethyl-		17.21
5172.		1	0	0	Isoquinoline, dimethyl-		17.21
5173.	64828-51-9	1	0	0	Isoquinoline, ethyl-		17.21
5174.	61010-32-0	0	1	0	Isoquinoline, 1-[(4-methoxy-3-nitrophenyl)methyl]-, mononitrate		10.2, 16.1
5175.	58853-80-8	1	0	0	Isoquinoline, methyl- {several methylquinolines detected in MSS}		17.21
5176.	1721-93-3	1	0	0	Isoquinoline, 1-methyl-		17.21
5177.	4965-09-7	1	0	0	Isoquinoline, 1-methyl-1,2,3,4-tetrahydro-		17.21
5178.	1125-80-0	1	0	0	Isoquinoline, 3-methyl-		17.21
5179.	64828-49-5	1	0	0	Isoquinoline, (1-methylethyl)-		17.21
5180.		1	0	0	Isoquinoline, methyltetrahydro-		17.21
5181.	64849-98-5	1	0	0	Isoquinoline, propyl-		17.21

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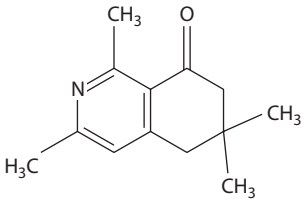
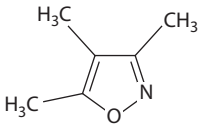
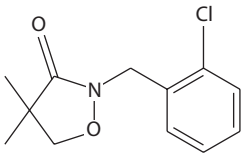
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5182.	29832-78-8	1	0	0	Isoquinoline, tetrahydro-		17.21
5183.	65312-75-6	1	0	0	Isoquinoline, tetrahydro methyl-		17.21
5184.	91-21-4	1	0	0	Isoquinoline, 1,2,3,4-tetrahydro-		17.21
5185.	36556-06-6	1	0	0	Isoquinoline, 5,6,7,8-tetrahydro-		17.21
5186.	64849-99-6	1	0	0	Isoquinolinecarbonitrile		11.2
5187.	1198-30-7	1	0	0	1-Isoquinolinecarbonitrile		11.2
5188.		0	1	0	5,6-Isoquinolinedione, 7,8-dihydro-1,3,7,7-tetramethyl-		3.13
5189.	55713-38-7	0	1	0	8(5*H*)-Isoquinolinone, 6,7-dihydro-1,3,6,6-tetramethyl- [6,7-dihydro- or 5,6,7,8-tetrahydro-?]		3.13
5190.	27137-10-6	1	0	0	Isotetradecanoic acid, methyl ester		5.3
5191.	556-61-6	0	1	0	Isothiocyanic acid, methyl- {Trapex®}	H_3C-N=S	18.1, 21.3
5192.	288-16-4	1	0	0	Isothiazole		18.1
5193.	34425-19-9	1	0	0	Isotriacontane		1.10
5194.	288-14-2	0	1	0	Isoxazole		17.15
5195.	300-87-8	0	1	0	Isoxazole, 3,5-dimethyl-		17.15
5196.	5765-44-6	1	0	0	Isoxazole, 5-methyl-		17.15
5197.	10557-82-1	1	0	0	Isoxazole, trimethyl- = isoxazole, 3,4,5-trimethyl-		17.15
5198.	81777-89-1	0	1	0	3-Isoxazolidinone, 2-[(2-chlorophenyl) methyl]-4,4-dimethyl- {Clomazone®}		17.15, 18.4, 21.3
5199.	1318-74-7	0	1	0	Kaolinite		20.6
5200.	9013-02-9	0	1	0	Kinase (phosphorylating), adenylate		22.2
5201.	9012-50-4	0	1	0	Kinase (phosphorylating), aspartate		22.2
5202.	9026-67-9	0	1	0	Kinase (phosphorylating), choline		22.2
5203.	9030-51-7	0	1	0	Kinase (phosphorylating), fructo-		22.2
5204.	9001-36-9	0	1	0	Kinase (phosphorylating), gluco-		22.2
5205.	9026-62-4	0	1	0	Kinase (phosphorylating), glucurono-		22.2
5206.	9001-51-8	0	1	0	Kinase (phosphorylating), hexo-		22.2
5207.	9032-66-0	0	1	0	Kinase (phosphorylating), nicotinamide adenine dinucleotide		22.2
5208.	9001-80-3	0	1	0	Kinase (phosphorylating), phosphofructo-		22.2
5209.	9032-96-6	0	1	0	Kinase (phosphorylating), phosphogluco-		22.2
5210.	150656-38-5	0	1	0	Kinase (phosphorylating), protein (tobacco BY-2 cell isoenzyme ZmPK1 reduced)		22.2
5211.	9001-59-6	0	1	0	Kinase (phosphorylating), pyruvate		22.2
5212.	9027-40-1	0	1	0	Kinase (phosphorylating), pyruvate-phosphate di-		22.2
5213.	9030-57-3	0	1	0	Kinase (phosphorylating), ribulo-		22.2
5214.	9031-51-0	0	1	0	Kinase (phosphorylating), shikimate		22.2
5215.		0	1	0	Kinase, protein		22.2

(*continued*)

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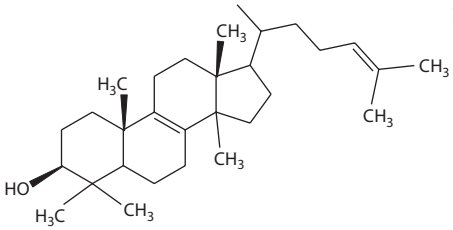
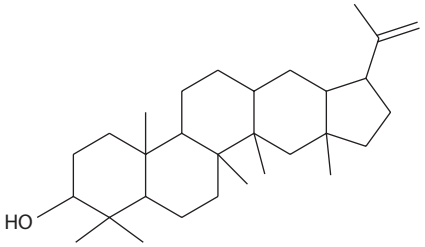
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5216.		0	1	0	*Klebsiella oxytoca*		22.2
5217.	9031-11-2	0	1	0	Lactase		22.2
5218.	63-42-3	0	1	0	Lactose		0.4, 2.5, 8.3, 10.2, 25.29
5219.	79-62-9	0	1	0	Lanost-8-en-3-ol, (3β)-		2.5, 2.7
5220.	6890-88-6	0	1	0	Lanost-8-en-3-ol, 24-methylene-, (3β)-		2.5, 2.7
5221.	26409-08-5	0	1	0	Lanost-9(11)-en-3-ol, 24,25-epoxy-, (3β)-		2.5, 2.7
5222.	79-63-0	0	1	0	Lanosta-8,24-dien-3-ol, (3β)- {lanosterol}		2.5, 2.7
5223.	67493-77-0	0	1	0	Lanostane-3,7,11-triol, 3,7-diacetate, (3β,7β,11β)-		2.5, 2.7, 5.3
5224.	70898-27-0	0	1	0	Lanostane-3,7-diol, (3β,7β)-		2.5, 2.7
5225.	7439-91-0	1	1	1	Lanthanum	La	20.5
5226.	13981-28-7	1	1	1	Lanthanum, isotope of mass 140	^{140}La	20.5
5227.	7439-92-1	1	1	1	Lead	Pb	0.4, 20.5, 23.5
5228.	14255-04-0	1	1	1	Lead, isotope of mass 210	^{210}Pb	20.5
5229.	15092-94-1	0	1	0	Lead, isotope of mass 212	^{212}Pb	20.5
5230.	15067-28-4	0	1	0	Lead, isotope of mass 214	^{214}Pb	20.5
5231.		0	1	0	Lead, isotope of mass 218	^{218}Pb	20.5
5232.	97281-47-5	0	1	0	Lecithins		12.2
5233.	7005-03-0	1	1	1	Leucine	$(H_3C)_2$═CH-CH_2-CH(NH_2)-COOH	0.4, 4.3, 4.10, 12.2, 24.3, 25.29
5234.	61-90-5	1	1	1	*L*-Leucine		4.3, 4.10, 12.2
5235.	139681-65-5	0	1	0	*L*-Leucine, *N*-[*N*-[*N*-[*N*-[*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-phenylalanyl)-*L*-seryl]-*L*-leucyl]-*L*-leucyl]-*L*-methionyl]-*L*-valyl]-*L*-valyl]-		4.3, 4.10, 12.2, 18.1
5236.	9005-53-2	0	1	0	Lignin		0.4, 8.3, 25.29
5237.	8068-04-0	0	1	0	Lignin, Klason		8.3
5238.	8068-00-6	0	1	0	Lignin, milled wood		8.3
5239.		0	1	0	Limulus amoebocyte lysate (LAL)		22.2
5240.	9001-62-1	0	1	0	Lipase {lipase, triacylglycerol}		0.4, 22.2
5241.		0	1	0	Lipopolysaccharide (LPS)		22.2
5242.	9029-60-1	0	1	0	Lipoxygenase		22.2
5243.	7439-93-2	1	1	1	Lithium	Li	0.4, 20.5
5244.	17341-24-1	0	1	0	Lithium, ion	Li^{+1}	20.5
5245.	12057-24-8	0	1	0	Lithium oxide	Li_2O	20.6
5246.	545-47-1	0	1	0	Lup-20(29)-en-3-ol, (3β)-		2.5, 2.7
5247.	7439-94-3	1	1	1	Lutecium	Lu	20.5
5248.	9045-78-7	0	1	0	Lyase, isocitrate		22.2

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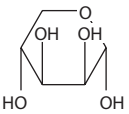
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5249.	9015-75-2	0	1	0	Lyase, pectate		22.2
5250.		0	1	0	*Lyngbya*		22.2
5251.	6899-06-5	0	1	0	Lysine {2,6-diaminohexanoic acid}	H_2N-$(CH_2)_4$-CH(NH_2)-COOH	0.4, 4.3, 4.10, 12.2
5252.	1190-94-9 28902-93-4	0	1	0	Lysine, hydroxy-		2.5. 4.3, 4.10, 12.2
5253.	56-87-1	0	1	0	*L*-Lysine	H_2N-$(CH_2)_4$-CH(NH_2)-COOH	4.3, 4.10, 12.2, 24.3, 25.29
5254.	1114-34-7	1	1	1	Lyxose		2.5, 8.3, 10.2
5255.	90803-60-4	0	1	0	M-1nkh		22.2
5256.	14428-12-7	0	1	0	Magnesate(1-), [9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(3-)-*N*23,*N*24,*N*25,*N*26]-, hydrogen, [*SP*-4-2-[3*S*-(3α,4β,21β)]]-{chlorophyllide b}		17.5, 20.6
5257.	14897-06-4	0	1	0	Magnesate(1-), [9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(3-)-*N*23,*N*24,*N*25,*N*26]-, hydrogen, [*SP*-4-2-[3*S*-(3α,4β,21β)]]-{chlorophyllide a}		17.5, 20.6
5258.	15611-43-5	0	1	0	Magnesate(3-), [18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12,17-tetramethyl-21*H*,23*H*-porphine-2-propanoato(5-)-*N*21,*N*22,*N*23,*N*24]-, trihydrogen, [*SP*-4-2-(2*S*-*trans*)]-{chlorophyllin}		17.5, 20.6
5259.	7439-95-4	1	1	1	Magnesium	Mg	0.4, 20.5
5260.	22537-22-0	0	1	0	Magnesium, ion	Mg^{+2}	20.5
5261.	7791-18-6	0	1	0	Magnesium chloride	$MgCl_2$	18.4, 20.6
5262.	1309-48-4	0	1	0	Magnesium oxide	MgO	20.6
5263.	479-61-8 42617-16-3	0	1	0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-*N*23,*N*24,*N*25,*N*26]-, [*SP*-4-2-[3*S*-[3α(2E,7*S**,11*S**),4β,21β]]]-{chlorophyll a}		0.4, 17.5, 20.6
5264.	519-62-0	0	1	0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-*N*23,*N*24,*N*25,*N*26]-, [*SP*-4-2-[3*S*-[3α(2E,7*S**,11*S**),4β,21β]]]-{chlorophyll b}		17.5, 20.6
5265.	7439-96-5	1	1	1	Manganese	Mn	0.4, 20.5, 26.9

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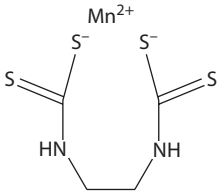
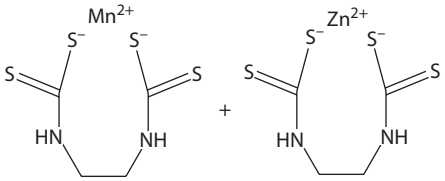
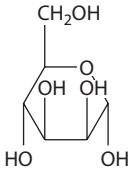
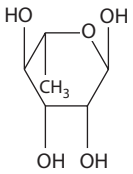
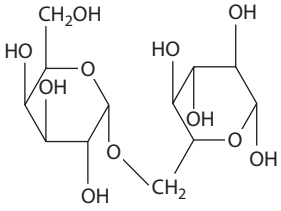
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5266.	13446-35-0	0	1	0	Manganese chloride	$MnCl_4$	18.4, 20.6
5267.	12427-38-2	0	1	0	Manganese, [[1,2-ethanediylbis [carbamodithioato]](2-)]- {Maneb®}		18.1, 20.6, 21.3
5268.	8018-01-7	0	1	0	Manganese, [[1,2-ethanediylbis [carbamodithioato]](2-)] + zinc, [[1,2-ethanediylbis-[carbamodithioato]] (2-)] {Mancozeb®}		18.1, 20.6, 21.3
5269.	16397-91-4	0	1	0	Manganese, ion	Mn^{+2}	20.5
5270.	14681-52-8	0	1	0	Manganese, isotope of mass 56	^{56}Mn	20.5
5271.	69-65-8	1	1	1	*D*-Mannitol {cordycepic acid}	$HOCH_2$-$(CHOH)_4$-CH_2OH	2.5, 8.3
5272.	31103-86-3	1	1	1	Mannose		2.5, 8.3, 10.2, 24.3, 25.29
5273.	3458-28-4	1	1	1	*D*-Mannose {seminose}		2.5, 8.3, 10.2
5274.	14307-02-9	0	1	0	*D*-Mannose, 2-amino-2-deoxy- {mannosamine}		2.5, 8.3, 10.2, 12.2
5275.	3615-41-6	1	1	1	*L*-Mannose, 6-deoxy- {α-rhamnose}		0.4, 2.5, 8.3, 10.2
5276.	9025-42-7	0	1	0	Mannosidase, α-		22.2
5277.	9024-05-9	0	1	0	*Megasphaera*		22.2
5278.	8049-97-6	0	1	0	Melanin		0.4, 22.2
5279.	585-99-9	0	1	0	Melibiose		2.5, 8.3, 10.2
5280.	7439-97-6	1	1	1	Mercury	Hg	0.4, 20.5, 23.5
5281.	13982-78-0	0	1	0	Mercury, isotope of mass 203	^{203}Hg	20.5
5282.	9002-91-9	0	1	0	Metaldehyde {acetaldehyde tetramer}		21.3
5283.	74-89-5	1	1	1	Methanamine {methylamine}	H_3C-NH_2	0.4, 12.2
5284.	75-50-3	1	1	1	Methanamine, *N,N*-dimethyl- {trimethylamine}	$(H_3C)_3{\equiv}N$	0.4, 12.2
5285.	124-40-3	1	1	1	Methanamine, *N*-methyl- {dimethylamine}	$(H_3C)_2{=}NH$	0.4, 12.2
5286.	62-75-9	1	1	1	Methanamine, *N*-methyl-*N*-nitroso- {NDMA}	$(H_3C)_2{=}N$-NO	12.2, 15.8, 23.5

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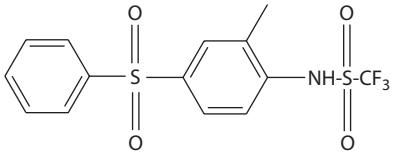
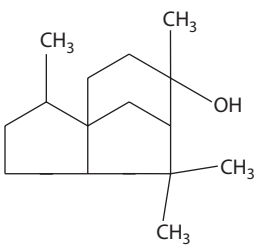
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5287.	107-43-7	0	1	0	Methanaminium, 1-carboxy-*N,N,N*-trimethyl-, inner salt {betaine}	$^{-}OOC\text{-}CH_2\text{-}N^{+}\equiv(CH_3)_3$	0.4, 12.2
5288.	74-82-8	1	0	0	Methane	CH_4	0.4, 1.10
5289.	74-83-9	1	1	1	Methane, bromo- {Brom-o-Gas®, Meth-o-Gas®, ProFum®, Terr-o-Gas®, Zytox®}	$H_3C\text{-}Br$	18.4, 21.3
5290.	74-87-3	1	1	1	Methane, chloro-	$H_3C\text{-}Cl$	18.4, 21.3
5291.	782-08-1	1	0	0	Methane, chlorobis(4-chlorophenyl)-		18.4
5292.	75-09-2	1	1	1	Methane, dichloro-	$H_2C{=}Cl_2$	18.4, 21.3
5293.	75-71-8	1	0	0	Methane, dichlorodifluoro-	CF_2Cl_2	18.4
5294.	74-88-4	1	1	1	Methane, iodo-	$H_3C\text{-}I$	18.4
5295.	624-83-9	1	0	0	Methane, isocyanato- {methyl isocyanate}	$H_3C\text{-}N{=}C{=}O$	5.3
5296.	75-52-5	1	0	0	Methane, nitro-	$H_3C\text{-}NO_2$	16.1, 23.5
5297.	76-06-2	0	1	0	Methane, nitrotrichloro- {Chloropicrin®}	$Cl_3{\equiv}C\text{-}NO_2$	16.1, 18.4, 21.3
5298.	115-10-6	1	1	1	Methane, oxybis- {dimethyl ether}	$H_3C\text{-}O\text{-}CH_3$	10.2
5299.	67-68-5	0	1	0	Methane, sulfinylbis-		18.1
5300.	75-18-3	1	1	1	Methane, thiobis- {methyl sulfide}	$(H_3C)_2{=}S$	18.1
5301.	67-66-3	1	1	1	Methane, trichloro- {chloroform}	$H\text{-}C{\equiv}Cl_3$	18.4, 21.3
5302.	75-69-4	1	1	1	Methane, trichlorofluoro-	$F\text{-}C{\equiv}Cl_3$	18.4
5303.	37924-13-3	0	1	0	Methanesulfonamide, trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl)- {Perfluidone®}		21.3
5304.	74-93-1	1	1	1	Methanethiol {methyl mercaptan}	$H_3C\text{-}SH$	18.1
5305.	475-20-7	0	1	0	1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1α,3aβ,4α,8aβ)]-		1.12
5306.	11028-42-5	0	1	0	1*H*-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl {cedrene}		1.12
5307.	469-61-4	0	1	0	1*H*-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,7β,8aα)]- {α-cedrene}		1.12
5308.	19870-75-8	0	1	0	1*H*-3a,7-Methanoazulene, 6-methoxy-octahydro-3,6,8,8-tetramethyl- {cedryl methyl ether}		10.2
5309.	77-53-2	0	1	0	1*H*-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,6α,7β,8aα)]-		2.5
5310.	4586-22-5	0	1	0	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, stereoisomer		2.5
5311.	17622-35-4	0	1	0	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, acetate, stereoisomer		5.3

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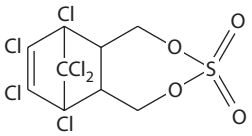
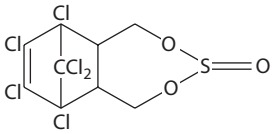
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5312.	1031-07-8	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3,3-dioxide {Thiodan® sulfate, Endosulfan® sulfate}		18.1, 18.4, 21.3
5313.	115-29-7	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide {Thiodan®, Thiosulfan®, Endosulfan®}		18.1, 18.4, 21.3, 25.29
5314.	33213-65-9	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aα,6β,9β,9aα)- {β-Endosulfan®}		18.1, 18.4, 21.3
5315.	959-98-8	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aβ,6α,9α,9aβ)- {α-Endosulfan®}		18.1, 18.4, 21.3
5316.	88125-11-5	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 1a,2,3,4,7a,7b-hexahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,7aα,7bα)]-		3.13
5317.	105300-09-2	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 1a-[(β-*D*-glucopyranosyloxy) methyl]octahydro-5,7b- dimethyl-[1aR-(1aa,2b,4ab,5a,7aa,7ba)]-		2.5, 3.13, 8.3, 10.2
5318.	125537-96-4	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 3-(β-*D*-glucopyranosyloxy) octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,3β,4aβ, 5α,7aα,7bα)]-		2.5, 3.13, 8.3, 10.2
5319.	125537-95-3	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 4-(β-*D*-glucopyranosyloxy) octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4β,4aβ,5α,7aα,7bα)]-		2.5, 3.13, 8.3, 10.2
5320.	105300-10-5	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 5-[(β-*D*-glucopyranosyloxy) methyl]octahydro-1a,7b-dimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		2.5, 3.13, 8.3, 10.2
5321.	88848-60-6	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, 6-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl) oxy]octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,6β,7aα,7bα)]-		2.5, 3.13, 8.3, 10.2
5322.	68690-84-6	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*] naphthalen-7-one, octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-		3.13

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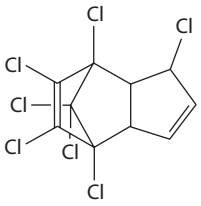
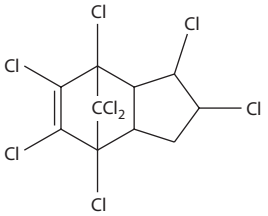
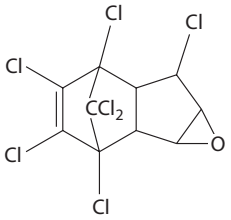
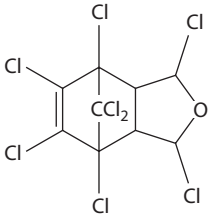
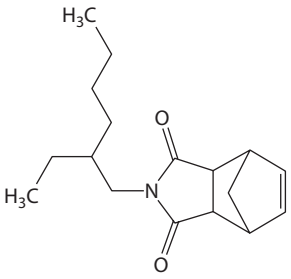
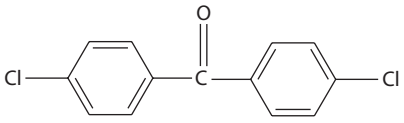
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5323.	76-44-8	1	1	1	4,7-Methano-1*H*-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- {Heptachlor®}		18.4, 21.3
5324.	5103-71-9	0	1	0	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- {α-Chlordane®}		18.4, 21.3
5325.	57-74-9 12789-03-6	0	1	0	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- {γ-Chlordane®}		18.4, 21.3
5326.	1024-57-3	1	1	1	2,5-Methano-2*H*-indeno[1,2-*b*]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)- {Heptachlor® epoxide}		10.2, 18.4, 21.3
5327.	297-78-9	1	1	1	4,7-Methanoisobenzofuran,1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro- {Isobenzan®, Telodrin®}		10.2, 18.4, 21.3
5328.	113-48-4	0	1	0	4,7-Methano-1*H*-isoindole-1,3(2*H*)-dione, 2-(2-ethylhexyl)-3a,4,7,7a-tetrahydro-		14.1, 21.3
5329.	67-56-1	1	1	1	Methanol	H_3C-OH	0.4, 2.5
5330.	5293-97-0	1	1	1	Methanone, bis(2-chlorophenyl)-		3.13, 18.4, 21.3
5331.	90-98-2	1	0	0	Methanone, bis(4-chlorophenyl)-		3.13, 18.4, 21.3
5332.	24966-13-0	1	0	0	Methanone, cyclopropyl-3-pyridinyl-		3.13, 17.7
5333.	119-61-9	1	1	1	Methanone, diphenyl- {benzophenone}	C_6H_5-CO-C_6H_5	3.13, 24.3, 25.29
5334.	5162-03-8	0	1	0	Methanone, (2-chlorophenyl)phenyl-		3.13, 18.4

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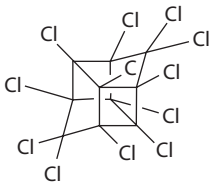
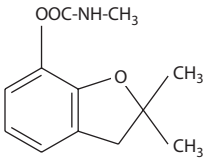
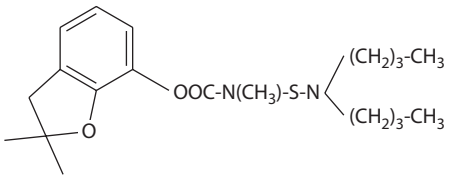
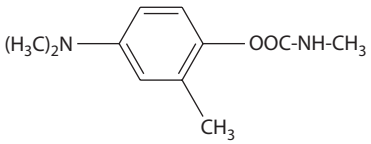
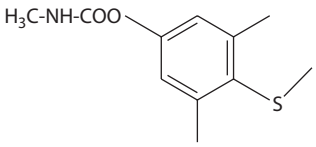
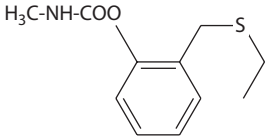
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5335.	2385-85-5	0	1	0	1,3,4-Metheno-1*H*-cyclobuta[*cd*]) pentalene, 1,1a,2,2,3,3a,4,5,5,5a,5b,6-dodecachlorooctahydro- {Mirex®}		21.3
5336.	7005-18-7	0	1	0	Methionine		4.3, 4.10, 18.1
5337.	63-68-3	0	1	0	*L*-Methionine	$H_3C\text{-}S\text{-}(CH_2)_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 4.3, 4.10, 18.1, 24.3, 25.29
5338.	20236-97-9	0	1	0	*D*-Methionine, *N*-(carboxyacetyl)-		4.3, 4.10, 18.1
5339.		1	0	0	Methoxy, amido-	$NH_2\text{-}CO\text{-}CH_2O$	27.1
5340.		1	0	0	Methoxy, amino-	$NH_2\text{-}CH_2O$	27.1
5341.		1	0	0	Methoxy, phenyl-	$C_6H_5\text{-}CH_2O$	27.1
5342.	2143-68-2	1	0	0	Methoxy radical	CH_3O	27.1
5343.	2229-07-4	1	0	0	Methyl radical	CH_3	27.1
5344.	1563-66-2	1	1	1	Methylcarbamic acid, 2,3-dihydro-2, 2-dimethyl-7-benzofuranyl ester Sometimes listed as 7-benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate {Furadan®, Carbofuran®}		5.3, 10.2, 21.3
5345.	55285-14-8	0	1	0	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl [(di-*N*-butylamino) thio] ester {Carbosulfan®}		5.3, 10.2, 12.2, 18.1, 21.3
5346.	2032-59-9	0	1	0	Methylcarbamicacid,4-(dimethylamino)-3-methylphenyl ester {Aminocarb®}		5.3, 12.2, 21.3
5347.	2032-65-7	0	1	0	Methylcarbamic acid, 3,5-dimethyl-4-(methylthio)phenyl ester {Methiocarb®}		5.3, 18.1, 21.3
5348.	16709-30-1	0	1	0	Methylcarbamicacid,2,2-dimethyl-3(2*H*)-oxobenzofuran-7-yl ester		3.13, 5.3, 10.2,
5349.	29973-13-5	0	1	0	Methylcarbamic acid, 2-((ethylthio) methyl)phenyl ester {Ethiofencarb®}		5.3, 18.1, 21.3
5350.	1822-74-8	1	0	0	Methyl ethenyl sulfide	$H_3C\text{-}S\text{-}CH{=}CH_2$	18.1
5351.	50936-45-3	0	1	0	Methyltransferase, caffeate		22.2
5352.	9012-25-3	0	1	0	Methyltransferase, catechol		22.2
5353.	152288-82-9	0	1	0	Methyltransferase, catechol (tobacco clone OMT3.4 isoenzyme II reduced)		22.2

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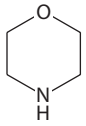
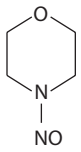
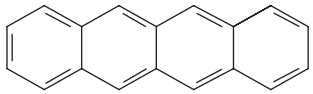
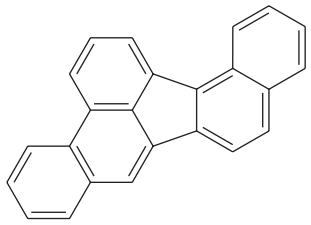
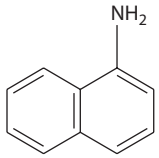
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5354.	9012-40-2	0	1	0	Methyltransferase, homocysteine {transmethylase}		18.1, 22.2
5355.	9027-77-4	0	1	0	Methyltransferase, methionine S-		18.1, 22.2
5356.	9055-07-6	0	1	0	Methyltransferase, protein (arginine)		22.2
5357.	9075-39-2	0	1	0	Methyltransferase, putrescine		22.2
5358.		0	1	0	*Microcystis*		22.2
5359.	7439-98-7	1	1	1	Molybdenum	Mo	0.4, 20.5
5360.	16065-87-5	0	1	0	Molybdenum, ion	Mo^{+6}	20.5
5361.	110-91-8	0	1	0	Morpholine {tetrahydro-2*H*-1, 2-oxazine, tetrahydro-}		10.2, 17.15
5362.	110488-70-5	0	1	0	Morpholine, 3-(3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl)- {Dimethomorph®, Acrobat®}		10.2, 17.15, 18.4, 21.3
5363.	147688-58-2	0	1	0	Morpholine, 2,2-dimethyl-		10.2, 17.15
5364.	59-89-2	1	1	1	Morpholine, 4-nitroso- {NMOR}		10.2, 15.8, 17.15, 23.5
5365.	70699-77-3	0	1	0	3-Morpholinepropanamide, 2-oxo-6-(1,2,3,4-tetrahydroxybutyl)-, [3S-[3α,6α(1R*,2S*,3S*)]]-		10.2, 13.1, 17.15
5366.	1318-94-1	0	1	0	Muscovite	$K_2O.3Al_2O_3.6SiO_2.2H_2O$	20.6
5367.	9047-56-7	0	1	0	Mutase		0.4, 22.2
5368.	9033-12-9	0	1	0	Mutase, ketone–aldehyde		0.4, 22.2
5369.		0	1	0	Mycorrhiza		22.2
5370.		0	1	0	*Myobacterium avium*		22.2
5371.	92-24-0	1	0	0	Naphthacene		1.20
5372.	5385-22-8	1	0	0	Naphth[1,2-*e*]acephenanthrylene {dibenzo[*b,j*]fluoranthene}		1.20
5373.	28258-64-2	1	0	0	Naphthalenamine, *N*-phenyl-		12.2
5374.	134-32-7	1	0	0	1-Naphthalenamine {naphthalene, 1-amino-, α-naphthylamine}		12.2, 23.5
5375.	2246-44-8	1	0	0	1-Naphthalenamine, 2-methyl-		12.2
5376.	90-30-2	1	0	0	1-Naphthalenamine, *N*-phenyl-		12.2

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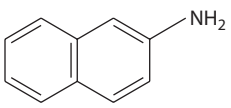
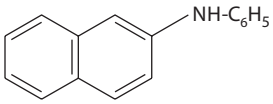
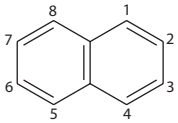
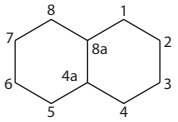
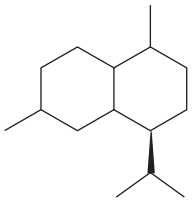
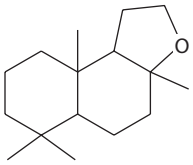
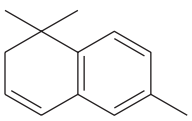
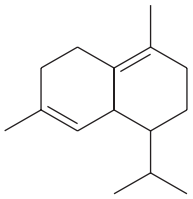
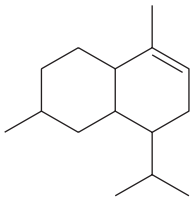
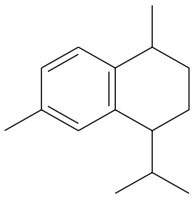
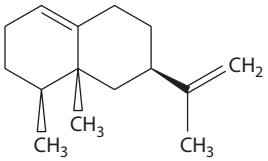
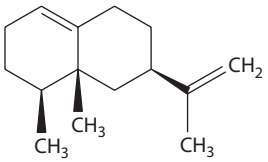
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5377.	91-59-8	1	0	0	2-Naphthalenamine {naphthalene, 2-amino-, β-naphthylamine}		12.2, 23.5
5378.	10546-24-4	1	0	0	2-Naphthalenamine, 3-methyl-		12.2
5379.	135-88-6	1	1	1	2-Naphthalenamine, *N*-phenyl-		12.2
5380.	91-20-3	1	1	1	Naphthalene		1.20, 25.29, 26.9
5381.		1	0	0	Naphthalene, alkyl-		1.20
5382.	91-17-8	1	0	0	Naphthalene, decahydro-		1.12
5383.	29350-73-0	0	1	0	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)- {δ-cadinene}		1.12, 24.3
5384.	3242-05-5	0	1	0	Naphthalene, decahydro-1,8a-dimethyl-7-(1-methylethyl)-, [1S-(1α,4aα,7α,8aα)]-		1.12
5385.	3738-00-9	0	1	0	Naphthalene, decahydro-1-ethoxido-2,5,5,8a-tetramethyl- {amberlyn, ambroxide DL}		10.2
5386.	31831-35-3	0	1	0	Naphthalene, diethyl-		1.20
5387.	29828-28-2	1	0	0	Naphthalene, dihydro-		1.20
5388.	72692-88-7	1	0	0	Naphthalene, dihydrodimethyl- {at least four isomers in MSS}		1.20
5389.	39292-53-0	1	0	0	Naphthalene, dihydromethyl- {at least three isomers in MSS}		1.20
5390.	2717-44-4	1	0	0	Naphthalene, 1,2-dihydro-3-methyl-		1.20
5391.	4373-13-1	1	0	0	Naphthalene, 1,2-dihydro-4-methyl-		1.20
5392.	67494-22-8	0	1	0	Naphthalene, 1,2-dihydro-5-methyl-3-(1-methylethenyl)-		1.20
5393.	2717-47-7	1	0	0	Naphthalene, 1,2-dihydro-6-methyl-		1.20
5394.		1	1	1	Naphthalene, dihydrotrimethyl- {at least two isomers in MSS}		1.20
5395.	30364-38-6	1	1	1	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-		1.20
5396.	4506-36-9	1	1	1	Naphthalene, 1,2-dihydro-1,5,8-trimethyl-		1.20
5397.	28804-88-8	1	1	1	Naphthalene, dimethyl-		1.20
5398.	573-98-8	1	1	1	Naphthalene, 1,2-dimethyl-		1.20

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5399.	575-41-7	1	1	1	Naphthalene, 1,3-dimethyl-		1.20
5400.	571-58-4	1	1	1	Naphthalene, 1,4-dimethyl-		1.20
5401.	571-61-9	1	1	1	Naphthalene, 1,5-dimethyl-		1.20
5402.	575-43-9	1	1	1	Naphthalene, 1,6-dimethyl-		1.20
5403.	575-37-1	1	1	1	Naphthalene, 1,7-dimethyl-		1.20
5404.	569-41-5	1	1	1	Naphthalene, 1,8-dimethyl-		1.20
5405.	581-40-8	1	1	1	Naphthalene, 2,3-dimethyl-		1.20
5406.	581-42-0	1	1	1	Naphthalene, 2,6-dimethyl-		1.20
5407.	582-16-1	1	1	1	Naphthalene, 2,7-dimethyl-		1.20
5408.	71630-68-7	1	0	0	Naphthalene, dimethyl-2-ethenyl-		1.20
5409.	65319-44-0	1	0	0	Naphthalene, dimethylethyl-		1.20
5410.	71607-89-1	1	0	0	Naphthalene, 1,4-dimethyl-2-ethyl-		1.20
5411.	66309-90-8	1	0	0	Naphthalene, 1,4-dimethyl-5-ethyl-		1.20
5412.	483-76-1	0	1	0	Naphthalene, 4,7-dimethyl-1,2,3,5,6,8a-hexahydro-1-(1-methylethyl)-, (1S-*cis*)- {δ-cadinene}		1.12
5413.	31983-22-9	0	1	0	Naphthalene, 4,7-dimethyl-1,2,4a,5,6,8a-hexahydro-1-(1-methylethyl)- {α-muurolene}		1.12
5414.	483-77-2	0	1	0	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-1,2,3,4-tetrahydro-, (1S-*Z*)-		1.20
5415.	4630-07-3	0	1	0	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7β,8a α] {valencene}		1.12, 24.3
5416.	10219-75-7	0	1	0	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7α,8aα] {eremophilene}		1.12
5417.	71607-60-8	1	0	0	Naphthalene, dimethyl-2-phenyl-		1.20
5418.		1	0	0	Naphthalene, dimethyltetrahydro- {at least three isomers in MSS}		1.20
5419.	51855-29-9 65338-07-0	1	0	0	Naphthalene, dimethyl-1,2,3,4-tetrahydro- {at least five isomers in MSS}		1.20
5420.		1	0	0	Naphthalene, ethenyl-		1.20
5421.	826-74-4	1	0	0	Naphthalene, 1-ethenyl-		1.20
5422.	827-54-3	1	0	0	Naphthalene, 2-ethenyl-		1.20

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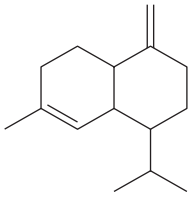
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5423.	64031-89-6	1	0	0	Naphthalene, 2-ethenylmethyl- {at least two isomers in MSS}		1.20
5424.	35737-86-1	1	0	0	Naphthalene, 2-ethenyl-1-methyl-		1.20
5425.	93-18-5	1	1	1	Naphthalene, 2-ethoxy- {β-naphthyl ethyl ether}		10.2, 24.3
5426.	27138-19-8	1	0	0	Naphthalene, ethyl-		1.20
5427.	1127-76-0	1	1	1	Naphthalene, 1-ethyl-		1.20
5428.	939-27-5	1	1	1	Naphthalene, 2-ethyl-		1.20
5429.	31391-42-1	1	0	0	Naphthalene, ethylmethyl-		1.20
5430.	17057-94-2	1	1	1	Naphthalene, 1-ethyl-3-methyl-		1.20
5431.	17057-92-0	1	1	1	Naphthalene, 1-ethyl-5-methyl-		1.20
5432.	31032-91-4	1	1	1	Naphthalene, 1-ethyl-6-methyl-		1.20
5433.	31032-92-5	1	1	1	Naphthalene, 1-ethyl-7-methyl-		1.20
5434.	61886-71-3	1	1	1	Naphthalene, 1-ethyl-8-methyl-		1.20
5435.	31032-94-7	1	1	1	Naphthalene, 2-ethyl-3-methyl-		1.20
5436.	17179-41-8	1	1	1	Naphthalene, 2-ethyl-4-methyl- {naphthalene, 3-ethyl-1-methyl-}		1.20
5437.	17059-53-9	1	1	1	Naphthalene, 2-ethyl-5-methyl- {naphthalene, 6-ethyl-1-methyl-}		1.20
5438.	7372-86-3	1	1	1	Naphthalene, 2-ethyl-6-methyl-		1.20
5439.	17059-55-1	1	1	1	Naphthalene, 2-ethyl-7-methyl-		1.20
5440.	77242-78-5	1	0	0	Naphthalene, hexamethyl-		1.20
5441.	2216-69-5	1	0	0	Naphthalene, 1-methoxy-		10.2
5442.	93-04-9	1	1	1	Naphthalene, 2-methoxy-		10.2
5443.	1321-94-4	1	1	1	Naphthalene, methyl-		1.20
5444.	90-12-0	1	1	1	Naphthalene, 1-methyl-		1.20
5445.	91-57-6	1	1	1	Naphthalene, 2-methyl-		1.20
5446.	29253-36-9	1	1	1	Naphthalene, (1-methylethyl)-		1.20
5447.	2027-17-0	0	1	0	Naphthalene, 2 (1-methylethyl)-		1.20
5448.	39029-41-9	0	1	0	Naphthalene, 7-methyl-4-methylene-1-(1-methylethyl)- 1,2,3,4,4a,5,6,8a-octahydro-, (1α,4aβ,8aα)- {γ-cadinene}		1.12
5449.		1	0	0	Naphthalene, methylphenyl-		1.20
5450.	71607-61-9	1	0	0	Naphthalene, methyl-2-phenyl-		1.20
5451.	34540-66-4	0	1	0	Naphthalene, methylpropyl-		1.20
5452.	1680-58-6	1	1	1	Naphthalene, 1-(1-methylpropyl)-		1.20
5453.	16727-91-6	1	1	1	Naphthalene, 1-(2-methylpropyl)-		1.20
5454.	71607-57-3	1	1	1	Naphthalene, methyltetrahydro- {at least three isomers in MSS}		1.20
5455.	31291-71-1	1	1	1	Naphthalene, methyl-1,2,3,4-tetrahydro-		1.20
5456.	1559-81-5	1	1	1	Naphthalene, 1-methyl-1,2,3,4-tetrahydro-		1.20
5457.	3877-19-8	1	1	1	Naphthalene, 2-methyl-1,2,3,4-tetrahydro-		1.20
5458.	2809-64-5	1	1	1	Naphthalene, 5-methyl-1,2,3,4-tetrahydro-		1.20
5459.	1680-51-9	1	1	1	Naphthalene, 6-methyl-1,2,3,4-tetrahydro- {naphthalene, 2-methyl-5,6,7,8-tetrahydro-}		1.20
5460.	86-57-7	1	1	1	Naphthalene, 1-nitro-		16.1
5461.	56908-81-7	1	1	1	Naphthalene, pentamethyl-		1.20
5462.	605-02-7	1	1	1	Naphthalene, 1-phenyl-		1.20
5463.	612-94-2	1	1	1	Naphthalene, 2-phenyl-		1.20

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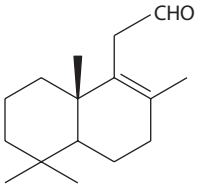
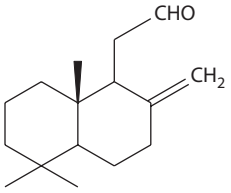
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5464.	71697-04-6	1	0	0	Naphthalene, phenyl-, monomethyl derivative		1.20
5465.	27378-74-1	0	1	0	Naphthalene, propyl-		1.20
5466.	2765-18-6	1	0	0	Naphthalene, 1-propyl-		1.20
5467.	2027-19-2	1	0	0	Naphthalene, 2-propyl-		1.20
5468.	119-64-2	1	1	1	Naphthalene, 1,2,3,4-tetrahydro- {tetralin}		1.20, 25.29
5469.	121214-18-4	1	0	0	Naphthalene, tetrahydrotrimethyl- {at least three isomers in MSS}		1.20
5470.	72843-02-8	1	0	0	Naphthalene,1,2,3,4-tetrahydrotrimethyl- {at least three isomers in MSS}		1.20
5471.	475-03-6	1	1	1	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl- {α-ionene}		1.20
5472.	21693-51-6	0	1	0	Naphthalene, 1,2,3,4-tetrahydro-1,5,8-trimethyl-		1.20
5473.	30316-36-0	0	1	0	Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-		1.20
5474.		0	1	0	Naphthalene, 1,2,3,4-tetrahydro-4,5,8-trimethyl-		1.20
5475.		0	1	0	Naphthalene, 1,2,3,4-tetrahydro-4,5,8-trimethyl- {isomer}		1.20
5476.	28652-74-6	1	1	1	Naphthalene, tetramethyl- {at least four isomers in MSS}		1.20
5477.	28652-77-9	1	1	1	Naphthalene, trimethyl- {at least 10 isomers in MSS}		1.20
5478.	2717-42-2	1	1	1	Naphthalene, 1,2,4-trimethyl-		1.20
5479.	3031-05-8	1	1	1	Naphthalene, 1,2,6-trimethyl-		1.20
5480.	486-34-0	1	1	1	Naphthalene, 1,2,7-trimethyl-		1.20
5481.	2131-39-7	1	1	1	Naphthalene, 1,3,5-trimethyl-		1.20
5482.	3031-08-1	1	1	1	Naphthalene, 1,3,6-trimethyl-		1.20
5483.	2131-41-1	1	0	0	Naphthalene, 1,4,5-trimethyl-		1.20
5484.	2131-42-2	1	1	1	Naphthalene, 1,4,6-trimethyl-		1.20
5485.	2245-38-7	1	1	1	Naphthalene, 1,6,7-trimethyl- {naphthalene, 2,3,5-trimethyl-}		1.20
5486.	829-26-5	1	1	1	Naphthalene, 2,3,6-trimethyl-		1.20
5487.	68985-11-5	0	1	0	1-Naphthaleneacetaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)-		3.12
5488.	3243-36-5	0	1	0	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-methylene-, [1S-(1α,4aβ,8aα)]-		3.12
5489.	68982-27-4	0	1	0	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-oxo-, [1R-(1α,4aβ,8aα)]-		3.12, 3.13
5490.	86-87-3	0	1	0	1-Naphthaleneacetic acid		4.3, 21.3
5491.	132-75-2	1	0	0	1-Naphthaleneacetonitrile		11.2

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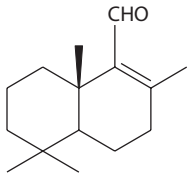
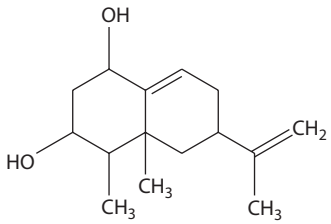
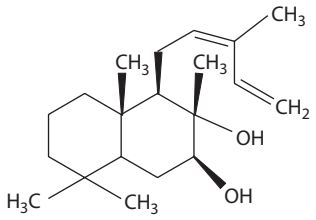
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5492.	25551-35-3	1	0	0	Naphthalenecarbonitrile		11.2
5493.		1	0	0	Naphthalenecarbonitrile, alkyl-		11.2
5494.	77417-07-3	1	0	0	Naphthalenecarbonitrile, methyl- {two isomers}		11.2
5495.	86-53-3	1	0	0	1-Naphthalenecarbonitrile		11.2
5496.	77417-07-3	1	0	0	1-Naphthalenecarbonitrile, 3-methyl-		11.2
5497.	23245-64-9	1	0	0	1-Naphthalenecarbonitrile, 5-nitro-		11.2, 16.1
5498.	613-46-7	1	0	0	2-Naphthalenecarbonitrile		11.2
5499.	68985-10-4	0	1	0	1-Naphthalenecarboxaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)-		3.12
5500.	31519-22-9	0	1	0	2-Naphthalenecarboxylic acid, 1, 4-dihydroxy-		4.3
5501.	79951-97-6	0	1	0	1,2-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl- {11-nor-8-drimanol}		2.5
5502.	79886-54-7	0	1	0	1,2-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl-, [1R-(1α,2β,4aβ,8aα)]-		2.5
5503.	37208-05-2	0	1	0	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [1R-(1α,3β,4β,4aα,6α)]-		2.5
5504.	114393-99-6	0	1	0	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, 3-acetate, [1R-(1α,3β,4.		2.5, 5.3
5505.	65513-74-8	0	1	0	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-6-[1-(hydroxymethyl) ethenyl]-4,4a-dimethyl-, (1α,3β,4β,4aα,6α)-		2.5
5506.	92-44-4	1	0	0	2,3-Naphthalenediol		9.22
5507.	27656-76-4	0	1	0	2,3-Naphthalenediol, 1,2α,3β,4,5,6,7,8-octahydro-7α-isopropenyl-1α-methyl-		2.5
5508.	18178-54-6	1	1	1	2,3-Naphthalenediol, 1,2,3,4,5,6,7, 8-octahydro-1-methyl-7-(1-methylethenyl)-, [1S-(1α,2β,3α,7β)]- {rishitin}		2.5
5509.	73496-12-5	0	1	0	2,3-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1S-[1α(*E*),2α,3β,4aβ,8aα]]-		2.5

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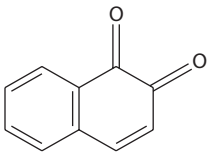
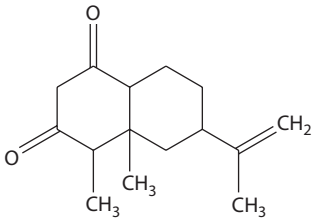
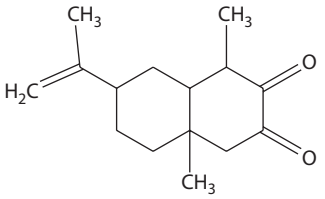
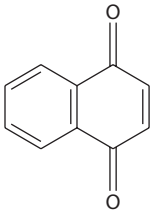
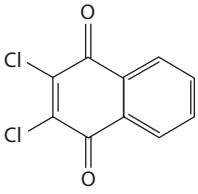
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5510.	524-42-5	1	0	0	1,2-Naphthalenedione {1,2-naphthoquinone}		9.24
5511.	60026-23-5	0	1	0	1,3(2*H*,5*H*)-Naphthalenedione, 6,7,8,8a-tetrahydro-4,8a-dimethyl-6-(1-methylethenyl)-		3.13
5512.	117769-22-9	0	1	0	2,3-Naphthalenedione, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-		3.13
5513.	88125-12-6	0	1	0	2,3-Naphthalenedione, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)-		3.13
5514.	130-15-4	1	0	0	1,4-Naphthalenedione {1,4-naphthoquinone}		9.24
5515.	117-80-6	0	1	0	1,4-Naphthalenedione, 2,3-dichloro- {Diclone®}		9.24, 18.4, 21.3
5516.	73850-17-6	1	0	0	1,4-Naphthalenedione, dimethyl-		9.24
5517.	2197-57-1	1	0	0	1,4-Naphthalenedione, 2,3-dimethyl-		9.24
5518.	482-70-2	1	0	0	1,4-Naphthalenedione, 2,7-dimethyl-		9.24
5519.	68860-42-4	1	1	1	1,4-Naphthalenedione, 2,3-dimethyl-6-(4,8,12-trimethyltridecyl)-, (R*,R*)-		9.24
5520.	481-39-0	0	1	0	1,4-Naphthalenedione, 5-hydroxy- {juglone}		9.22, 9.24
5521.		1	0	0	1,4-Naphthalenedione, methyl-		9.24
5522.	58-27-5	1	0	0	1,4-Naphthalenedione, 2-methyl-		9.24
5523.	84-80-0	0	1	0	1,4-Naphthalenedione, 2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [R-[R*,R*-(*E*)]]- {vitamin K1}		9.24
5524.	73850-15-4	1	0	0	1,4-Naphthalenedione, tetramethyl-		9.24
5525.	73850-16-5	1	0	0	1,4-Naphthalenedione, trimethyl-		9.24
5526.	20490-42-0	1	1	1	1,4-Naphthalenedione, 2,3,6-trimethyl-		9.24

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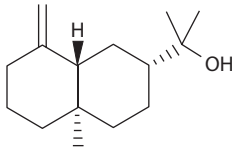
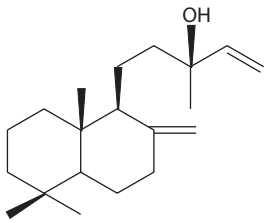
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5527.	59832-90-5	1	0	0	1,4-Naphthalenedione, 2,6,7-trimethyl-		9.24
5528.	102977-87-7	0	1	0	2-Naphthaleneethanol,3,4-dihydro-1,5,6-trimethyl-		2.5
5529.	52617-99-9	0	1	0	1-Naphthalenemethanol, decahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [1S-(1α,2β,4aβ,8aα)]-		2.5
5530.	473-15-4	0	1	0	2-Naphthalenemethanol, 1,2α,3,4,4a,5,6,7,8,8aα-decahydro-α,α,4aβ-trimethyl-8-methylene- {β-eudesmol}		2.5
5531.	29484-46-6	0	1	0	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl-, [2S-(2α,4aβ,8aβ)]-		2.5
5532.	37574-03-1	0	1	0	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl- {*trans*-occidentalol}		2.5
5533.	473-17-6	0	1	0	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl-, [2R-(2α,4aβ,8aβ)]- {occidentalol}		2.5
5534.	87797-89-5	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,6-tetramethyl-, (R)-		2.5
5535.	117065-22-2	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,6-tetramethyl-, (±)-		2.5
5536.	5986-36-7	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,8-tetramethyl-, (R)-		2.5
5537.	61263-48-7	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,8-tetramethyl-, acetate, (R)-		5.3
5538.	87797-88-4	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,7,8-tetramethyl-, (R)-		2.5
5539.	117065-21-1	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,7,8-tetramethyl-, (±)-		2.5
5540.	121269-01-0	0	1	0	2-Naphthalenemethanol, 3,4-dihydro-1,5,6-trimethyl-		2.5
5541.	10267-21-7	0	1	0	1-Naphthalenepentanol, decahydro-2-hydroxy-γ,2,5,5,8a-pentamethyl-, [1R-[1α(S*),2β,4aβ,8aα]]		2.5
5542.		0	1	0	1-Naphthalene-2-pentenol, decahydro-γ,2,5,5,8a-pentamethyl-		2.5
5543.		0	1	0	1-Naphthalene-2-pentenol, 3,4,4a,5,6,7,8,8a-octahydro-γ,2,5,5,8a-pentamethyl-		2.5
5544.	596-85-0	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-α,5,5,8a-tetramethyl-2-methylene-, [1S-[1α(S*),4aβ,8aα]]- {manool}		2.5
5545.	4630-08-4	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-α,2,5,5,8a-pentamethyl-, [1R-[1α(S*),2β,4aβ,8aα]]- {episclareol}		2.5

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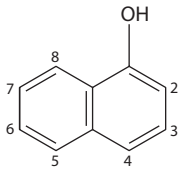
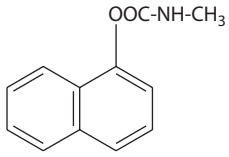
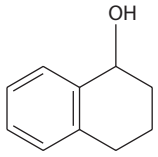
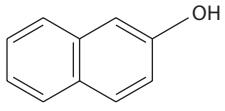
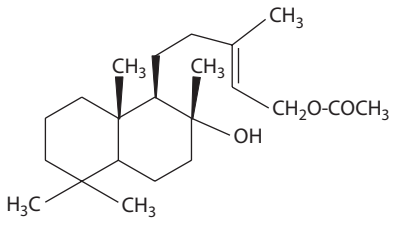
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5546.	515-03-7	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-α,2,5,5,8a-pentamethyl-, [1R-[1α(R*),2β,4aβ,8aα]]- {sclareol}		2.5
5547.	57567-06-3	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-7-hydroxy-α,5,5,8a-tetramethyl-2-methylene-		2.5
5548.	1321-67-1	1	0	0	Naphthalenol {naphthol}		9.22
5549.	121198-51-4	0	1	0	Naphthalenol, 6,8-dimethyl-		9.22
5550.	121198-52-5	0	1	0	Naphthalenol, 7,8-dimethyl-		9.22
5551.	90-15-3	1	0	0	1-Naphthalenol {1-naphthol = α-naphthol}		9.22
5552.	40529-54-2	1	0	0	1-Naphthalenol, dimethyl-		9.22
5553.	59534-35-9	1	0	0	1-Naphthalenol, methyl-		9.22
5554.		1	0	0	1-Naphthalenol, methyl-nitro-		9.22, 16.1
5555.	7469-77-4	1	0	0	1-Naphthalenol, 2-methyl-		9.22
5556.	63-25-2	1	1	1	1-Naphthalenol, methylcarbamate {Sevin®, Carbaryl®}		5.3, 21.3, 25.29
5557.	529-33-9	1	0	0	1-Naphthalenol, 1,2,3,4-tetrahydro-		2.5
5558.	55591-08-7	0	1	0	1-Naphthalenol,1,2,3,4-tetrahydro-2,5,8-trimethyl-		2.5
5559.	30316-22-4	1	0	0	1-Naphthalenol,1,2,3,4-tetrahydro-3,5,8-trimethyl-		2.5
5560.	66324-66-1	0	1	0	1-Naphthalenol,1,2,3,4-tetrahydro-4,5,8-trimethyl-		2.5
5561.	67494-23-9	0	1	0	1-Naphthalenol, 1,2,3,4-tetrahydro-8-methyl-2-(1-methylethenyl)-, (*Z*)-(±)		2.5
5562.	135-19-3	1	1	1	2-Naphthalenol {2-naphthol = β-naphthol}		9.22, 21.3
5563.	31149-06-1	0	1	0	2-Naphthalenol, 1-[5-(acetyloxy)-3-methyl-3-pentenyl]decahydro-2,5,5,8a-tetramethyl-, [1R-[1α(*E*),2β,4aβ,8aα]]-		2.5, 5.3

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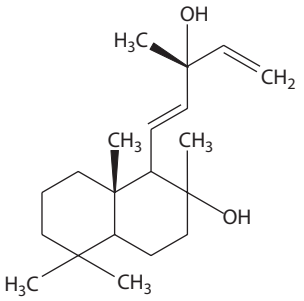
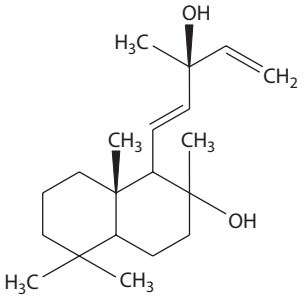
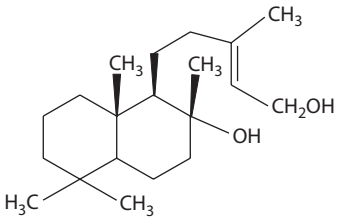
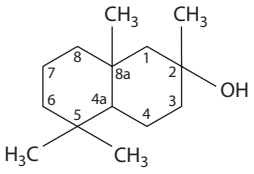
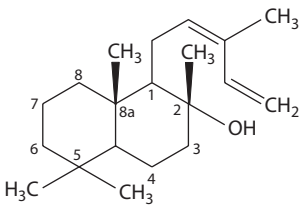
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5564.	66890-73-1	0	1	0	2-Naphthalenol,decahydro-1-(3-hydroxy-3-methyl-1,4-pentadienyl)-2,5,5,8a-tetramethyl-, [1R-[1α(1*E*,3S*), 2β,4aβ,8aα]]-		2.5
5565.	66966-02-7	0	1	0	2-Naphthalenol, decahydro-1-(3-hydroxy-3-methyl-1,4-pentadienyl)-2,5,5,8a-tetramethyl-, [1R-[1α(1*E*,3R*), 2β,4aβ,8aα]]-		2.5
5566.	10267-31-9	0	1	0	2-Naphthalenol, decahydro-1-(5-hydroxy-3-methyl-3-pentenyl)-2,5,5,8a-tetramethyl-, [1R-[1α(*E*), 2β,4aβ,8aα]]-		2.5
5567.	22343-28-8	0	1	0	2-Naphthalenol, decahydro-1-(5-hydroxy-3-methyl-3-pentenyl)-2,5,5,8a-tetramethyl-, [1R-(1α,2β,4aβ,8aα)]-		2.5
5568.	53163-43-2	0	1	0	2-Naphthalenol, decahydro-1,2,5,5, 8a-pentamethyl-, [1R-(1α,2β,4aβ,8aα)]-		2.5
5569.	36211-21-9	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-		2.5
5570.	49749-17-9	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-, (2α,4aα,8aβ)-(±)-		2.5
5571.	42569-63-1	1	0	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-1, 3-pentadienyl)-, [1R-[1α(1*E*,3*E*),2β,4aβ,8aα]]-		2.5
5572.	1616-86-0	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-(1α,2β,4aβ,8aα)]- {*Z*-abienol}		2.5, 21.3

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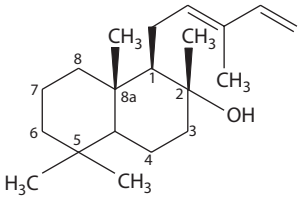
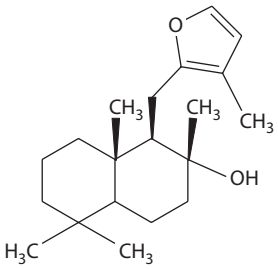
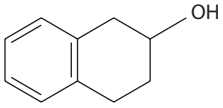
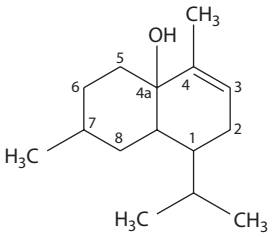
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5573.	17990-15-7	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-,[1R-[1α(*E*),2β,4aβ,8aα]]-		2.5
5574.	17990-16-8	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-,[1R-[1α(Z),2β,4aβ,8aα]]-		2.5
5575.	62121-32-8	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-[(3-methyl-2-furanyl) methyl]-, [1R-(1α,2β,4aβ,8aα)]-		2.5, 10.2
5576.	82451-46-5	0	1	0	2-Naphthalenol, decahydro-4a,8,8-trimethyl-3-methylene-4-(3-methyl-2,4-pentadienyl)-, [2S-[2α,4α(*E*),4aα,8aβ]]-		2.5
5577.	82458-63-7	0	1	0	2-Naphthalenol, decahydro-4a,8,8-trimethyl-3-methylene-4-(3-methylene-4-pentenyl)-, [2S-(2α,4α,4aα,8aβ)]-		2.5
5578.	58239-50-2	0	1	0	2-Naphthalenol, decahydro-5,5,8a-trimethyl-, [2R-(2α,4aα,8aβ)]-		2.5
5579.	73850-19-8	1	0	0	2-Naphthalenol, dimethyl-		9.22
5580.	54703-51-4	1	0	0	2-Naphthalenol, 1,8-dimethyl-		9.22
5581.	59534-36-0	1	0	0	2-Naphthalenol, methyl-		9.22
5582.	1076-26-2	1	0	0	2-Naphthalenol, 1-methyl-		9.22
5583.	71369-76-1	1	0	0	2-Naphthalenol, tetrahydro-		9.22
5584.	530-91-6	1	0	0	2-Naphthalenol, 1,2,3,4-tetrahydro-		2.5
5585.	1125-78-6	1	0	0	2-Naphthalenol, 5,6,7,8-tetrahydro-		9.22
5586.		1	0	0	2-Naphthalenol, 5,6,7,8-tetramethyl-		9.22
5587.	73850-18-7	1	0	0	2-Naphthalenol, trimethyl-		9.22
5588.	30889-50-0	1	0	0	2-Naphthalenol, 3,5,8-trimethyl-		9.22
5589.	17910-08-6	0	1	0	4a(2*H*)-Naphthalenol, 1,5,6,7,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1α,4aβ,7α,8aα)]-		2.5

(*continued*)

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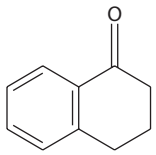
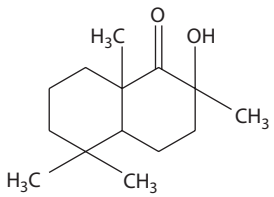
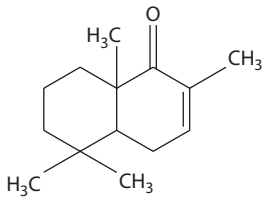
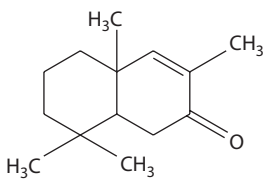
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5590.	529-34-0	1	0	0	1(2*H*)-Naphthalenone, 3,4-dihydro- {1-tetralone}		3.13
5591.	117210-52-3	0	1	0	1(2*H*)-Naphthalenone, 3,4-dihydro-5-methyl-3-(1-methylethenyl)-		3.13
5592.		1	0	0	1(2*H*)-Naphthalenone,3,4-dihydro-4,5,6-trimethyl-		3.13
5593.	27410-97-5	1	0	0	1(2*H*)-Naphthalenone,3,4-dihydro-4,5,7-trimethyl-		3.13
5594.	41720-93-8	0	1	0	1(2*H*)-Naphthalenone, 3,4,4a,5, 6,7-hexahydro-3-hydroxy-4,4a-dimethyl-6-(1-methylethenyl)-, [3R-(3α,4α,4aβ,6β)]-		2.5, 3.13
5595.	52811-60-6	1	1	1	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl-		2.5, 3.13
5596.	55497-93-3	0	1	0	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [2R-(2α,4aα,8aβ)]-		2.5, 3.13
5597.	25487-94-9	0	1	0	1(4*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)-		3.13
5598.	57601-69-1	0	1	0	1(4*H*)-Naphthalenone, 2-hydroxy-4,4,7-trimethyl-		3.13
5599.	117472-47-6	0	1	0	1(4*H*)-Naphthalenone, 5,6,7,8-tetrahydro-8-methyl-5-(1-methylethenyl)-		3.13
5600.	29210-91-1	1	0	0	2(1*H*)-Naphthalenone, 3,4-dihydro-4,4,7-trimethyl-		3.13
5601.	55733-01-2	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8, 8a-hexahydro-3,4,4a,8,8-pentamethyl-, (4aS-*trans*)-		3.13
5602.	76739-26-9	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4,4a,8,8-pentamethyl-		3.13
5603.		0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8, 8a-hexahydro-3-hydroxy-3,4a,8,8-tetramethyl- {two isomers reported}		2.5, 3.13
5604.	51020-10-1	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4a,8,8-tetramethyl-, (4aR-*trans*)- {isonordrimenone}		3.13

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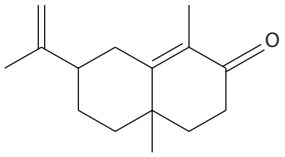
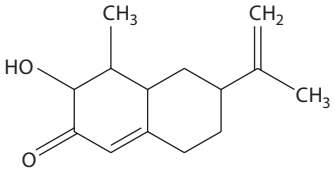
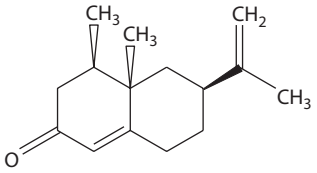
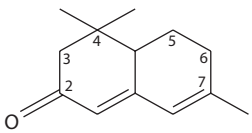
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5605.	72446-33-4	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4a,8,8-tetramethyl-4-(3-oxobutyl)-, (4aS-*trans*)-		3.13
5606.	14506-68-4	0	1	0	2(1*H*)-Naphthalenone, 1-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-5,5,8a-trimethyl-, [1R-[1α(R*),4aβ,8aα]]-		2.5, 3.13
5607.	57567-07-4	0	1	0	2(1*H*)-Naphthalenone, 8-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-4,4,8a-trimethyl-7-methylene-		2.5, 3.13
5608.	473-08-5	1	1	1	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)-{bicyclo[4.4.0]dec-1-en-3-one, 2,6-dimethyl-9-isopropenyl-}		3.13
5609.	60026-22-4	1	0	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-{6-epicyperone-1}		3.13
5610.	55051-94-0	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-3-hydroxy-4-methyl-6-(1-methylethenyl)-, [3R-(3α,4β,4aβ,6α)]-		2.5, 3.13
5611.	4674-50-4	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4α,4aα,6β)]-{bicyclo[4.4.0]dec-1-en-3-one, 5,6-dimethyl-8-isopropenyl-}{nootkatone}		3.13
5612.	102977-86-6	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,8-dimethyl-7-(1-methylethenyl)-		3.13
5613.	38044-00-7	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-		2.5, 3.13
5614.	5835-19-8	0	1	0	2(3*H*)-Naphthalenone, 4,4a.5.6-tetrahydro-4,4,7-trimethyl-		3.13
5615.	39815-74-2	0	1	0	2(3*H*)-Naphthalenone, 4,6,7,8-tetrahydro-4,4,7-trimethyl-		3.13
5616.	17081-85-5	0	1	0	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-1,4a-dimethyl-7-(1-methylethenyl)-(4aS-*cis*)-{1,2-dehydro-α-cyperone}		3.13

(*continued*)

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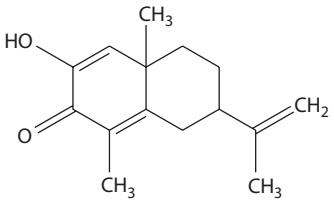
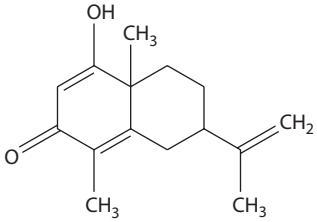
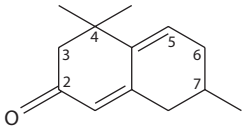
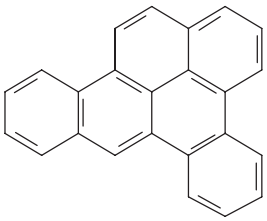
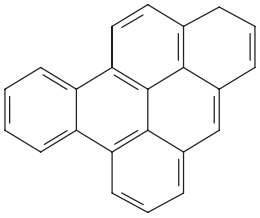
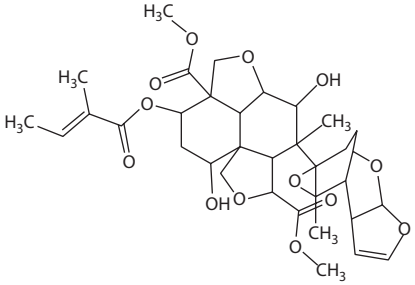
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5617.	68420-60-0	0	1	0	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-3-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)-		2.5, 3.13
5618.	38043-97-9	1	1	1	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-4-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-, (4aR-*cis*)- {1-keto-α-cyperone}		2.5, 3.13
5619.		0	1	0	2(6*H*)-Naphthalenone, 3,4,7,8-tetrahydro-4,4,7-trimethyl-		3.13
5620.	1338-24-5	0	1	0	Naphthenic acid		4.3
5621.	192-65-4	1	0	0	Naphtho[1,2,3,4-*def*]chrysene {dibenzo[*a,e*]pyrene}		1.20, 23.5
5622.	190-99-8	1	0	0	1*H*-Naphtho[3,2,1,8-*defg*]chrysene {1,2,5,6-dibenzopyrene}		1.20
5623.	11141-17-6	0	1	0	1*H*,7*H*-Naphtho[1,8*a*,8-*bc*:4,4*a*-*c*′] difuran-3,7a-dicarboxylic acid, (3S,3aR,4S, 5S,5aR, 5a[1]R 7aS,8R,10S,10aS)-8-acetoxy-3,3a,4,5a,5a[1],7a,8,9, 10-decahydro-3,5-dihydroxy-4-{(1S,3S,7S,8R,9S,11R)-7-hydroxy-9-methyl-2,4, 10-trioxatetracyclo[6.3.1.$0^{3,7}$.$0^{9,11}$] dodeca-5-en-11-yl}-4-methyl-10[(*E*)-2-methylbut-2-enoyloxy]-, dimethyl ester {Azadirachtin® A and B, Neem®}		21.3
5624.	64083-16-5	1	0	0	Naphthofuran		10.2
5625.		1	0	0	Naphthofuran, dimethyl-		10.2
5626.		1	0	0	Naphthofuran, methyl-		10.2
5627.	234-03-7	1	0	0	Naphtho[1,2-*b*]furan		10.2
5628.	71607-62-0	1	0	0	Naphtho[1,2-*b*]furan, dimethyl-		10.2

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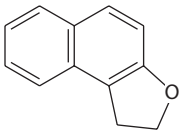
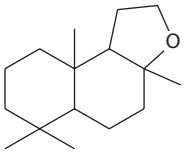
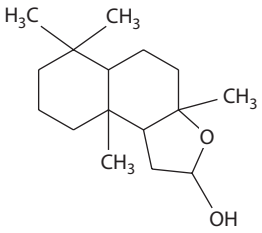
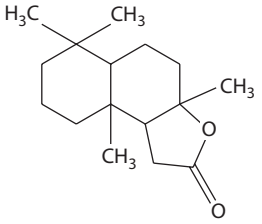
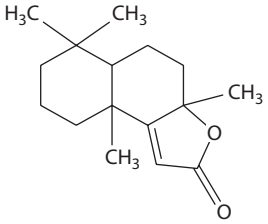
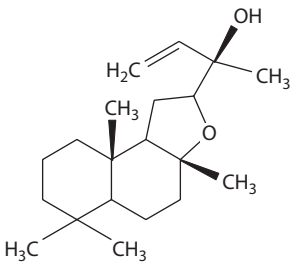
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5629.	25826-63-5	1	0	0	Naphtho[1,2-*b*]furan, 2-methyl-		10.2
5630.	232-95-1	1	0	0	Naphtho[2,1-*b*]furan		10.2
5631.	65588-69-4 6790-58-5	0	1	0	Naphtho[2,1-*b*]furan, dodecahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]-{ambroxide, ambroxyl}		10.2
5632.	52811-62-8	1	1	1	Naphtho[2,1-*b*]furan-2-ol, dodecahydro-3a,6,6,9a-tetramethyl- {sclaral}		2.5, 10.2
5633.	30450-17-0	0	1	0	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aS-(3aα,5aα,9aβ,9bα)]-		10.2
5634.	564-20-5	1	1	1	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]-{1,5,5,9-tetramethyl-13-oxatricyclo[8,3,0,0(4,9)]tridecane} {sclareolide}		6.3, 24.3, 25.29
5635.		1	1	1	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]-{1,5,5,9-tetramethyl-13-oxatricyclo [8,3,0,0(4,9)]tridecane}, labeled with ^{14}C {sclareolide-^{14}C}		6.3, 25.29
5636.	52811-59-3	1	1	1	Naphtho[2,1-*b*]furan-2(3a*H*)-one, 4, 5,5a,6,7,8,9,9a-octahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα)]-		6.3
5637.	56682-25-8	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2R-[2α(R*), 3aβ,5aα,9aβ,9bα]]-		2.5, 10.2

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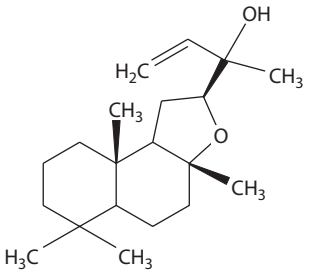
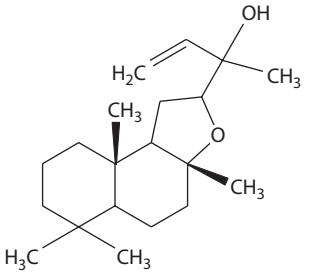
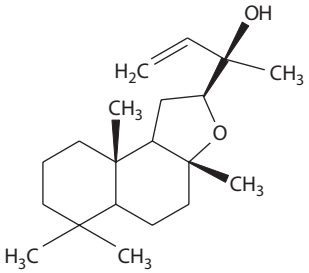
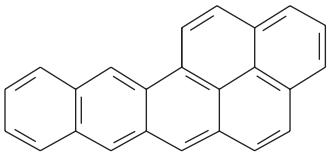
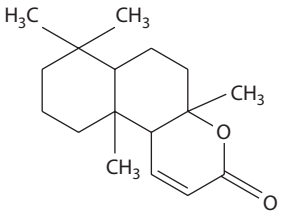
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5638.	56711-38-7	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2R-[2α(S*),3aβ,5aα,9aβ,9bα]]-		2.5, 10.2
5639.	56711-39-8	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(S*),3aα,5aβ,9aα,9bβ]]-		2.5, 10.2
5640.	56711-40-1	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(R*),3aα,5aβ,9aα,9bβ]]-		2.5, 10.2
5641.	196-42-9	1	0	0	Naphtho[2,1,8-*qra*]naphthacene		1.20
5642.	52811-58-2	1	1	1	*3H*-Naphtho[2,1-*b*]pyran-3-one, 4a,5,6,6a,7,8,9,10,10a,10b-decahydro-4a,7,7,10a-tetramethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]- {dehydroambreinolide}		6.3
5643.	468-84-8	1	1	1	3*H*-Naphtho[2,1-*b*]pyran-3-one, dodecahydro-4a,7,7,10a-tetramethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]- {ambreinolide}		6.3
5644.	5153-92-4	1	1	1	1*H*-Naphtho[2,1-*b*]pyran, 4a,5,6,6a,7,8,9,10,10a,10b-decahydro-3,4a,7,7,10a-pentamethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]-		10.2
5645.	6252-26-2	0	1	0	1*H*-Naphtho[2,1-*b*]pyran, dodecahydro-3,4a,7,7,10a-pentamethyl-		10.2

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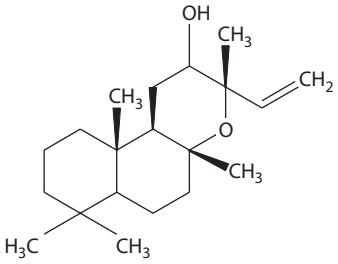
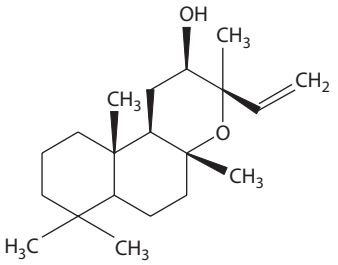
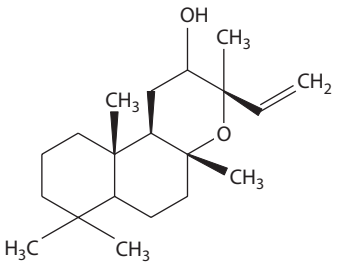
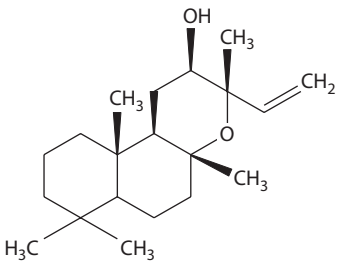
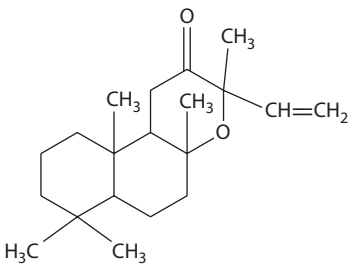
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5646.	596-84-9	0	1	0	1*H*-Naphtho[2,1-*b*]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aβ,6aα,10aβ,10bα)]-		10.2
5647.	59170-14-8	1	1	1	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3β,4aβ,6aα,10aβ,10bα)]- {labd-14-ene, 8,13-epoxy-12α-hydroxy-} {12α-hydroxy-13-epimanoyl oxide}		2.5, 10.2
5648.	64681-69-2	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2R-(2α,3α,4aα,6aβ,10aα,10bβ)]-		2.5, 10.2
5649.	64681-70-5	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3α,4aβ,6aα,10aβ,10bα)]-		2.5, 10.2
5650.	67528-84-1	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2R-(2α,3β,4aα,6aβ,10aα,10bβ)]-		2.5, 10.2
5651.	38017-17-3	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl- {8,13-epoxylabd-14-en-12-one}		3.13, 10.2

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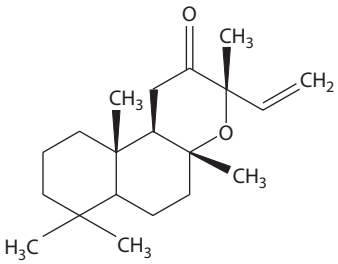
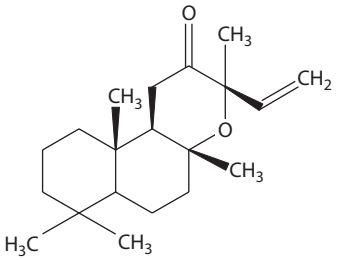
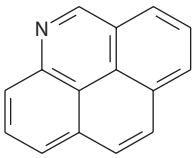
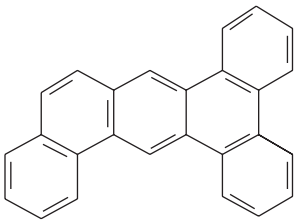
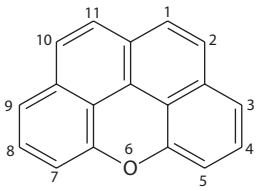
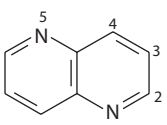
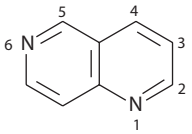
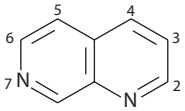
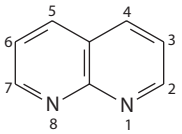
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5652.	37551-73-8	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]-		3.13, 10.2
5653.	37551-74-9	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aα,6aβ,10aα,10bβ)]-		3.13, 10.2
5654.	68985-12-6	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7, 10a-pentamethyl-		3.13, 10.2
5655.	313-80-4	1	0	0	Naphtho[2,1,8-*def*]quinoline {1-azapyrene}		17.21
5656.		1	0	0	Naphtho[2,1,8-*def*]quinoline, dimethyl-		17.21
5657.		1	0	0	Naphtho[2,1,8-*def*]quinoline, methyl-		17.21
5658.		1	0	0	Naphtho[2,1,8-*def*]quinoline, trimethyl-		17.21
5659.	215-26-9	1	0	0	Naphtho[1,2-*b*]triphenylene {tribenz[*a,c,h*]anthracene}		1.20
5660.	191-37-7	1	0	0	Naphtho[2,1,8,7-*klmn*]xanthene		10.2
5661.		1	0	0	Naphthyridine		17.21
5662.		1	0	0	Naphthyridine, C_2-alkyl-		17.21
5663.		1	0	0	Naphthyridine, 3-butanoyl-		3.13, 17.21
5664.		1	0	0	Naphthyridine, 3-methyl-		17.21
5665.	254-79-5	1	0	0	1,5-Naphthyridine {1,5-diazanaphthalene, pyrido[3,2-*b*]pyridine}		17.21
5666.	18937-71-8	1	0	0	1,5-Naphthyridine, 3-methyl-		17.21

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5667.	253-72-5	1	0	0	1,6-Naphthyridine {1,6-diazanaphthalene, pyrido[4,3-*b*]pyridine}		17.21
5668.	14757-43-8	1	0	0	1,6-Naphthyridine, 3-methyl-		17.21
5669.	253-69-0	1	0	0	1,7-Naphthyridine {1,7-diazanaphthalene, pyrido[3,4-*b*]pyridine}		17.21
5670.	254-60-4	1	0	0	1,8-Naphthyridine {1,8-diazanaphthalene, pyrido[2,3-*b*]pyridine}		17.21
5671.		1	0	0	1,8-Naphthyridine, 3-butanoyl-		3.13, 17.21
5672.	14757-45-0	1	0	0	1,8-Naphthyridine, 2,6-dimethyl-		17.21
5673.	14759-22-9	1	0	0	1,8-Naphthyridine, 3-methyl-		17.21
5674.	40000-89-3	1	0	0	1,8-Naphthyridin-2(1*H*)-one, 3-methyl-		17.13, 17.23
5675.	8002-65-1	0	1	0	Neem oil		21.3
5676.	7440-00-8	1	1	1	Neodymium	Ne	20.5
5677.	7440-02-0	1	1	1	Nickel	Ni	0.4, 20.5
5678.	13463-39-3 12612-55-4	1	0	0	Nickel carbonyl	$Ni(CO)_4$	20.6
5679.	37211-05-5	0	1	0	Nickel chloride	NiCl	18.4, 20.6
5680.	7440-03-1	1	0	0	Niobium	Nb	20.5
5681.	14797-55-8	1	1	1	Nitrate	NO_3^-	0.4, 20.5
5682.	125239-87-4	1	0	0	Nitrate, peroxy-		20.6
5683.	7697-37-2	1	1	1	Nitric acid	$HO\text{-}NO_2$	0.4, 20.6
5684.	6484-52-2	0	1	0	Nitric acid, ammonium salt		20.6
5685.	10124-37-5	0	1	0	Nitric acid, calcium salt	$Ca{=}(O\text{-}NO_2)_2$	20.6
5686.	3251-23-8	0	1	0	Nitric acid, copper salt	$Cu{=}(O\text{-}NO_2)_2$	20.6
5687.	10099-74-8	0	1	0	Nitric acid, lead salt		20.6
5688.	10377-60-3	0	1	0	Nitric acid, magnesium salt	$Mg{=}(O\text{-}NO_2)_2$	20.6
5689.	598-58-3	1	0	0	Nitric acid, methyl ester	$H_3C\text{-}O\text{-}NO_2$	5.3
5690.	7757-79-1	0	1	0	Nitric acid, potassium salt	$KO\text{-}NO_2$	0.4, 20.6
5691.	7761-88-8	0	1	0	Nitric acid, silver salt		20.6
5692.	7631-99-4	0	1	0	Nitric acid, sodium salt	$NaO\text{-}NO_2$	20.6
5693.	10102-45-1	0	1	0	Nitric acid, thallium salt		20.6
5694.	10102-06-4	0	1	0	Nitric acid, uranium salt		20.6
5695.	7779-88-6	0	1	0	Nitric acid, zinc salt		20.6
5696.	14797-65-0	1	1	1	Nitrite	$O{=}N\text{-}O^{-1}$	20.5
5697.	19059-14-4	1	0	0	Nitrite, peroxy-		20.6
5698.		1	0	0	Nitrite radical	O-N=O	27.1
5699.	7727-37-9	1	1	1	Nitrogen	N_2	0.4, 19.5, 20.5
5700.	11104-93-1	1	0	0	Nitrogen oxide		19.5
5701.	10024-97-2	1	1	1	Nitrogen oxide {nitrous oxide}	N_2O	19.5
5702.	10102-43-9	1	1	1	Nitrogen oxide {nitric oxide}	NO	19.5, 23.5, 27.1
5703.	10102-44-0	1	0	0	Nitrogen oxide {nitrogen dioxide}	NO_2	19.5
5704.		1	1	1	Nitrogen oxides	$N_2O + NO + NO_2$	19.5, 23.5
5705.	35576-91-1	1	0	0	Nitrosamide	$H_2N\text{-}N{=}O$	15.8
5706.		1	1	1	*N*-Nitrosamines {general discussion}		15.8
5707.	7782-77-6	1	0	0	Nitrous acid	HO-N=O	20.6

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5708.	109-95-5	1	0	0	Nitrous acid, ethyl ester	H_3C-CH_2-ON=O	5.3
5709.	624-91-9	1	1	1	Nitrous acid, methyl ester	H_3C-ON=O	5.3
5710.	630-03-5	1	1	1	Nonacosane	H_3C-$(CH_2)_{27}$-CH_3	0.4, 1.10
5711.	1560-75-4	1	1	1	Nonacosane, 2-methyl-	$(H_3C)_2$=CH-$(CH_2)_{26}$-CH_3	1.10
5712.	14167-67-0	1	1	1	Nonacosane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{25}$-CH_3	1.10
5713.	4250-38-8	1	1	1	Nonacosanoic acid	H_3C-$(CH_2)_{27}$-COOH	4.3
5714.	121878-05-5	1	1	1	Nonacosanoic acid, docosyl ester	H_3C-$(CH_2)_{27}$-COO-$(CH_2)_{21}$-CH_3	5.3
5715.	121877-94-9	1	1	1	Nonacosanoic acid, eicosyl ester	H_3C-$(CH_2)_{27}$-COO-$(CH_2)_{19}$-CH_3	5.3
5716.	39815-65-1	0	1	0	Nonacosanoic acid, 4-(2-hydroxyethyl) phenyl ester		5.3
5717.	6624-76-6	0	1	0	1-Nonacosanol	H_3C-$(CH_2)_{27}$-CH_2OH	2.5
5718.	18835-35-3	1	0	0	1-Nonacosene	H_2C=CH-$(CH_2)_{26}$-CH_3	1.11
5719.		1	0	0	1-Nonacosene, 2-methyl-	H_2C=$C(CH_3)$-$(CH_2)_{26}$-CH_3	1.11
5720.		1	0	0	2-Nonacoscene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{25}$-CH_3	1.11
5721.		1	0	0	2-Nonacoscene, (*E*)-		1.11
5722.		1	0	0	2-Nonacosene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{25}$-CH_3	1.11
5723.		1	0	0	2-Nonacosene, 27-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{23}$-$CH(CH_3)$-CH_2-CH_3	1.11
5724.		1	0	0	2-Nonacosene, 27-methyl-, (*E*)-		1.11
5725.		1	0	0	2-Nonacosene, 28-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{24}$-$CH(CH_3)_2$	1.11
5726.		1	0	0	2-Nonacosene, 28-methyl-, (*E*)-		1.11
5727.	629-92-5	1	1	1	Nonadecane	H_3C-$(CH_2)_{17}$-CH_3	1.10
5728.		1	0	0	Nonadecane, methyl-		1.10
5729.	6418-45-7	0	1	0	Nonadecane, 3-methyl-	H_3C-$(CH_2)_{15}$-$CH(CH_3)$-CH_2-CH_3	1.10
5730.	646-30-0	1	1	1	Nonadecanoic acid	H_3C-$(CH_2)_{17}$-COOH	4.3
5731.	42232-76-8	1	1	1	Nonadecanoic acid, docosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{21}$-CH_3	5.3
5732.	42232-66-6	1	1	1	Nonadecanoic acid, dodecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{11}$-CH_3	5.3
5733.	36610-54-5	1	1	1	Nonadecanoic acid, eicosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{19}$-CH_3	5.3
5734.	42232-75-7	1	1	1	Nonadecanoic acid, heneicosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{20}$-CH_3	5.3
5735.		1	1	1	Nonadecanoic acid, heptacosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{26}$-CH_3	5.3
5736.	36610-51-2	1	1	1	Nonadecanoic acid, heptadecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{16}$-CH_3	5.3
5737.		1	1	1	Nonadecanoic acid, hexacosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{25}$-CH_3	5.3
5738.	36610-50-1	1	1	1	Nonadecanoic acid, hexadecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{15}$-CH_3	5.3
5739.	1731-94-8	0	1	0	Nonadecanoic acid, methyl ester	H_3C-$(CH_2)_{17}$-COO-CH_3	5.3
5740.	36610-53-4	1	1	1	Nonadecanoic acid, nonadecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{18}$-CH_3	5.3
5741.	36610-52-3	1	1	1	Nonadecanoic acid, octadecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{17}$-CH_3	5.3
5742.		1	1	1	Nonadecanoic acid, pentacosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{24}$-CH_3	5.3
5743.	36610-49-8	1	1	1	Nonadecanoic acid, pentadecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{14}$-CH_3	5.3
5744.	121877-66-5	1	1	1	Nonadecanoic acid, tetracosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{23}$-CH_3	5.3
5745.	36610-48-7	1	1	1	Nonadecanoic acid, tetradecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{13}$-CH_3	5.3
5746.	42232-77-9	1	1	1	Nonadecanoic acid, tricosyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{22}$-CH_3	5.3
5747.	36610-47-6	1	1	1	Nonadecanoic acid, tridecyl ester	H_3C-$(CH_2)_{17}$-COO-$(CH_2)_{12}$-CH_3	5.3
5748.	53254-53-8	1	1	1	Nonadecanoic acid, 17-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COOH	4.3
5749.	121877-54-1	1	1	1	Nonadecanoic acid, 17-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COO-$(CH_2)_{20}$-CH_3	5.3
5750.	121877-69-8	1	1	1	Nonadecanoic acid, 17-methyl-, tetracosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COO-$(CH_2)_{23}$-CH_3	5.3
5751.	121877-59-6	1	1	1	Nonadecanoic acid, 17-methyl-, tricosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{15}$-COO-$(CH_2)_{22}$-CH_3	5.3
5752.	6250-72-2	1	1	1	Nonadecanoic acid, 18-methyl-	$(H_3C)_2$=CH-$(CH_2)_{16}$-COOH	4.3
5753.	145090-31-9	0	1	0	Nonadecanoic acid, 18-methyl-, 2-(acetyloxy)-1-(hydroxymethyl)ethyl ester		5.3
5754.		1	1	1	Nonadecanoic acid, 18-methyl-, eicosyl ester	$(H_3C)_2$=CH-$(CH_2)_{16}$-COO-$(CH_2)_{19}$-CH_3	5.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5755.	150643-41-7	0	1	0	Nonadecanoic acid, 18-methyl-, ester with 1,2,3-propanetriol monoacetate mono(16-methylheptadecanoate)		5.3
5756.	121877-51-8	1	1	1	Nonadecanoic acid, 18-methyl-, heneicosyl ester	$(H_3C)_2$═CH-$(CH_2)_{16}$-COO-$(CH_2)_{20}$-CH_3	5.3
5757.	121877-37-0	1	1	1	Nonadecanoic acid, 18-methyl-, nonadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{16}$-COO-$(CH_2)_{18}$-CH_3	5.3
5758.	71607-90-4	1	0	0	Nonadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
5759.	52783-43-4	1	0	0	Nonadecanol		2.5
5760.	1454-84-8	1	1	1	1-Nonadecanol	H_3C-$(CH_2)_{17}$-CH_2OH	2.5
5761.	6809-52-5	1	1	1	5,9,13,17-Nonadecatetraen-2-one, 6,10,14,18-tetramethyl-		3.13
5762.	27400-77-7	1	0	0	Nonadecene	H-$(CH_2)_n$-CH═CH-$(CH_2)_{(17-n)}$-H	1.11
5763.	18435-45-5	1	1	1	1-Nonadecene	H_2C═CH-$(CH_2)_{16}$-CH_3	1.11
5764.	52254-50-9	1	0	0	1-Nonadecene, 2-methyl-	H_2C═$C(CH_3)$-$(CH_2)_{16}$-CH_3	1.11
5765.		1	0	0	2-Nonadecene, (*Z*)-	H_3C-CH═CH-$(CH_2)_{15}$-CH_3	1.11
5766.	94434-40-9	1	0	0	2-Nonadecene, (*E*)-		1.11
5767.	110746-39-9	1	0	0	2-Nonadecene, 2-methyl-	H_3C-$C(CH_3)$═CH-$(CH_2)_{15}$-CH_3	1.11
5768.		1	0	0	2-Nonadecene, 17-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{13}$-$CH(CH_3)$-CH_2-CH_3	1.11
5769.		1	0	0	2-Nonadecene, 17-methyl-, (*E*)-		1.11
5770.		1	0	0	2-Nonadecene, 18-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{14}$-$CH(CH_3)_2$	1.11
5771.		1	0	0	2-Nonadecene, 18-methyl-, (*E*)-		1.11
5772.	6750-03-4 5910-87-2	1	1	1	2,4-Nonadienal, (*E,E*)-		3.12
5773.		0	1	0	2,4-Nonadienal, 6-methyl-		3.12
5774.		0	1	0	2,4-Nonadienal, 8-methyl-		3.12
5775.	26370-28-5	0	1	0	2,6-Nonadienal {leaf aldehyde violet}		3.12
5776.	557-48-2	0	1	0	2,6-Nonadienal, (*E,Z*)-		3.12, 24.3, 25.29
5777.	129777-21-5	0	1	0	2,6-Nonadienal, 2-methyl-5-(1-methylethyl)-8-oxo-, (*E,E*)-(+)-		3.12, 3.13
5778.	71030-52-9	0	1	0	Nonadiene		1.11
5779.	51109-34-3	0	1	0	Nonadienoic acid		4.3
5780.		0	1	0	2,4-Nonadienoic acid, 2,3-dimethyl-		4.3
5781.	60026-10-0	1	1	1	2,6-Nonadienoic acid		4.3
5782.	23605-13-2	0	1	0	2,6-Nonadienoic acid, (*E,Z*)-		4.3
5783.	70898-29-2	0	1	0	2,7-Nonadienoic acid, (*E,Z*)-		4.3
5784.		0	1	0	4,6-Nonadienoic acid		4.3
5785.	63450-36-2	0	1	0	Nonadien-1-ol		2.5
5786.	7786-44-9	0	1	0	2,6-Nonadien-1-ol		2.5
5787.	28069-72-9	0	1	0	2,6-Nonadien-1-ol, (*E,Z*)-		2.5
5788.	56805-23-3	0	1	0	3,6-Nonadien-1-ol		2.5
5789.	53046-97-2	0	1	0	3,6-Nonadien-1-ol, (*Z,Z*)-		2.5
5790.	38713-12-1	0	1	0	3,7-Nonadien-1-ol, 4,8-dimethyl- {homogeraniol}		2.5
5791.	459-88-1	0	1	0	3,7-Nonadien-1-ol, 4,8-dimethyl-, (*E*)-		2.5
5792.	150405-75-7	0	1	0	6,8-Nonadien-2-ol, 8-methyl-5-(3-methylbutyl)-		2.5
5793.	40525-38-0	1	1	1	6,8-Nonadien-2-ol, 8-methyl-5-(1-methylethyl)- {solanol}		2.5

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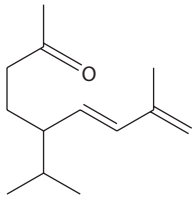
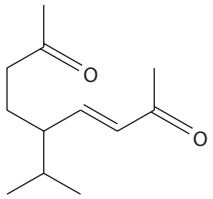
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5794.	64130-24-1	1	1	1	6,8-Nonadien-2-ol, 8-methyl-5-(1-methylethyl)- {solanol isomer}		2.5
5795.	817-88-9	0	1	0	3,7-Nonadien-2-one, 4,8-dimethyl-		3.13
5796.		0	1	0	3,8-Nonadien-2-one, 4,8-dimethyl-		3.13
5797.	123695-65-8	1	0	0	5,7-Nonadien-2-one, 8-hydroxy-5-(1-methylethyl)-, (*E,Z*)-		3.13
5798.	39012-18-5	1	1	1	5,7-Nonadien-2-one, 8-methyl-5-(1-methylethyl)- {isosolanone}		3.13
5799.	60714-16-1	0	1	0	6,8-Nonadien-2-one, 6-methyl-5-(1-methylethenyl)-		3.13
5800.	40286-47-3	0	1	0	6,8-Nonadien-2-one, 8-methyl-5-(methylethyl)-		3.13
5801.	2278-53-7	0	1	0	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [R-(*E*)]-		3.13
5802.	1937-54-8	1	1	1	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [S-(*E*)]- {solanone}		3.13, 24.3
5803.	54868-48-3	0	1	0	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, (*E*)-		3.13
5804.	124-19-6	1	1	1	Nonanal {pelargonaldehyde}	H_3C-$(CH_2)_7$-CH═O	3.12, 24.3, 25.29
5805.	111-84-2	1	1	1	Nonane	H_3C-$(CH_2)_7$-CH_3	1.10
5806.		1	0	0	Nonane, 4-acetyl-2,6,8-trimethyl-		3.13
5807.	871-83-0	1	0	0	Nonane, 2-methyl-		1.10
5808.	51655-64-2	1	0	0	Nonane, 3-methylene-		1.11
5809.	123-99-9	1	1	1	Nonanedioic acid {azelaic acid}	HOOC-$(CH_2)_7$-COOH	4.3
5810.	3937-56-2	0	1	0	1,9-Nonanediol	$HOCH_2$-$(CH_2)_7$-CH_2OH	2.5
5811.	55023-56-8	1	1	1	2,8-Nonanediol, 5-(1-methylethyl)-		2.5
5812.		0	1	0	2,5-Nonanedione		3.13
5813.		0	1	0	2,7-Nonanedione, 8-hydroxy-8-methyl-5-(1-methylethyl)-		2.5, 3.13
5814.	55023-57-9	1	1	1	2,8-Nonanedione, 5-(1-methylethyl)- {norsolanadione}		3.13
5815.	38284-28-5	0	1	0	2,5,8-Nonanetrione		3.13
5816.	112-05-0	1	1	1	Nonanoic acid {pelargonic acid}	H_3C-$(CH_2)_7$-COOH	4.3, 24.3, 25.29
5817.	123-29-5	0	1	0	Nonanoic acid, ethyl ester	H_3C-$(CH_2)_7$-COO-C_2H_5	5.3, 24.3, 25.29
5818.	1731-84-6	0	1	0	Nonanoic acid, methyl ester	H_3C-$(CH_2)_7$-COO-CH_3	5.3
5819.	41653-89-8	0	1	0	Nonanoic acid, 7-methyl-		4.3
5820.	6064-52-4	0	1	0	Nonanoic acid, 4-oxo-		3.13, 4.3
5821.	143-08-8	1	1	1	1-Nonanol	H_3C-$(CH_2)_7$-CH_2OH	2.5
5822.	628-99-9	1	0	0	2-Nonanol		2.5
5823.	624-51-1	1	0	0	3-Nonanol		2.5
5824.	19870-37-2	1	0	0	4-Nonanol, 2,6,8-trimethyl-		2.5
5825.	821-55-6	1	1	1	2-Nonanone	H_3C-$(CH_2)_6$-CO-CH_3	3.13, 24.3, 25.29

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5826.	58002-07-6	0	1	0	2-Nonanone, 6,7-epoxy-8-hydroxy-5-(1-methylethyl)-		3.13, 10.2
5827.	55023-54-6	1	1	1	2-Nonanone,8-hydroxy-5-(1-methylethyl)-		3.13
5828.	123-18-2	1	0	0	4-Nonanone, 2,6,8-trimethyl		3.13
5829.		0	1	0	5-Nonanone, 2,8-dimethyl-7,8-epoxy-		3.13, 10.2
5830.	68-26-8	0	1	0	2,4,6,8-Nonatetraen-1-ol, 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (all-*E*)- {retinol}		2.5, 26.9
5831.	7194-86-7	1	1	1	Nonatriacontane	H_3C-$(CH_2)_{37}$-CH_3	1.10
5832.	17609-32-4	0	1	0	3,5,7-Nonatrien-2-one		3.13
5833.	2463-53-8	1	1	1	2-Nonenal	H_3C-$(CH_2)_5$-CH═CH-CH═O	3.12, 24.3
5834.	18829-56-6	0	1	0	2-Nonenal, (*E*)-		3.12, 24.3
5835.		0	1	0	2-Nonenal, 2,3-dimethyl-8-oxo-		3.12, 3.13
5836.	2277-19-2	0	1	0	6-Nonenal, (*Z*)-		3.12
5837.	124-11-8	1	0	0	1-Nonene	H_3C-$(CH_2)_6$-CH═CH_2	1.11
5838.	2216-39-8	1	0	0	2-Nonene	H_3C-$(CH_2)_5$-CH═CH-CH_3	1.11
5839.	17003-99-5	1	0	0	2-Nonene, 3-methyl-		1.11
5840.	53966-53-3	1	0	0	3-Nonene, 2-methyl-	H_3C-$(CH_2)_4$-CH═CH-CH═$(CH_3)_2$	1.11
5841.	2198-23-4	1	0	0	4-Nonene		1.11
5842.	55023-53-5	1	1	1	3-Nonene-2,8-diol, 5-(1-methylethyl)-		2.5
5843.	38372-56-4	1	1	1	3-Nonene-2,8-dione {norsolanadione}		3.13
5844.	35953-21-0 60619-46-7 101159-09-5	1	1	1	3-Nonene-2,8-dione, 5-(1-methylethyl)-, [S-(*E*)]- {norsolanadione, oxysolanone}		3.13
5845.	37822-76-7	0	1	0	Nonenoic acid, methyl ester		5.3
5846.	3760-11-0	1	1	1	2-Nonenoic acid	H_3C-$(CH_2)_5$-CH═CH-COOH	4.3
5847.	14812-03-4	0	1	0	2-Nonenoic acid, (*E*)-		4.3
5848.	111-79-5	0	1	0	2-Nonenoic acid, methyl ester		5.3
5849.	4124-88-3	0	1	0	3-Nonenoic acid		4.3
5850.	41653-98-9	0	1	0	3-Nonenoic acid, (*Z*)-		4.3
5851.	41653-99-0	0	1	0	6-Nonenoic acid, (*Z*)-		4.3
5852.	31642-67-8	0	1	0	8-Nonenoic acid		4.3
5853.	31502-14-4	0	1	0	2-Nonen-1-ol	H_3C-$(CH_2)_5$-CH═CH-CH_2OH	2.5
5854.	10340-23-5	0	1	0	3-Nonen-1-ol, (*Z*)-		2.5
5855.	68985-18-2	0	1	0	2-Nonen-4-one, 3-methyl-, (*E*)-		3.13
5856.	65017-85-8	0	1	0	2-Nonen-4-one, 8-hydroxy-3-methyl-, (*E*)-		2.5, 3.13
5857.	122881-64-5	0	1	0	3-Nonen-8-one, 1,2-dihydroxy-2-methyl-5-(1-methylethyl)-		2.5, 3.13
5858.		0	1	0	5-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-		2.5, 3.13
5859.	55023-59-1	0	1	0	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-		2.5, 3.13
5860.	57934-86-8	0	1	0	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (*E*)-(±)-		2.5, 3.13
5861.	60828-13-9	0	1	0	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (6*E*)-		2.5, 3.13
5862.	55023-52-4	0	1	0	6-Nonen-2-one, 8-hydroxy-5-(1-methylethyl)-		2.5, 3.13
5863.	77288-95-0	0	1	0	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [R-[R*,S*-(*E*)]]-		2.5, 3.13
5864.	77288-96-1	0	1	0	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [S-[R*,R*-(*E*)]]-		2.5, 3.13
5865.	3452-09-3	1	0	0	1-Nonyne	H_3C-$(CH_2)_6$-C≡CH	1.11

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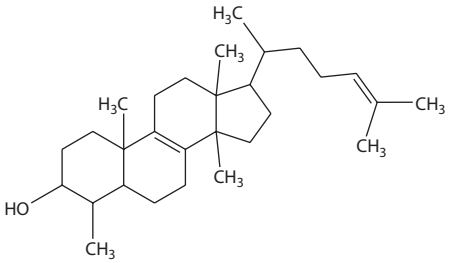
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5866.	18444-66-1	0	1	0	19-Norlanosta-1,5,23-triene-3,11,22-trione, 25-(acetyloxy)-2, 16,20-trihydroxy-9-methyl-, (9β,10α,16α,23*E*)-		2.5, 2.7, 3.13, 5.3
5867.	17278-28-3	0	1	0	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3, 16,20-trihydroxy-9-methyl-, (3α,9β,10α,16α,23*E*)-		2.5, 2.7, 3.13, 5.3
5868.	89647-62-1	0	1	0	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16, 20-trihydroxy-9-methyl-, (3β,9β,10α,16α,23*E*)-		2.5, 2.7, 3.13, 5.3
5869.	51013-77-5	0	1	0	31-Norlanosterol		2.5, 2.7
5870.	5157-09-5	0	1	0	Norleucine {2-aminohexanoic acid}	H_3C-$(CH_2)_3$-$CH(NH_2)$-COOH	4.3, 4.10, 12.2
5871.		0	1	0	*Novosphingobium aromaticivorans*		22.2
5872.	9026-81-7	0	1	0	Nuclease		22.2
5873.	9003-98-9	0	1	0	Nuclease, deoxyribo-		22.2
5874.	9055-11-2	0	1	0	Nuclease, endo-		22.2
5875.	59977-50-3	0	1	0	Nuclease, mammalian deoxyribonucleate-nicking endo-		22.2
5876.	9025-44-9	0	1	0	Nucleosidase		22.2
5877.	9033-33-4	0	1	0	Nucleotidase		22.2
5878.	9012-90-2	0	1	0	Nucleotidyltransferase, deoxyribonucleate {polymerase, nucleic acid deoxyribo}		22.2
5879.	9068-38-6	0	1	0	Nucleotidyltransferase, deoxyribonucleate, RNA-dependent		22.2
5880.	9014-24-8	0	1	0	Nucleotidyltransferase, ribonucleate		22.2
5881.	9026-28-2	0	1	0	Nucleotidyltransferase, ribonucleate, RNA-dependent		22.2
5882.	66328-00-5	1	0	0	2,6,10,14,18,22,26-Octacosaheptaene, 2,6,10,14,18,22,26-heptamethyl-, (all-*E*)-		1.11
5883.	630-02-4	1	1	1	Octacosane	H_3C-$(CH_2)_{26}$-CH_3	1.10
5884.	1560-98-1	1	1	1	Octacosane, 2-methyl-	$(H_3C)_2$═CH-$(CH_2)_{25}$-CH_3	1.10
5885.	65820-58-8	1	1	1	Octacosane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{24}$-CH_3	1.10
5886.	506-48-9	1	1	1	Octacosanoic acid	H_3C-$(CH_2)_{26}$-COOH	4.3
5887.	121878-02-2	1	1	1	Octacosanoic acid, docosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{21}$-CH_3	5.3
5888.		1	1	1	Octacosanoic acid, dodecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{11}$-CH_3	5.3
5889.	121877-91-6	1	1	1	Octacosanoic acid, eicosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{19}$-CH_3	5.3
5890.		1	1	1	Octacosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl octacosanoate}		2.7, 5.3
5891.	121877-95-0	1	1	1	Octacosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{20}$-CH_3	5.3
5892.		1	1	1	Octacosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{26}$-CH_3	5.3
5893.		1	1	1	Octacosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{16}$-CH_3	5.3

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5894.		1	1	1	Octacosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{25}$-CH_3	5.3
5895.	80756-16-7	1	1	1	Octacosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{15}$-CH_3	5.3
5896.		1	1	1	Octacosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{18}$-CH_3	5.3
5897.	95415-29-5	1	1	1	Octacosanoic acid, octadecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{17}$-CH_3	5.3
5898.		1	1	1	Octacosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{24}$-CH_3	5.3
5899.		1	1	1	Octacosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{14}$-CH_3	5.3
5900.	80252-40-0	1	1	1	Octacosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{23}$-CH_3	5.3
5901.	28570-28-7	1	1	1	Octacosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{13}$-CH_3	5.3
5902.		1	1	1	Octacosanoic acid, tricosyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{22}$-CH_3	5.3
5903.		1	1	1	Octacosanoic acid, tridecyl ester	H_3C-$(CH_2)_{26}$-COO-$(CH_2)_{12}$-CH_3	5.3
5904.	121878-04-4	1	1	1	Octacosanoic acid, 26-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{24}$-COO-$(CH_2)_{21}$-CH_3	5.3
5905.	557-61-9	1	1	1	1-Octacosanol {montanyl alcohol}	H_3C-$(CH_2)_{26}$-CH_2OH	2.5
5906.		0	1	0	1-Octacosanol, 26-methyl-		2.5
5907.		0	1	0	1-Octacosanol, 27-methyl-		2.5
5908.	18835-34-2	1	0	0	1-Octacosene	H_3C-$(CH_2)_{25}$-CH=CH_2	1.11
5909.		1	0	0	1-Octacosene, 2-methyl-	H_2C=$C(CH_3)$-$(CH_2)_{25}$-CH_3	1.11
5910.		1	0	0	2-Octacosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{24}$-CH_3	1.11
5911.		1	0	0	2-Octacosene, (*E*)-		1.11
5912.		1	0	0	2-Octacosene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{24}$-CH_3	1.11
5913.		1	0	0	2-Octacosene, 26-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{23}$-$CH(CH_3)$-CH_2-CH_3	1.11
5914.		1	0	0	2-Octacosene, 26-methyl-, (*E*)-		1.11
5915.		1	0	0	2-Octacosene, 27-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{23}$-$CH(CH_3)_2$	1.11
5916.		1	0	0	2-Octacosene, 27-methyl-, (*E*)-		1.11
5917.	26764-25-0	1	1	1	Octadecadienoic acid		4.3
5918.	28984-77-2	0	1	0	Octadecadienoic acid, (Z,Z)-		4.3
5919.	97145-16-9	0	1	0	Octadecadienoic acid, 1-[[[(2-aminoethoxy) hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl ester, (all-*Z*)-		5.3, 12.2
5920.	97190-11-9	0	1	0	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) hexadecanoate		5.3, 12.2
5921.	97190-13-1	0	1	0	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecanoate, (*Z,Z*)-		5.3, 12.2
5922.	28061-47-4	0	1	0	Octadecadienoic acid, methyl ester		5.3
5923.	97210-24-7	0	1	0	Octadecadienoic acid, monoester with 1,2,3-propanetriol 1,1′-(hydrogen phosphate)mono-3-hexadecenoate, [R-[R*,S*-(*E*)]]-		5.3
5924.	60-33-3	1	1	1	9,12-Octadecadienoic acid, (*Z,Z*)- {linoleic acid}		4.3
5925.	506-21-8	1	1	1	9,12-Octadecadienoic acid, (*E,E*)- {linoleic acid}	H_3C-$(CH_2)_4$-CH=CH-CH_2-CH=CH-$(CH_2)_7$-COOH	0.4, 4.3, 24.3, 25.29
5926.	26836-36-2	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, diester with 1,2,3-propanetriol monohexadecanoate {palmitodilinolein}		5.3

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5927.	28409-91-8	0	1	0	9,12-Octadecadienoic acid-, diester with 1,2,3-propanetriol mono-9-octadecenoate {oleodilinolein}?		5.3
5928.	29590-02-1	0	1	0	9,12-Octadecadienoic acid-, diester with 1,2,3-propanetriol monooctadecanoate {stearodilinolein}		5.3
5929.	26836-35-1	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, ester with 1,2,3-propanetriol monohexadecanoate mono[(*Z*)-9-octadecenoate]		5.3
5930.	544-35-4	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, ethyl ester {ethyl linoleate}	H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COO-C_2H_5	5.3
5931.	4546-59-2	0	1	0	9,12-Octadecadienoic acid, 18-hydroxy-, (*Z,Z*)-		4.3
5932.	2462-85-3	0	1	0	9,12-Octadecadienoic acid, methyl ester		5.3
5933.	112-63-0	1	1	1	9,12-Octadecadienoic acid (*Z,Z*)-, methyl ester {methyl linoleate}	H_3C-$(CH_2)_4$-CH═CH-CH_2-CH═CH-$(CH_2)_7$-COO-CH_3	5.3, 24.3
5934.	26836-38-4	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol monooctadecanoate mono-9-octadecenoate, (*Z*)-		5.3
5935.	28880-78-6	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol bis[(Z)-9-octadecenoate]		5.3
5936.	26836-30-6 99431-70-6	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitolinolein}		5.3
5937.	26836-32-8	0	1	0	9,12-Octadecadienoic acid, monoester with propanetriol monohexadecanoate and monooctadecanoate {palmitostearolinolein}		5.3
5938.	34521-51-2	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dioctadecanoate		5.3
5939.	70495-60-2	1	1	1	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15,19,23,27,31, 35-nonamethyl- 2,6,10,14,18,22,26,30, 34-hexatriacontanonaenyl ester {solanesyl octadecadienoate}		5.3
5940.	53950-59-7	1	0	0	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
5941.	506-43-4	0	1	0	9,12-Octadecadien-1-ol, (*Z,Z*)-		2.5
5942.	56847-03-1	1	0	0	Octadecadienoic acid, methyl ester		5.3
5943.	593-45-3	1	1	1	Octadecane	H_3C-$(CH_2)_{16}$-CH_3	1.10
5944.	1560-88-9	0	1	0	Octadecane, 2-methyl-	H_3C-$(CH_2)_{15}$-CH═$(CH_3)_2$	1.10
5945.	6561-44-0	0	1	0	Octadecane, 3-methyl-	H_3C-$(CH_2)_{14}$-$CH(CH_3)$-CH_2-CH_3	1.10

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
5946.	554-62-1	0	1	0	1,3,4-Octadecanetriol, 2-amino-, [2S-(2R*,3R*,4S*)]-		2.5, 12.2
5947.	57-11-4	1	1	1	Octadecanoic acid {stearic acid}	H_3C-$(CH_2)_{16}$-COOH	0.4, 4.3, 25.29, 26.9
5948.	26855-40-3	0	1	0	Octadecanoic acid, diester with 1,2,3-propanetriol dihexadecanoate {dipalmitostearin}?		5.3
5949.	22413-03-2	1	1	1	Octadecanoic acid, docosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{21}$-CH_3	5.3
5950.	5303-25-3	1	1	1	Octadecanoic acid, dodecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{11}$-CH_3	5.3
5951.	22413-02-1	1	1	1	Octadecanoic acid, eicosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{19}$-CH_3	5.3
5952.	111-61-5	1	1	1	Octadecanoic acid, ethyl ester {ethyl stearate}	H_3C-$(CH_2)_{16}$-COO-CH_2-CH_3	5.3, 24.3
5953.	42232-59-7	1	1	1	Octadecanoic acid, heneicosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{20}$-CH_3	5.3
5954.	121877-78-9	1	1	1	Octadecanoic acid, heptacosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{26}$-CH_3	5.3
5955.	18299-82-6	1	1	1	Octadecanoic acid, heptadecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{16}$-CH_3	5.3
5956.	58886-94-5	1	1	1	Octadecanoic acid, hexacosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{25}$-CH_3	5.3
5957.	1190-63-2	1	1	1	Octadecanoic acid, hexadecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{15}$-CH_3	5.3
5958.	1330-70-7	0	1	0	Octadecanoic acid, hydroxy-		2.5, 4.3
5959.	3155-42-8	0	1	0	Octadecanoic acid, 18-hydroxy-	$HOCH_2$-$(CH_2)_{16}$-COOH	2.5, 4.3
5960.	112-61-8	1	1	1	Octadecanoic acid, methyl ester	H_3C-$(CH_2)_{16}$-COO-CH_3	5.3
5961.	121877-86-9	1	1	1	Octadecanoic acid, nonacosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{28}$-CH_3	5.3
5962.	36610-45-4	1	1	1	Octadecanoic acid, nonadecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{18}$-CH_3	5.3
5963.	70495-59-9	1	1	1	Octadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecanoate}		5.3
5964.	63317-82-8	1	1	1	Octadecanoic acid, octacosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{27}$-CH_3	5.3
5965.	2778-96-3	1	1	1	Octadecanoic acid, octadecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{17}$-CH_3	5.3
5966.	121877-65-4	1	1	1	Octadecanoic acid, pentacosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{24}$-CH_3	5.3
5967.	18299-80-4	1	1	1	Octadecanoic acid, pentadecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{14}$-CH_3	5.3
5968.	42232-61-1	1	1	1	Octadecanoic acid, tetracosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{23}$-CH_3	5.3
5969.	17661-50-6	1	1	1	Octadecanoic acid, tetradecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{13}$-CH_3	5.3
5970.	63317-83-9	1	1	1	Octadecanoic acid, triacontyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{29}$-CH_3	5.3
5971.	42232-60-0	1	1	1	Octadecanoic acid, tricosyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{22}$-CH_3	5.3
5972.	31556-45-3	1	1	1	Octadecanoic acid, tridecyl ester	H_3C-$(CH_2)_{16}$-COO-$(CH_2)_{12}$-CH_3	5.3
5973.	17001-28-4	1	1	1	Octadecanoic acid, 16-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{14}$-COOH IVA-3	
5974.	121877-53-0	1	1	1	Octadecanoic acid, 16-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{14}$-COO-$(CH_2)_{21}$-CH_3	5.3
5975.	121877-75-6	1	1	1	Octadecanoic acid, 16-methyl-, hexacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{14}$-COO-$(CH_2)_{25}$-CH_3	5.3
5976.	2724-59-6	0	1	0	Octadecanoic acid, 17-methyl-	$(H_3C)_2$=CH-$(CH_2)_{15}$-COOH	4.3
5977.		0	1	0	Octadecanoic acid, 17-methyl-, methyl ester	$(H_3C)_2$=CH-$(CH_2)_{15}$-COO-CH_3	5.3
5978.	62172-54-7	1	0	0	Octadecanoicacid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
5979.	112-92-5	1	1	1	1-Octadecanol {stearyl alcohol}	H_3C-$(CH_2)_{16}$-CH_2OH	2.5
5980.	2490-01-9	0	1	0	1-Octadecanol, 16-methyl-		2.5
5981.	51592-59-7	0	1	0	3,6,9,12,15-Octadecapentaenoic acid, (all-*Z*)-		4.3
5982.	25448-06-0	0	1	0	Octadecatetraenoic acid		4.3
5983.	25448-03-7	0	1	0	Octadecatrienoic acid		4.3
5984.	27213-43-0	0	1	0	Octadecatrienoic acid, (*Z,Z,Z*)-		4.3

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	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
5985.	97190-08-4	0	1	0	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecadienoate, (all-*Z*)-		5.3, 12.2
5986.	97229-62-4	0	1	0	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) 2(or 3)-hexadecanoate, (*Z,Z,Z*)-		5.3, 12.2
5987.	97229-63-5	0	1	0	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1,1′-(hydrogen phosphate) 2(or 3)-(3-hexadecenoate), [R-(R*,S*)]-		5.3
5988.	29565-44-4	0	1	0	Octadecatrienoic acid, methyl ester		5.3
5989.	13296-76-9	1	0	0	9,11,13-Octadecatrienoic acid		4.3
5990.	463-40-1	1	1	1	9,12,15-Octadecatrienoic acid, (*Z,Z,Z*)- {linolenic acid}	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COOH	0.4, 4.3, 24.3
5991.		1	1	1	9,12,15-Octadecatrienoic acid, docosyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{21}$-CH_3	5.3
5992.		1	1	1	9,12,15-Octadecatrienoic acid, dodecyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{11}$-CH_3	5.3
5993.		1	1	1	9,12,15-Octadecatrienoic acid, eicosyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{19}$-CH_3	5.3
5994.	1191-41-9	0	1	0	9,12,15-Octadecatrienoic acid, ethyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-$COOC_2H_5$	5.3
5995.		1	1	1	9,12,15-Octadecatrienoic acid, heneicosyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{20}$-CH_3	5.3
5996.		1	1	1	9,12,15-Octadecatrienoic acid, heptacosyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{26}$-CH_3	5.3
5997.		1	1	1	9,12,15-Octadecatrienoic acid, heptadecyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{16}$-CH_3	5.3
5998.		1	1	1	9,12,15-Octadecatrienoic acid, hexacosyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{25}$-CH_3	5.3
5999.		1	1	1	9,12,15-Octadecatrienoic acid, hexadecyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{15}$-CH_3	5.3
6000.	51327-73-2	0	1	0	9,12,15-Octadecatrienoic acid, 18-hydroxy-, (*Z,Z,Z*)-	$HOCH_2$-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COOH	4.3
6001.	7361-80-0	1	1	1	9,12,15-Octadecatrienoic acid, methyl ester {methyl linolenate}	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-$COOCH_3$	5.3
6002.	301-00-8	1	1	1	9,12,15-Octadecatrienoic acid, methyl ester, (*Z,Z,Z*)- {methyl linolenate}	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-CH_3	5.3, 24.3
6003.		1	1	1	9,12,15-Octadecatrienoic acid, nonadecyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{18}$-CH_3	5.3
6004.	28973-74-2	1	1	1	9,12,15-Octadecatrienoic acid, 3,7,11,15,19,23,27,31, 35-nonamethyl-2,6,10, 14,18,22,26,30, 34-hexatriacontanonaenyl ester {solanesyl octadecatrienoate}		5.3
6005.	17673-60-8	1	1	1	9,12,15-Octadecatrienoic acid, octadecyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{17}$-CH_3	5.3
6006.		1	1	1	9,12,15-Octadecatrienoic acid, pentacosyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{24}$-CH_3	5.3
6007.		1	1	1	9,12,15-Octadecatrienoic acid, pentadecyl ester, (*Z,Z,Z*)-	H_3C-($CH_2CH{=}CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{14}$-CH_3	5.3

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6008.		1	1	1	9,12,15-Octadecatrienoic acid, tetracosyl ester, (*Z,Z,Z*)-	H_3C-(CH_2CH=$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{23}$-CH_3	5.3
6009.		1	1	1	9,12,15-Octadecatrienoic acid, tetradecyl ester, (*Z,Z,Z*)-	H_3C-(CH_2CH=$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{13}$-CH_3	5.3
6010.		1	1	1	9,12,15-Octadecatrienoic acid, tricosyl ester, (*Z,Z,Z*)-	H_3C-(CH_2CH=$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{22}$-CH_3	5.3
6011.		1	1	1	9,12,15-Octadecatrienoic acid, tridecyl ester, (*Z,Z,Z*)-	H_3C-(CH_2CH=$CH)_3$-$(CH_2)_7$-COO-$(CH_2)_{12}$-CH_3	5.3
6012.	30452-68-7	1	0	0	9,12,15-Octadecatrienoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(E,Z,Z,Z)]]-		5.3
6013.	506-44-5	1	0	0	9,12,15-Octadecatrien-1-ol, (*Z,Z,Z*)-		2.5
6014.	56554-87-1	0	1	0	16-Octadecenal		3.12
6015.	27070-58-2	1	0	0	Octadecene	H-$(CH_2)_n$-CH=CH-$(CH_2)_{(16-n)}$-H	1.11
6016.	112-88-9	1	0	0	1-Octadecene	H_2C=CH-$(CH_2)_{15}$-CH_3	1.11
6017.	61868-20-0	1	0	0	1-Octadecene, 2-methyl-	H_2C=C(CH_3)-$(CH_2)_{15}$-CH_3	1.11
6018.		1	0	0	2-Octadecene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{14}$-CH_3	1.11
6019.	7206-18-0	1	0	0	2-Octadecene, (*E*)-		1.11
6020.		1	0	0	2-Octadecene, 2-methyl-	H_3C-C(CH_3)=CH-$(CH_2)_{14}$-CH_3	1.11
6021.		1	0	0	2-Octadecene, 16-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{12}$-CH(CH_3)-CH_2-CH_3	1.11
6022.		1	0	0	2-Octadecene, 16-methyl-, (*E*)-		1.11
6023.		1	0	0	2-Octadecene, 17-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{13}$-CH(CH_3)$_2$	1.11
6024.		1	0	0	2-Octadecene, 17-methyl-, (*E*)		1.11
6025.	26764-26-1	1	1	1	Octadecenoic acid {oleic acid}		4.3, 24.3, 25.29
6026.	112-79-8	1	1	1	Octadecenoic acid, (*E*)- {elaidic acid}		4.3
6027.	27104-13-8	0	1	0	Octadecenoic acid, (*Z*)-		4.3
6028.	93976-10-4	1	1	1	Octadecenoic acid, docosyl ester, (*Z*)-		5.3
6029.		1	1	1	Octadecenoic acid, heneicosyl ester, (*Z*)-		5.3
6030.	93976-08-0	1	1	1	Octadecenoic acid, hexacosyl ester, (*Z*)-		5.3
6031.	27234-05-5	0	1	0	Octadecenoic acid, methyl ester		5.3
6032.	93976-09-1	1	1	1	Octadecenoic acid, tetracosyl ester, (*Z*)-		5.3
6033.	112-80-1	1	1	1	9-Octadecenoic acid (*Z*)- {oleic acid}	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COOH	0.4, 4.3
6034.	71607-93-7	1	1	1	9-Octadecenoic acid (*Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester		5.3
6035.	57840-35-4	1	0	0	9-Octadecenoic acid (*Z*)-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
6036.	27071-84-7	0	1	0	9-Octadecenoic acid, diester with 1,2,3-propanetriol monohexadecanoate {palmitodiolein}		5.3
6037.		1	1	1	9-Octadecenoic acid (*Z*)-, docosyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{21}$-CH_3	5.3
6038.	36078-10-1	1	1	1	9-Octadecenoic acid (*Z*)-, dodecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{11}$-CH_3	5.3
6039.	22393-88-0	1	1	1	9-Octadecenoic acid (*Z*)-, eicosyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{19}$-CH_3	5.3
6040.	111-62-6	1	1	1	9-Octadecenoic acid (*Z*)-, ethyl ester {ethyl oleate}	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-C_2H_5	5.3, 24.3
6041.		1	1	1	9-Octadecenoic acid (*Z*)-, heptacosyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{26}$-CH_3	5.3
6042.	22393-86-8	1	1	1	9-Octadecenoic acid (*Z*)-, hexadecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{16}$-CH_3	5.3
6043.	112-62-9	1	1	1	9-Octadecenoic acid (*Z*)-, methyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-CH_3	5.3

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6044.	28409-94-1	0	1	0	9-Octadecenoic acid-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitoolein}		5.3
6045.		1	1	1	9-Octadecenoic acid (*Z*)-, nonadecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{18}$-CH_3	5.3
6046.	71607-93-7 73037-55-5	1	1	1	9-Octadecenoic acid (*Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester {solanesyl oleate}		5.3
6047.	17673-49-3	1	1	1	9-Octadecenoic acid (*Z*)-, octadecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{17}$-CH_3	5.3
6048.		1	1	1	9-Octadecenoic acid (*Z*)-, pentacosyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{24}$-CH_3	5.3
6049.	69454-18-8	1	1	1	9-Octadecenoic acid (*Z*)-, pentadecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{14}$-CH_3	5.3
6050.		1	1	1	9-Octadecenoic acid (*Z*)-, tetracosyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{23}$-CH_3	5.3
6051.	22393-85-7	1	1	1	9-Octadecenoic acid (*Z*)-, tetradecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{13}$-CH_3	5.3
6052.		1	1	1	9-Octadecenoic acid (*Z*)-, tricosyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{22}$-CH_3	5.3
6053.	75164-73-7	1	1	1	9-Octadecenoic acid (*Z*)-, tridecyl ester	H_3C-$(CH_2)_7$-CH=CH-$(CH_2)_7$-COO-$(CH_2)_{12}$-CH_3	5.3
6054.	104077-09-0	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-,1-(hydroxymethyl)-2-[(1-oxo-9-octadecenyl)oxy] ethyl ester, (*Z,Z,Z*)-		2.5, 5.3
6055.	104077-10-3	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-		2.5, 5.3
6056.	104100-34-7	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-1,3-propanediyl ester, (all-*Z*)-		2.5, 5.3
6057.	104077-06-7	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-3-[(1-oxo-9-octadecenyl) oxy]propyl ester, (*Z,Z,Z*)-		2.5, 5.3
6058.	104077-07-8	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-		2.5, 5.3
6059.	104077-11-4	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-		2.5, 5.3
6060.	104077-12-5	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl) oxy]-9-octadecenyl] oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-		2.5, 5.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6061.	104100-35-8	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 2-hydroxy-1,3-propanediyl ester, (all-*Z*)-		2.5, 5.3
6062.	104077-08-9	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[[1-oxo-18- [(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-		2.5, 5.3
6063.	104077-13-6	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-		2.5, 5.3
6064.	24753-52-4	0	1	0	9-Octadecenoic acid, 18-hydroxy-, (*Z*)-		2.5, 4.3
6065.	2462-84-2	0	1	0	9-Octadecenoic acid, methyl ester		5.3
6066.	593-47-5	0	1	0	9-Octadecen-1-ol		2.5
6067.	71899-42-8	0	1	0	5-Octadecyne	$H_3C\text{-}(CH_2)_3\text{-}C{\equiv}C\text{-}(CH_2)_{11}\text{-}CH_3$	1.11
6068.	141-27-5	1	1	1	2,6-Octadienal, 3,7-dimethyl-		3.12
6069.	5392-40-5	1	1	1	2,6-Octadienal, 3,7-dimethyl-, (*E*)- {*trans*-citral, *trans*-gerianal}		3.12, 24.3, 25.29
6070.	106-26-3	1	0	0	2,6-Octadienal, 3,7-dimethyl-, (*Z*)-		3.12
6071.	71607-91-5	1	0	0	1,6-Octadiene, 4,7-dimethyl- {2,5-dimethyl-2,7-octadiene}	$H_2C{=}CH\text{-}C(CH_3){=}CH\text{-}CH_2\text{-}CH{=}C(CH_3)_2$	1.11
6072.	123-35-3	1	1	1	1,6-Octadiene, 7-methyl-3-methylene- {myrcene}	$H_2C{=}CH\text{-}C(=CH_2)\text{-}(CH_2)_2\text{-}CH{=}C(CH_3)_2$	1.11
6073.	2216-70-8	1	0	0	2,4-Octadiene, 7-methyl-	$H_3C\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_2\text{-}CH(CH_3)_2$	1.11
6074.	40195-09-3	1	0	0	1,6-Octadiene, 2,7-dimethyl- = {2,7-dimethyl-2,7-octadiene}	$H_2C{=}C(CH_3)\text{-}(CH_2)_3\text{-}CH{=}C(CH_3)_2$	1.11
6075.	128241-35-0	1	0	0	1,6-Octadiene, 3,7-dimethyl- = {2,6-dimethyl-2,7-octadiene}	$H_2C{=}CH\text{-}CH(CH_3)\text{-}(CH_2)_2\text{-}CH{=}C(CH_3)_2$	1.11
6076.	71607-92-6	1	0	0	2,5-Octadiene, 7-methyl-	$H_3C\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}CH\text{-}CH(CH_3)_2$	1.11
6077.	2792-39-4	1	0	0	2,6-Octadiene, 2,6-dimethyl-		1.11
6078.	18476-57-8	1	0	0	2,6-Octadiene, 4,5-dimethyl-		1.11
6079.	66957-95-7	0	1	0	2,7-Octadiene-1,6-diol, 2, 6-dimethyl-, [S-(*E*)]-		2.5
6080.		0	1	0	Octadienoic acid		4.3
6081.	459-80-3	0	1	0	2,6-Octadienoic acid, 3,7-dimethyl- {geranic acid}		4.3
6082.	4698-08-2	0	1	0	2,6-Octadienoic acid, 3,7-dimethyl-, (*E*)-		4.3
6083.	4613-38-1	0	1	0	2,6-Octadienoic acid, 3,7-dimethyl-, (*Z*)-		4.3
6084.	64090-50-2	0	1	0	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-		4.3
6085.	54557-54-9	0	1	0	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-, (*E*)-		4.3

(*continued*)

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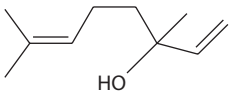
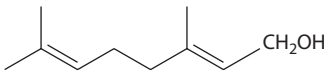
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6086.	70687-51-3	0	1	0	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-, methyl ester		5.3
6087.	78-70-6	1	1	1	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool}		0.4, 2.5, 24.3, 25.29
6088.		1	1	1	1,6-Octadien-3-ol, 3,7-dimethyl-, labeled with ^{14}C {linalool-^{14}C}		2.5, 25.29
6089.	126-91-0	1	1	1	1,6-Octadien-3-ol, 3,7-dimethyl- {*l*-linalool}		2.5
6090.	115-95-7	0	1	0	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate {linalyl acetate}		5.3, 24.3, 25.29
6091.	115-99-1	0	1	0	1,6-Octadien-3-ol, 3,7-dimethyl-, formate {linalyl formate}		5.3
6092.	106-24-1	1	1	1	2,6-Octadien-1-ol, 3,7-dimethyl-, (*E*)- {geraniol}		2.5, 24.3, 25.29
6093.	106-25-2	1	1	1	2,6-Octadien-1-ol, 3,7-dimethyl-, (*Z*)- {nerol}		2.5, 24.3, 25.29
6094.	38284-27-4	0	1	0	3,5-Octadien-2-one		3.13
6095.	30086-02-3	0	1	0	3,5-Octadien-2-one, (*E,E*)-		3.13
6096.	124-13-0	1	1	1	Octanal	$H_3C\text{-}(CH_2)_6\text{-}CH{=}O$	3.12, 24.3, 25.29
6097.		0	1	0	Octanal, 2,7-dimethyl-7-hydroxy-		2.5, 3.12
6098.	107-75-5	0	1	0	Octanal, 3,7-dimethyl-7-hydroxy- {hydroxycitronellal}		2.5, 3.12
6099.	111-86-4	1	1	1	1-Octanamine	$H_3C\text{-}(CH_2)_6\text{-}CH_2\text{-}NH_2$	12.2
6100.	111-65-9	1	1	1	Octane	$H_3C\text{-}(CH_2)_6\text{-}CH_3$	1.10
6101.		1	0	0	Octane, dimethyl-	$C_6H_{12}{=}(CH_3)_2$	1.10
6102.	61193-19-9	1	0	0	Octane, methyl-	$C_7H_{15}\text{-}CH_3$	1.10
6103.	2216-33-3	1	0	0	Octane, 3-methyl-		1.10
6104.	2216-34-4	0	1	0	Octane, 4-methyl-		1.10
6105.	505-48-6	1	0	0	Octanedioic acid {suberic acid}		4.3
6106.	20653-90-1	0	1	0	2,3-Octanediol		2.5
6107.	585-25-1	1	1	1	2,3-Octanedione		3.13
6108.	65716-44-1	0	1	0	2,7-Octanedione, 3,3-dimethyl-		3.13
6109.	124-12-9	1	0	0	Octanenitrile		11.2
6110.	124-07-2	1	1	1	Octanoic acid {caprylic acid}	$H_3C\text{-}(CH_2)_6\text{-}COOH$	0.4, 4.3, 21.3, 24.3, 25.29
6111.	14352-59-1	0	1	0	Octanoic acid, 3,3-dimethyl-		4.3
6112.	106-32-1	1	1	1	Octanoic acid, ethyl ester {ethyl caprylate}		5.3, 24.3, 25.29
6113.	111-11-5	0	1	0	Octanoic acid, methyl ester {methyl caprylate}		5.3
6114.	3004-93-1	0	1	0	Octanoic acid, 2-methyl-		4.3
6115.	2035-99-6	0	1	0	Octanoic acid, 3-methylbutyl ester		5.3
6116.	16493-80-4	0	1	0	Octanoic acid, 4-ethyl-		4.3
6117.	6061-10-5	0	1	0	Octanoic acid, 3-methyl-		4.3
6118.	504-99-4	0	1	0	Octanoic acid, 6-methyl-		4.3
6119.	693-19-6	0	1	0	Octanoic acid, 7-methyl-		4.3
6120.	70898-30-5	1	1	1	Octanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester, (all-*E*)- {solanesyl octanoate}		5.3

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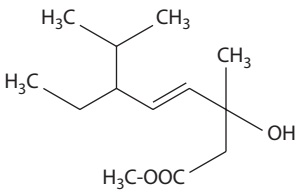
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6121.	96937-51-8	1	0	0	Octanoic acid, oxo-		3.13, 4.3
6122.	638-25-5	0	1	0	Octanoic acid, pentyl ester		5.3
6123.	70898-31-6	0	1	0	Octanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
6124.	111-87-5	1	1	1	1-Octanol {caprylic alcohol}	H_3C-$(CH_2)_6$-CH_2OH	2.5, 21.3, 24.3, 25.29
6125.	106-21-8	1	1	1	1-Octanol, 3,7-dimethyl- {tetrahydrogeraniol}		2.5
6126.	20780-49-8	0	1	0	1-Octanol, 3,7-dimethyl-, acetate {tetrahydrogeranyl acetate}		5.3
6127.	123-96-6	1	0	0	2-Octanol	H_3C-$(CH_2)_5$-CHOH-CH_3	2.5
6128.	589-98-0	0	1	0	3-Octanol		2.5
6129.	78-69-3	0	1	0	3-Octanol, 3,7-dimethyl- {tetrahydrolinalool}		2.5
6130.	1674-37-9	1	0	0	1-Octanone, 1-phenyl- {octanophenone}		3.13
6131.	111-13-7	1	1	1	2-Octanone {hexyl methyl ketone}	H_3C-$(CH_2)_5$-CO-CH_3	3.13, 24.3
6132.	102488-04-0	0	1	0	2-Octanone, 3,3-dimethyl-7-hydroxy-		2.5, 3.13
6133.	65716-45-2	0	1	0	2-Octanone, 7-hydroxy-3,3-dimethyl-,(±)-		2.5, 3.13
6134.	106-68-3	0	1	0	3-Octanone {ethyl amyl ketone}		3.13
6135.	7194-85-6	1	1	1	Octatriacontane	H_3C-$(CH_2)_{36}$-CH_3	1.10
6136.	929-20-4	1	0	0	1,3,6-Octatriene	H_2C=CH-CH=CH-CH_2-CH=CH-CH_3	1.11
6137.	13877-91-3	1	1	1	1,3,6-Octatriene, 3,7-dimethyl- {ocimene}	H_2C=CH-C(CH_3)=CH-CH_2-CH=C(CH_3)$_2$	1.11, 24.3, 25.29
6138.	3779-61-1	0	1	0	1,3,6-Octatriene, 3,7-dimethyl-, (*E*)-		1.11
6139.	673-84-7	1	0	0	2,4,6-Octatriene, 2,6-dimethyl- {alloöcimene}	(H_3C)$_2$=C=CH-CH=CH-C(CH_3)=CH-CH_3	1.11
6140.	29414-56-0	1	0	0	1,5,7-Octatrien-3-ol, 2,6-dimethyl-		2.5
6141.	2548-87-0	0	1	0	2-Octenal		3.12
6142.	73757-28-5	0	1	0	2-Octenal, 2-propyl-		3.12
6143.		0	1	0	2-Octenal, 4-(1-methylethyl)-		3.12
6144.	106-23-0	1	1	1	6-Octenal, 3,7-dimethyl- {citronellal}	(H_3C)$_2$=C=CH-(CH_2)$_2$-CH(CH_3)-CH_2-CH=O	3.12, 24.3, 25.29
6145.	71607-54-0	1	0	0	Octene, methyl-		1.11
6146.	111-66-0	1	0	0	1-Octene {caprylene}	H_2C=CH-(CH_2)$_5$-CH_3	1.11
6147.	4588-18-5	1	0	0	1-Octene, 2-methyl-	H_2C=C(CH_3)-(CH_2)$_5$-CH_3	1.11
6148.	111-67-1	1	0	0	2-Octene	H_3C-CH=CH-(CH_2)$_4$-CH_3	1.11
6149.	592-99-4	1	0	0	4-Octene	H_3C-(CH_2)$_2$-CH=CH-(CH_2)$_2$-CH_3	1.11
6150.	28962-27-8	1	0	0	Octenoic acid		4.3
6151.	1470-50-4	0	1	0	2-Octenoic acid		4.3
6152.		0	1	0	2-Octenoicacid, 4-(1-methylethyl)-7-oxo-		3.13, 4.3
6153.		0	1	0	4-Octenoic acid, 3-hydroxy-3-methyl- 6-(1-methylethyl)-		2.5, 4.3
6154.		0	1	0	4-Octenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-, methyl ester		2.5, 5.3
6155.	41654-08-4	0	1	0	4-Octenoic acid, 6-ethyl-3-hydroxy-3,7-dimethyl-		2.5
6156.	63892-00-2	0	1	0	5-Octenoic acid		4.3
6157.	41653-97-8	0	1	0	5-Octenoic acid, (*Z*)-		4.3

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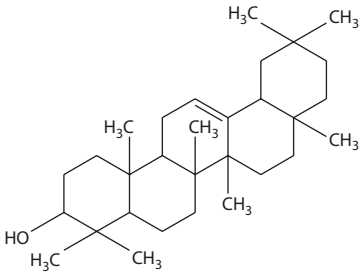
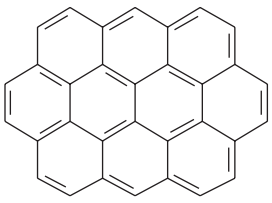
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6158.	502-47-6	0	1	0	6-Octenoic acid, 3,7-dimethyl-		4.3
6159.	18719-24-9	0	1	0	7-Octenoic acid		4.3
6160.	3391-86-4	0	1	0	1-Octen-3-ol		2.5, 24.3, 25.29
6161.	18409-17-1	0	1	0	2-Octen-1-ol, (*E*)-	H_3C-$(CH_2)_4$-CH=CH-CH_2OH	2.5
6162.	76649-14-4	0	1	0	3-Octen-2-ol		2.5
6163.	106-22-9	1	1	1	6-Octen-1-ol, 3,7-dimethyl- {*dl*-citronellol}		2.5, 24.3, 25.29
6164.	6812-78-8 141-25-3	0	1	0	7-Octen-1-ol, 3,7-dimethyl- {rhodinol}		2.5
6165.	1669-44-9	0	1	0	3-Octen-2-one		3.13
6166.	14129-48-7	0	1	0	4-Octen-3-one		3.13
6167.	124354-88-7	0	1	0	Octen-4-one, 2,6-dimethyl-, monoepoxy derivative		3.13, 10.2
6168.		1	0	0	Octyne		1.11
6169.	111-12-6	0	1	0	2-Octynoic acid, methyl ester	H_3C-$(CH_2)_4$-C≡C-COO-CH_3	5.3
6170.	508-02-1	0	1	0	Olean-12-en-28-oic acid, 3-hydroxy-, (3β)-		2.5, 2.7, 4.3
6171.	471-53-4	1	0	0	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-		2.5, 2.7, 3.13, 4.3
6172.	559-70-6	1	1	1	Olean-12-en-3-ol, (3β)- {β-amyrin}		2.5, 2.7
6173.	7006-33-9	1	1	1	Ornithine {2,3-diaminopentanoic acid}	H_2N-$(CH_2)_3$-CH(NH_2)-COOH	4.3, 4.10, 12.2
6174.	70-26-8	1	1	1	*L*-Ornithine		4.3, 4.10, 12.2
6175.	20197-09-5	0	1	0	*L*-Ornithine, *N*2-(1-carboxyethyl)-, (R)-		4.3, 4.10, 12.2
6176.	372-75-8	0	1	0	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline}	H_2N-CO-NH-$(CH_2)_3$-CH(NH_2)-COOH	0.4, 4.3, 4.10, 12.2, 13.1
6177.	7440-04-2	1	1	1	Osmium	Os	20.5
6178.	141093-09-6	0	1	0	1-226-Osmotin (*Nicotiana tabacum* samsun clone pMOG404 reduced)		22.2
6179.	141093-08-5	0	1	0	Osmotin (*Nicotiana tabacum* samsun clone pMOG404 reduced)		22.2
6180.	143638-31-7	0	1	0	Osmotin (*Nicotiana tabacum* samsun clone pTOL1 precursor reduced)		22.2
6181.	143638-32-8	0	1	0	Osmotin (*Nicotiana tabacum* samsun clone pTOL1 reduced)		22.2
6182.	131553-54-3	0	1	0	Osmotin (*Nicotiana tabacum* samsun reduced)		22.2
6183.	142583-50-4	0	1	0	Osmotin (tobacco clone pVK5 precursor reduced)		22.2
6184.	142583-51-5	0	1	0	Osmotin (tobacco clone pVK5 reduced)		22.2
6185.	190-26-1	1	0	0	Ovalene		1.20

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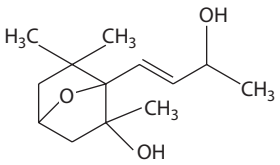
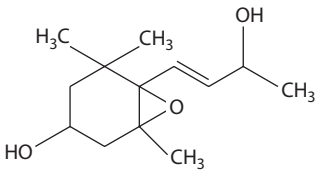
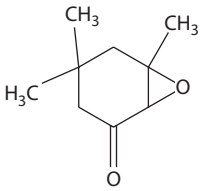
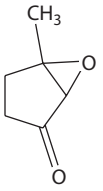
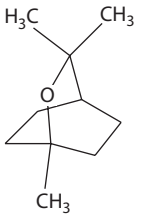
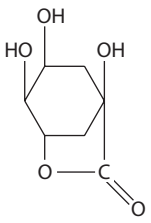
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6186.	38284-11-6	0	1	0	7-Oxabicyclo[4.1.0]heptane-2,5-dione, 1,3,3-trimethyl-		3.13, 10.2
6187.	73051-73-7	0	1	0	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-		2.5, 10.2
6188.	102518-80-9	0	1	0	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-[1 R[1AL]]		2.5, 10.2
6189.	68573-20-6	0	1	0	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-		2.5, 10.2
6190.	72777-88-9	0	1	0	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-		2.5, 10.2
6191.	10276-21-8	1	0	0	7-Oxabicyclo[4.1.0]heptan-2-one, 4,4,6-trimethyl-		3.13, 10.2
6192.	17024-44-1	1	0	0	6-Oxabicyclo[3.1.0]hexan-4-one, 1-methyl-		3.13, 10.2
6193.	63626-79-9	1	0	0	3-Oxabicyclo[3.3.1]nonan-2-one, 9-hydroxy-5-methyl-		2.5, 6.3
6194.	470-82-6	1	1	1	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- {eucalyptol, 1.8-cineole}		10.2, 24.3, 25.29
6195.		1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 6-hydroxy-3-methyl-		2.5, 6.3
6196.	72693-08-4	1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 8-hydroxy-1-methyl-		2.5, 6.3
6197.	640-06-2	1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy- {cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, γ-lactone, quinic acid lactone, quinide}		2.5, 6.3

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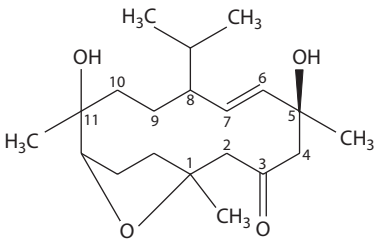
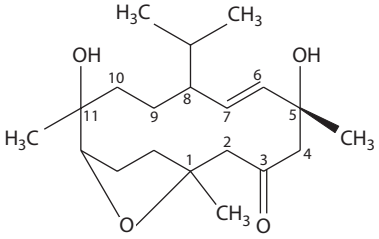
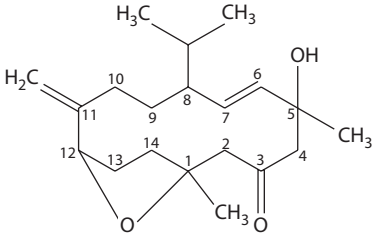
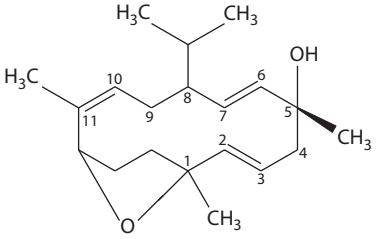
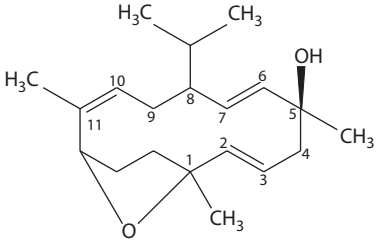
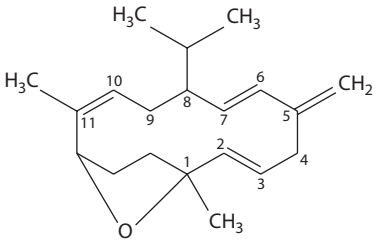
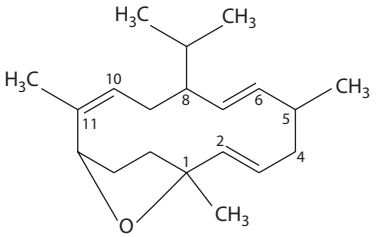
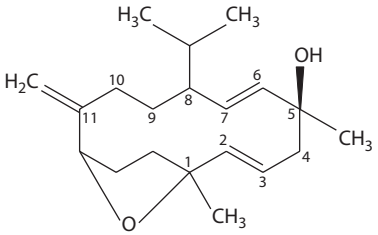
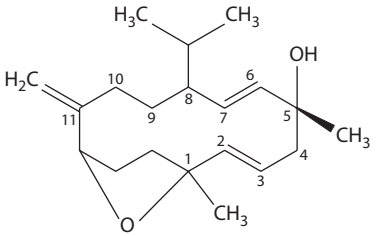
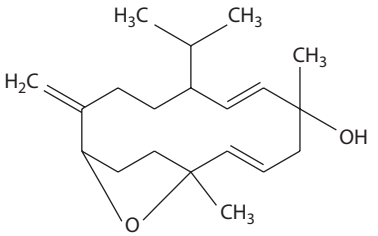
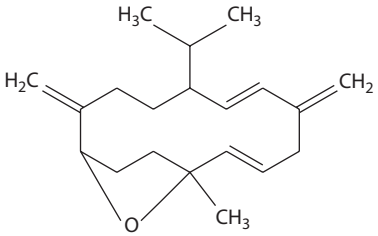
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6198.	27783-00-2	1	1	1	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy-, (exo,exo)-		2.5, 6.3
6199.	665-27-0	1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy-, [1S-(exo,exo)]-		2.5, 10.2
6200.	98064-77-8	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,11R*,		2.5, 3.13, 10.2
6201.	98167-33-0	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,11S*,12S*)]-		2.5, 3.13, 10.2
6202.	98064-76-7	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one, 5-hydroxy-1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,1)]-		2.5, 3.13, 10.2
6203.	121927-14-8	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-ene-2,3,5-triol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2S*,3R*,5S*,6*E*,8*)]		2.5, 10.2
6204.	57760-48-2	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8S*,10*E*,12S*)]-		2.5, 10.2
6205.	60047-18-9	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)-		2.5, 10.2
6206.	60026-18-8	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,11-dimethyl-5-methylene-8-(1-methylethyl)-		10.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6207.	69010-30-6	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,11-dimethyl-5-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,6*E*,8S*,10*Z*,12S*)]-		10.2
6208.		1	1	1	15-Oxabicyclo[10.2.1] pentadeca-2,6,10-triene, 1,5,11-trimethyl-8-(1-methylethyl)-		10.2
6209.	57688-98-9	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8R*,10S*)]-		2.5, 10.2
6210.	57760-47-1	1	1	1	15-Oxabicyclo[10.2.1] pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,5R*,6*E*,8S*,12S*)]-		2.5, 10.2
6211.	60047-16-7	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-		2.5, 10.2
6212.	102977-88-8	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 5-methyl-11-methylene-8-(1-methylethyl)-		2.5, 10.2
6213.	72693-05-1	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-diene, 1-methyl-5,11-bis (methylene)-8-(1-methylethyl)-		10.2

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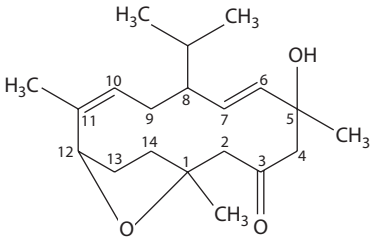
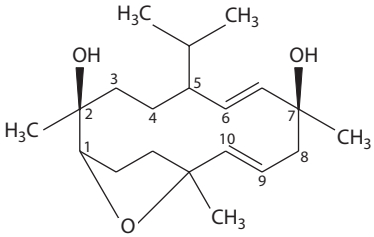
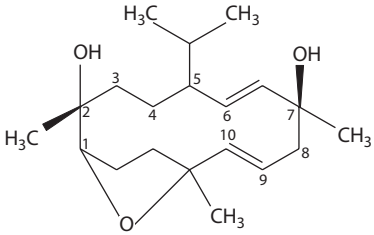
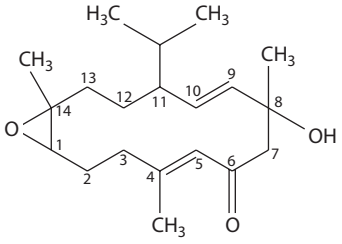
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6214.	58947-96-9	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-2-one, 8-hydroxy-8,12-dimethyl-5-(1-methylethyl)-		2.5, 3.13, 10.2
6215.	98064-75-6	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-3-one, 5-hydroxy-1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,5S*,6*E*,8S*,10*E*,		2.5, 3.13, 10.2
6216.	66890-76-4	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol, 2,8,12-trimethyl-5-(1-methylethyl)-, [1S-(1R*,2S*,5R*,6*E*,8R*,10*E*,12S*)]-		2.5, 10.2
6217.	66966-04-9	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol, 2,8,12-trimethyl-5-(1-methylethyl)-, [1S-(1R*,2R*,5R*,6*E*,8R*,10*E*,12S*)]-		2.5, 10.2
6218.	119613-99-9	0	1	0	15-Oxabicyclo[12.1.0]pentadec-9-en-5-one, 11,13-dihydroxy-1, 11-dimethyl-8-(1-methylethyl)-, [1S-(1R*,8R*,9*E*,11R*,13S*,14S*)]-		2.5, 3.13, 10.2
6219.	98064-73-4	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one, 8-hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,8R*,9*E*,11R*)]		2.5, 3.13, 10.2
6220.	152209-53-5	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 11-(1-hydroxy-1-methylethyl)-4,8,14-trimethyl-, [1S-(1R*,4*E*,6S*,8R*,9*E*,11S*,14R*)]-		2.5, 10.2
6221.	70969-36-7	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-		2.5, 10.2

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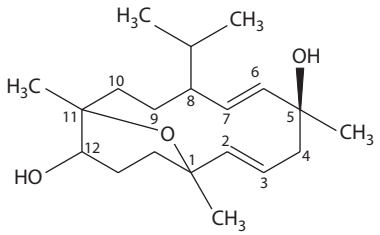
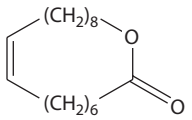
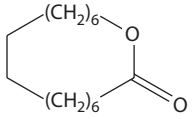
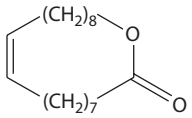
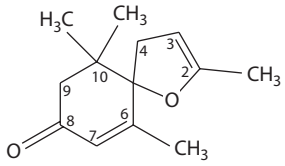
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6222.	75281-93-5	0	1	0	15-Oxabicyclo[12.1.0] pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,6S*,8S*,9*E*,11R*,14R*)]-		2.5, 10.2
6223.	75281-99-1	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,6S*,8R*,9*E*,11R*,14R*)]-		2.5, 10.2
6224.	75282-00-7	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-, [1R-(1R*,4*E*,6R*,8S*,9*E*,11S*,14R*)]-		2.5, 10.2
6225.	62498-80-0	0	1	0	15-Oxabicyclo[9.3.1] pentadeca-2,6-diene-5,12-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8R*,11S*,12S*)]-		2.5, 10.2
6226.	123-69-3	1	0	0	Oxacycloheptadec-8-en-2-one, (*Z*)-{ambrettolide}		6.3
6227.	106-02-5	0	1	0	Oxacyclohexadecan-2-one {ω-pentadecalactone, exaltolide}		6.3, 24.3, 25.29
6228.	68985-15-9	0	1	0	Oxacyclononadec-10-en-2-one, (*E*)-		6.3
6229.	60918-97-0	0	1	0	1,3,4-Oxadiazol-2-amine, *N*-(4-bromophenyl)-5-(1-naphthalenylmethyl)-		12.2, 17.15, 18.4
6230.	72962-43-7	0	1	0	β-homo-7-Oxaergostan-6-one,2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R, 23R,24S)-		2.5, 2.7, 3.13
6231.	80722-28-7	0	1	0	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-		3.13, 10.2
6232.	85248-56-2	0	1	0	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-, (S)- {8,9-dehydrotheaspirone}		3.13, 10.2

(*continued*)

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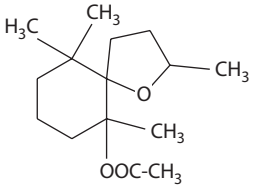
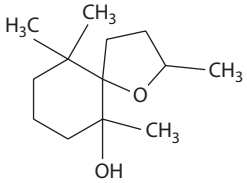
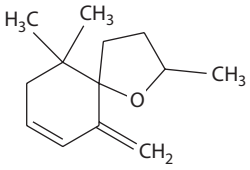
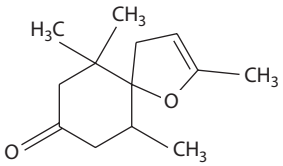
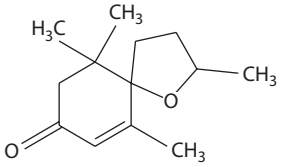
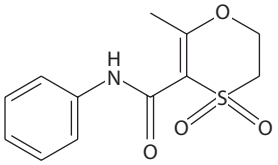
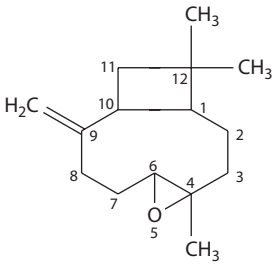
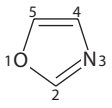
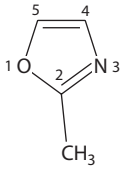
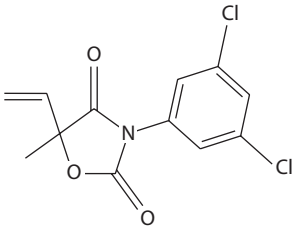
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6233.	57893-27-3	0	1	0	1-Oxaspiro[4.5]decane, 6-acetoxy-2,6,10,10-tetramethyl- {6-acetoxydihydrotheaspirane}		5.3, 10.2
6234.	65620-50-0	0	1	0	1-Oxaspiro[4.5]decane, 6-hydroxy-2,6,10,10-tetramethyl- {6-hydroxydihydrotheaspirane}		2.5, 10.2
6235.	65416-59-3	0	1	0	1-Oxaspiro[4.5]dec-7-ene, 6-methylene 2,10,10-trimethyl- {vitispirane}		10.2
6236.	38713-26-7	0	1	0	1-Oxaspiro[4.5]dec-2-en-8-one, 2,6,6,10-tetramethyl-		3.13, 10.2
6237.	19377-59-4	0	1	0	1-Oxaspiro[4.5]dec-6-en-8-one, 2,6,10,10-tetramethyl-		3.13, 10.2
6238.	5259-88-1	0	1	0	1,4-Oxathiin-3-carboxamide 4,4-dioxide, 5,6-dihydro-2-methyl-*N*-phenyl- {Oxycarboxin®}		10.2, 13.1, 18.1, 21.3
6239.	1139-30-6	0	1	0	5-Oxatricyclo[8.2.0.04,6] dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- {β-caryophyllene oxide}		10.2, 24.3, 25.29
6240.	15769-88-7	1	1	1	2*H*-1,2-Oxazine, tetrahydro-2-methyl-6-(3-pyridinyl)-, (–)-		17.7
6241.	71607-95-9	1	0	0	2*H*-1,2-Oxazine, tetrahydro-3-(1-methylethyl)-6-(3-pyridinyl)-		17.7
6242.	288-42-6	1	0	0	Oxazole		17.15

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6243.		1	0	0	Oxazole, 2-butyl-4,5-dimethyl-		17.15
6244.		1	0	0	Oxazole, 5-butyl-2,4-dimethyl-		17.15
6245.		1	0	0	Oxazole, 2-butyl-4-methyl-		17.15
6246.		1	0	0	Oxazole, 4-butyl-2-methyl-		17.15
6247.	7208-05-1	1	0	0	Oxazole, 2,4-dimethyl-		17.15
6248.	33318-74-0	1	0	0	Oxazole, 2,4-dimethyl-5-ethyl-		17.15
6249.		1	0	0	Oxazole, 2,4-dimethyl-5-(2-methylpropyl)-		17.15
6250.		1	0	0	Oxazole, 2,4-dimethyl-5-propyl-		17.15
6251.	23012-11-5	1	0	0	Oxazole, 2,5-dimethyl-		17.15
6252.		1	0	0	Oxazole, 2,5-dimethyl-4-ethyl-		17.15
6253.		1	0	0	Oxazole, 2,5-dimethyl-4-(2-methylpropyl)-		17.15
6254.	20654-94-8 20662-83-3	1	0	0	Oxazole, 4,5-dimethyl-		17.15
6255.	53833-30-0	1	0	0	Oxazole, 4,5-dimethyl-2-ethyl-		17.15
6256.		1	0	0	Oxazole, 4,5-dimethyl-2-(1-methylpropyl)-		17.15
6257.		1	0	0	Oxazole, 4,5-dimethyl-2-(2-methylpropyl)-		17.15
6258.	24667-03-6	1	0	0	Oxazole, 2-ethyl-4-methyl-		17.15
6259.	42463-54-7	1	0	0	Oxazole, 2-ethyl-5-methyl-		17.15
6260.	53833-20-8	1	0	0	Oxazole, 4-ethyl-2-methyl-		17.15
6261.	53833-28-6	1	0	0	Oxazole, 4-ethyl-5-methyl-		17.15
6262.	53833-29-7	1	0	0	Oxazole, 5-ethyl-2-methyl-		17.15
6263.	29584-92-7	1	0	0	Oxazole, 5-ethyl-4-methyl-		17.15
6264.	23012-10-4	1	0	0	Oxazole, 2-methyl-		17.15
6265.		1	0	0	Oxazole, 2-(2-methylpropyl)-		17.15
6266.		1	0	0	Oxazole, 2-(3-methylbutyl)-		17.15
6267.		1	0	0	Oxazole, 2-methyl-4-(2-methylpropyl)-		17.15
6268.		1	0	0	Oxazole, 4-(2-methylpropyl)-		17.15
6269.		1	0	0	Oxazole, 4-methyl-2-(2-methylpropyl)-		17.15
6270.		1	0	0	Oxazole, 4-methyl-5-(2-methylpropyl)-		17.15
6271.		1	0	0	Oxazole, 4-methyl-2-propyl-		17.15
6272.	27744-95-2	1	0	0	Oxazole, 4-methyl-5-propyl-		17.15
6273.	53833-31-1	1	0	0	Oxazole, 5-methyl-2-propyl-		17.15
6274.		1	0	0	Oxazole, 4-pentyl-		17.15
6275.	20662-84-4	1	1	1	Oxazole, trimethyl- = 2,4,5-trimethyloxazole		17.15
6276.	2346-26-1	1	0	0	2,4-Oxazolidinedione		14.1, 17.15
6277.	50471-44-8	0	1	0	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- {Vinclozolin®}		14.1, 17.15, 18.4, 21.3
6278.		1	0	0	2,4-Oxazolidinedione, 5-ethyl-1-methyl-		14.1, 17.15
6279.	27770-23-6	1	0	0	2,4-Oxazolidinedione, 5-methyl-		14.1, 17.15
6280.	58628-98-1	1	0	0	2-Oxazolidinone, 4.5-dimethyl-		14.1, 17.15

(*continued*)

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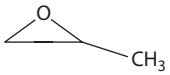
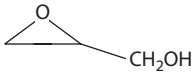
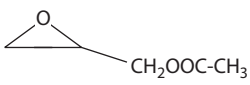
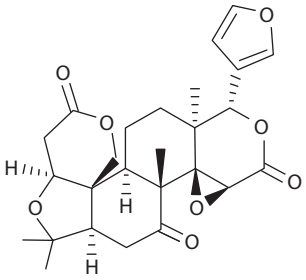
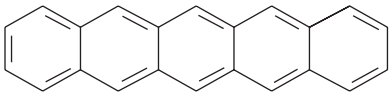
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6281.	9035-73-8	0	1	0	Oxidase		0.4, 22.2
6282.	9029-44-1	0	1	0	Oxidase, ascorbate		0.4, 22.2
6283.	9028-67-5	0	1	0	Oxidase, choline		22.2
6284.	9076-84-0	0	1	0	Oxidase, coproporphyrinogen		22.2
6285.	9001-16-5	0	1	0	Oxidase, cytochrome c {cytochrome oxidase}		0.4, 22.2
6286.	9001-53-0	0	1	0	Oxidase, diamine		22.2
6287.	9028-71-1	0	1	0	Oxidase, glycolate		22.2
6288.	9027-85-4	0	1	0	Oxidase, indoleacetate		22.2
6289.	55326-39-1	0	1	0	Oxidase, isopentenyladenosine		22.2
6290.	37259-79-3	0	1	0	Oxidase, methylputrescine		22.2
6291.	9001-96-1	0	1	0	Oxidase, pyruvate		22.2
6292.	9032-21-7	0	1	0	Oxidase, reduced nicotinamide adenine dinucleotide		22.2
6293.	9032-22-8	0	1	0	Oxidase, reduced nicotinamide adenine dinucleotide phosphate		22.2
6294.	9014-35-1	0	1	0	Oxidase, succinate		22.2
6295.	69671-26-7	0	1	0	Oxidase, ubiquinol		22.2
6296.	9002-12-4	0	1	0	Oxidase, urate		22.2
6297.	9002-17-9	0	1	0	Oxidase, xanthine		22.2
6298.	75-21-8	1	0	0	Oxirane {ethylene oxide}		10.2, 23.5
6299.	106-89-8	0	1	0	Oxirane, (chloromethyl)-		10.2, 18.4
6300.	558-30-5	1	0	0	Oxirane, 2,2-dimethyl- {isobutylene oxide}		10.2
6301.	7200-26-2	1	0	0	Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-, (all-*E*)-		10.2
6302.	3234-28-4	1	0	0	Oxirane, dodecyl- {tetradecane, 1,2-epoxy}		10.2
6303.	75-56-9	1	0	0	Oxirane, methyl- {propylene oxide}		10.2, 23.5
6304.	96-09-3	1	1	1	Oxirane, phenyl- {phenylethylene oxide}		10.2
6305.	77341-24-3	0	1	0	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-		2.5, 10.2
6306.	77288-97-2	0	1	0	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-, [2α(αS*,δR*),3α]-		2.5, 10.2
6307.	77288-94-9	0	1	0	Oxiranebutanol, 3-(1-hydroxyethyl)-α-methyl-δ-(1-methylethyl)-		2.5, 10.2
6308.	77-83-8	0	1	0	Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester {ethyl methylphenylglycidate}		5.3, 10.2
6309.	61892-62-4	0	1	0	2,3-Oxiranedimethanol, monopropanoate		2.5, 5.3, 10.2
6310.	556-52-5	1	0	0	Oxiranemethanol {glycidol}		2.5, 10.2
6311.	6387-89-9	0	1	0	Oxiranemethanol, acetate {glycidyl acetate}		5.3, 10.2

(continued)

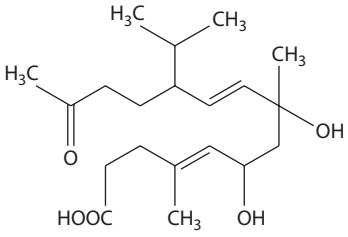
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6312.	51297-34-8	0	1	0	Oxiranemethanol, 3-(1-ethyl-2-methylpropyl)-α,α-dimethyl-		2.5, 10.2
6313.	1180-71-8	1	0	0	11*H*,13*H*-Oxireno[d]pyrano[4′,3′:3,3a]isobenzofuro[5,4-f][2]benzopyran-4,6,13(2H,5aH)-trione, 8-(3-furyl)decahydro-2,2,4a,8a-tetramethyl- {limonin}		3.13, 6.3, 10.2
6314.	430-75-1	0	1	0	Oxyacetate {glyoxylate}	O═CH-CO_2^-	20.6
6315.	7782-44-7	1	1	1	Oxygen	O_2	0.4, 19.5, 20.5
6316.	7782-44-7	1	1	1	Oxygen (diradical)		27.1
6317.	9029-57-6	0	1	0	Oxygenase,2,5-dihydroxypyridine5,6-di-		22.2
6318.	152060-37-2	0	1	0	Oxygenase, benzoate 2-mono-		22.2
6319.	9077-75-2	0	1	0	Oxygenase, cinnamate 4-mono- {hydroxylase cinnamate}		22.2
6320.	9068-40-0	0	1	0	Oxygenase, *p*-coumarate 3-mono-		22.2
6321.	9028-06-2	0	1	0	Oxygenase, protocollagen proline di-		22.2
6322.	39335-11-0	0	1	0	Oxygenase, ribulose diphosphate		22.2
6323.	10028-15-6	0	1	0	Ozone	O_3	19.5,
6324.	7440-05-3	1	1	1	Palladium	Pd	20.5
6325.		0	1	0	*Pantoea*		22.2
6326.	142193-29-1	0	1	0	Parasiticein		22.2
6327.	142193-19-9	0	1	0	Parasiticein (*Phytophthora parasitica* reduced)		22.2
6328.	9046-40-6	0	1	0	Pectic acid		0.4, 2.5, 4.3, 8.3
6329.		0	1	0	Pectic acid, labeled with ^{14}C {pectic acid-^{14}C}		2.5, 4.3, 8.3, 25.29
6330.		0	1	0	Pectic acid, calcium magnesium salt		2.5, 8.3, 20.6
6331.	65028-58-2	0	1	0	Pectic acid, magnesium salt		2.5, 8.3, 20.6
6332.	9000-69-5	0	1	0	Pectin		0.4, 2.5, 8.3, 24.3, 25.29
6333.		0	1	0	Pectin, labeled with ^{14}C {pectin-^{14}C}		2.5, 8.3, 25.29
6334.	9047-18-1	0	1	0	Pectinic acid		2.5, 4.3, 8.3
6335.	135-48-8	1	0	0	Pentacene {benzo[*b*]naphthacene}		1.20
6336.	629-99-2	1	1	1	Pentacosane	H_3C-$(CH_2)_{23}$-CH_3	1.10, 25.29
6337.	629-87-8	1	1	1	Pentacosane, 2-methyl-	H_3C-$(CH_2)_{22}$-CH═$(CH_3)_2$	1.10
6338.	6902-54-1	1	1	1	Pentacosane, 3-methyl-		1.10
6339.	506-38-7	1	1	1	Pentacosanoic acid	H_3C-$(CH_2)_{23}$-COOH	4.3
6340.	121877-88-1	1	1	1	Pentacosanoic acid, docosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{21}$-CH_3	5.3
6341.		1	1	1	Pentacosanoic acid, dodecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{11}$-CH_3	5.3
6342.	121877-80-3	1	1	1	Pentacosanoic acid, eicosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{19}$-CH_3	5.3
6343.		1	1	1	Pentacosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{20}$-CH_3	5.3
6344.		1	1	1	Pentacosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{26}$-CH_3	5.3
6345.		1	1	1	Pentacosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{16}$-CH_3	5.3
6346.		1	1	1	Pentacosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{25}$-CH_3	5.3
6347.		1	1	1	Pentacosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{15}$-CH_3	5.3
6348.		1	1	1	Pentacosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{18}$-CH_3	5.3

(*continued*)

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
6349.		1	1	1	Pentacosanoic acid, octadecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{17}$-CH_3	5.3
6350.	10482-74-3	1	1	1	Pentacosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{24}$-CH_3	5.3
6351.		1	1	1	Pentacosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{14}$-CH_3	5.3
6352.		1	1	1	Pentacosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{23}$-CH_3	5.3
6353.		1	1	1	Pentacosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{13}$-CH_3	5.3
6354.		1	1	1	Pentacosanoic acid, tricosyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{32}$-CH_3	5.3
6355.		1	1	1	Pentacosanoic acid, tridecyl ester	H_3C-$(CH_2)_{23}$-COO-$(CH_2)_{12}$-CH_3	5.3
6356.		0	1	0	Pentacosanoic acid, 23-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{21}$-COOH	4.3
6357.	121877-85-8	1	1	1	Pentacosanoic acid, 23-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{21}$-COO-$(CH_2)_{20}$-CH_3	5.3
6358.		0	1	0	Pentacosanoic acid, 24-methyl-		4.3
6359.	129074-11-9	1	0	0	Pentacosanol		2.5
6360.	26040-98-2	0	1	0	1-Pentacosanol	H_3C-$(CH_2)_{23}$-CH_2OH	2.5
6361.	63785-24-0	0	1	0	1-Pentacosanol, 24-methyl-	$(H_3C)_2$=CH-$(CH_2)_{22}$-CH_2OH	2.5
6362.	30551-31-6	1	0	0	Pentacosene		1.11
6363.	16980-85-1	1	0	0	1-Pentacosene	H_3C-$(CH_2)_{22}$-CH=CH_2	1.11
6364.		1	0	0	1-Pentacosene, 2-methyl-	H_2C=CH-$(CH_2)_{22}$-CH_3	1.11
6365.		1	0	0	2-Pentacosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{21}$-CH_3	1.11
6366.		1	0	0	2-Pentacosene, (*E*)-		1.11
6367.		1	0	0	2-Pentacosene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{21}$-CH_3	1.11
6368.		1	0	0	2-Pentacosene, 23-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{19}$-$CH(CH_3)$-CH_2-CH_3	1.11
6369.		1	0	0	2-Pentacosene, 23-methyl-, (*E*)-		1.11
6370.		1	0	0	2-Pentacosene, 24-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{20}$-$CH(CH_3)_2$	1.11
6371.		1	0	0	2-Pentacosene, 24-methyl-, (*E*)-		1.11
6372.	102673-27-8	0	1	0	4,9-Pentadecadienal, 6-(acetyloxy)-8-hydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4*E*,6R*,8R*,9*E*,11S*)]-		2.5, 3.12, 3.13, 5.3
6373.	95360-16-0	0	1	0	4,9-Pentadecadienal, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4*E*,6R*,8S*,9*E*,11S*)]-		2.5, 3.12, 3.13
6374.		1	0	0	Pentadecadiene, 2,6,10,14-tetramethyl-		1.11
6375.	70898-33-8	1	0	0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-		2.5, 3.13, 4.3
6376.	102734-50-9	0	1	0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, methyl ester, [6R-(4*E*,6R*,8S*,9*E*,11S*)]-		2.5, 3.13, 5.3
6377.	102734-47-4	0	1	0	4,9-Pentadecadienoic acid, 6, 8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-		2.5, 3.13, 4.3
6378.	102734-49-6	0	1	0	4,9-Pentadecadienoic acid, 6, 8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo- {isomer}		2.5, 3.13, 4.3
6379.	102734-51-0	0	1	0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, methyl ester, [6R-(4*E*,6R*,8R*,9*E*,11S*)]-		2.5, 3.13, 5.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6380.	152209-55-7	0	1	0	6,11-Pentadecadien-2-one, 8,10,15-trihydroxy-8,12-dimethyl-5-(1-methylethyl)-, [5S-(5R*,6*E*,8R*,10S*,11*E*)]-		2.5, 3.13
6381.	2765-11-9	0	1	0	Pentadecanal	H_3C-$(CH_2)_{13}$-CH═O	3.12
6382.	68982-28-5	0	1	0	Pentadecanal, 2-ethylidene-6,10,14-trimethyl-		3.12
6383.	629-62-9	1	1	1	Pentadecane	H_3C-$(CH_2)_{13}$-CH_3	1.10
6384.		0	1	0	Pentadecane, 4-acetoxy-		5.3
6385.	1560-93-6	1	1	1	Pentadecane, 2-methyl-	H_3C-$(CH_2)_{12}$-CH═$(CH_3)_2$	1.10
6386.	2882-96-4	1	1	1	Pentadecane, 3-methyl-	H_3C-$(CH_2)_{11}$-$CH(CH_3)$-CH_2-CH_3	1.10
6387.	1921-70-6	1	0	0	Pentadecane, 2,6,10,14-tetramethyl- {pristane}		1.10
6388.	3892-00-0	1	0	0	Pentadecane, 2,6,10-trimethyl- {norpristane}		1.10
6389.	1460-18-0	1	0	0	Pentadecanedioic acid	HOOC-$(CH_2)_{13}$-COOH	4.3
6390.	1002-84-2	1	1	1	Pentadecanoic acid	H_3C-$(CH_2)_{13}$-COOH	4.3
6391.	42232-23-5	1	1	1	Pentadecanoic acid, docosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{21}$-CH_3	5.3
6392.	42232-14-4	1	1	1	Pentadecanoic acid, dodecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{11}$-CH_3	5.3
6393.	36617-37-5	1	1	1	Pentadecanoic acid, eicosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{19}$-CH_3	5.3
6394.	41114-00-5	0	1	0	Pentadecanoic acid, ethyl ester	H_3C-$(CH_2)_{13}$-COO-CH_2-CH_3	5.3
6395.	42232-22-4	1	1	1	Pentadecanoic acid, heneicosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{20}$-CH_3	5.3
6396.		1	1	1	Pentadecanoic acid, heptacosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{26}$-CH_3	5.3
6397.	36617-34-2	1	1	1	Pentadecanoic acid, heptadecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{16}$-CH_3	5.3
6398.		1	1	1	Pentadecanoic acid, hexacosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{25}$-CH_3	5.3
6399.	36617-33-1	1	1	1	Pentadecanoic acid, hexadecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{15}$-CH_3	5.3
6400.	7132-64-1	1	1	1	Pentadecanoic acid, methyl ester	H_3C-$(CH_2)_{13}$-COO-CH_3	5.3
6401.	36617-36-4	1	1	1	Pentadecanoic acid, nonadecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{18}$-CH_3	5.3
6402.	36617-35-3	1	1	1	Pentadecanoic acid, octadecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{17}$-CH_3	5.3
6403.		1	1	1	Pentadecanoic acid, pentacosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{24}$-CH_3	5.3
6404.	36617-32-0	1	1	1	Pentadecanoic acid, pentadecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{14}$-CH_3	5.3
6405.	121877-44-9	1	1	1	Pentadecanoic acid, tetracosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{23}$-CH_3	5.3
6406.	36617-31-9	1	1	1	Pentadecanoic acid, tetradecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{13}$-CH_3	5.3
6407.	42232-24-6	1	1	1	Pentadecanoic acid, tricosyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{22}$-CH_3	5.3
6408.	36617-30-8	1	1	1	Pentadecanoic acid, tridecyl ester	H_3C-$(CH_2)_{13}$-COO-$(CH_2)_{12}$-CH_3	5.3
6409.		1	1	1	Pentadecanoic acid, 13-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COOH	4.3
6410.	121877-18-7	1	1	1	Pentadecanoic acid, 13-methyl-, heptadecyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COO-$(CH_2)_{16}$-CH_3	5.3
6411.	121877-55-2	1	1	1	Pentadecanoic acid, 13-methyl-, pentacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COO-$(CH_2)_{24}$-CH_3	5.3
6412.	121877-43-8	1	1	1	Pentadecanoic acid, 13-methyl-, tricosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{11}$-COO-$(CH_2)_{32}$-CH_3	5.3
6413.	4669-02-7	1	1	1	Pentadecanoic acid, 14-methyl-	$(H_3C)_2$═CH-$(CH_2)_{12}$-COOH	4.3
6414.	121877-31-4	1	1	1	Pentadecanoic acid, 14-methyl-, docosyl ester	$(H_3C)_2$═CH-$(CH_2)_{12}$-COO-$(CH_2)_{21}$-CH_3	5.3
6415.	121877-27-8	1	1	1	Pentadecanoic acid, 14-methyl-, eicosyl ester	$(H_3C)_2$═CH-$(CH_2)_{12}$-COO-$(CH_2)_{19}$-CH_3	5.3
6416.	121877-13-2	1	1	1	Pentadecanoic acid, 14-methyl-, heptadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{12}$-COO-$(CH_2)_{16}$-CH_3	5.3
6417.	121877-20-1	1	1	1	Pentadecanoic acid, 14-methyl-, octadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{12}$-COO-$(CH_2)_{17}$-CH_3	5.3
6418.	121877-47-2	1	1	1	Pentadecanoic acid, 14-methyl-, tetracosyl ester	$(H_3C)_2$═CH-$(CH_2)_{12}$-COO-$(CH_2)_{23}$-CH_3	5.3

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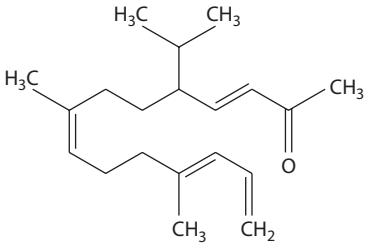
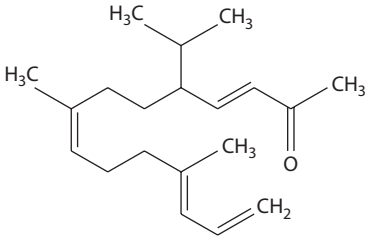
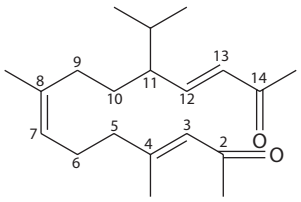
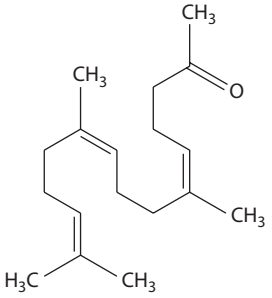
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6419.	121877-38-1	1	1	1	Pentadecanoic acid, 14-methyl-, tricosyl ester	$(H_3C)_2$═CH-$(CH_2)_{12}$-COO-$(CH_2)_{22}$-CH_3	5.3
6420.		0	1	0	Pentadecanoic acid, 3,7,11,15,19,23,27, 31,35-nonamethyl-2,6,10,14, 18,22,26, 30,34-hexatriacontanonaenyl ester {solanesyl pentadecanoate}		5.3
6421.	71607-96-0	1	0	0	Pentadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
6422.	629-76-5	1	1	1	1-Pentadecanol	H_3C-$(CH_2)_{13}$-CH_2OH	2.5
6423.	20194-48-3	0	1	0	1-Pentadecanol, 14-methyl-	$(H_3C)_2$═CH-$(CH_2)_{12}$-CH_2OH	2.5
6424.	2345-28-0	0	1	0	2-Pentadecanone	H_3C-$(CH_2)_{12}$-CO-CH_3	3.13
6425.	502-69-2	1	1	1	2-Pentadecanone, 6,10,14-trimethyl- {phytone, hexahydrofarnesyl acetone}	H-[CH_2-$CH(CH_3)$-CH_2-CH_2]$_3$-CH_2-CO-CH_3	3.13
6426.	16825-16-4	0	1	0	2-Pentadecanone, 6,10,14-trimethyl-, [R-(R*,R*)]-		3.13
6427.	81345-07-5	1	0	0	3,8,12,14-Pentadecatetraen-2-one, 8,12-dimethyl-5-(1-methylethyl)-, (*E,E,E*)-		3.13
6428.	81345-08-6	1	0	0	3,8,12,14-Pentadecatetraen-2-one, 8,12-dimethyl-5-(1-methylethyl)-, (*E,Z,E*)-		3.13
6429.	41429-55-4	0	1	0	3,7,12-Pentadecatriene-2,14-dione, 4,8-dimethyl-11-(1-methylethyl)-, (*E,Z,E*)-		3.13
6430.	57760-50-6	0	1	0	3,7,12-Pentadecatriene-2,14-dione, 4,8-dimethyl-11-(1-methylethyl)-, [S-(*E,E,E*)]-		3.13
6431.	762-29-8	1	1	1	5,9,13-Pentadecatrien-2-one, 6,10, 14-trimethyl- {farnesyl acetone} {three isomers}		3.13

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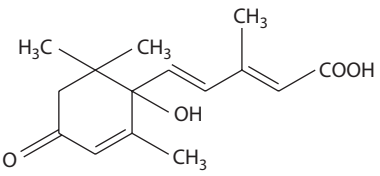
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6432.	1117-52-8	1	1	1	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (*E,E*)-		3.13
6433.	27251-68-9	1	1	1	Pentadecene	$H\text{-}(CH_2)_n\text{-}CH{=}CH\text{-}(CH_2)_{(13\text{-}n)}\text{-}H$	1.11
6434.	13360-61-7	1	1	1	1-Pentadecene	$H_3C\text{-}(CH_2)_{12}\text{-}CH{=}CH_2$	1.11
6435.	29833-69-0	1	1	1	1-Pentadecene, 2-methyl-	$H_2C{=}C(CH_3)\text{-}(CH_2)_{11}\text{-}CH_3$	1.11
6436.		1	1	1	2-Pentadecene, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{11}\text{-}CH_3$	1.11
6437.	74392-36-2	1	1	1	2-Pentadecene, (*E*)-		1.11
6438.		1	1	1	2-Pentadecene, 2-methyl-	$H_2C{=}C(CH_3)\text{-}(CH_2)_{12}\text{-}CH_3$	1.11
6439.		1	1	1	2-Pentadecene, 13-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_9\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1.11
6440.		1	1	1	2-Pentadecene, 13-methyl-, (*E*)-		1.11
6441.		1	1	1	2-Pentadecene, 14-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{10}\text{-}CH(CH_3)_2$	1.11
6442.		1	1	1	2-Pentadecene, 14-methyl-, (*E*)-		1.11
6443.	2140-82-1 60976-73-0	1	1	1	1-Pentadecene, 2,6,10,14-tetramethyl- {norphytene}	$H_2C{=}C(CH_3)\text{-}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\}_3\text{-}H$	1.11
6444.	36232-37-8	1	0	0	6-Pentadecene, 2,6,10,14-tetramethyl-	$(H_3C)_2CH\text{-}(CH_2)_3\text{-}C(CH_3){=}CH_2\text{-}\{(CH_2)_2\text{-}CH(CH_3)\text{-}CH_2\}_2\text{-}H$	1.11
6445.	26444-04-2	1	1	1	Pentadecenoic acid		4.3
6446.	31422-28-3	0	1	0	Pentadecenoic acid, methyl ester		5.3
6447.	17351-34-7	0	1	0	14-Pentadecenoic acid		4.3
6448.	764-40-9	1	1	1	2,4-Pentadienal	$H_2C{=}CH\text{-}CH{=}CH\text{-}CH{=}O$	3.12
6449.	41050-31-1	1	0	0	Pentadiene		1.11
6450.	51064-12-1	1	0	0	Pentadiene, methyl-		1.11
6451.	591-95-7	1	0	0	1,2-Pentadiene {ethylallene}	$H_3C\text{-}CH_2\text{-}CH{=}C{=}CH_2$	1.11
6452.	504-60-9	1	1	1	1,3-Pentadiene {piperylene}	$H_3C\text{-}CH{=}CH\text{-}CH{=}CH_2$	1.11
6453.	2004-70-8	1	0	0	1,3-Pentadiene, (*E*)-		1.11
6454.	1574-41-0	1	0	0	1,3-Pentadiene, (*Z*)-		1.11
6455.	1118-58-7	1	0	0	1,3-Pentadiene, 2-methyl-	$H_3C\text{-}CH{=}CH\text{-}C(CH_3){=}CH_2$	1.11
6456.	4549-74-0	1	0	0	1,3-Pentadiene, 3-methyl-		1.11
6457.	2787-45-3	1	0	0	1,3-Pentadiene, 3-methyl-, (*Z*)-		1.11
6458.	2787-43-1	1	0	0	1,3-Pentadiene, 3-methyl-, (*E*)-		1.11
6459.	926-56-7	0	1	0	1,3-Pentadiene, 4-methyl-	$H_3C\text{-}C(CH_3){=}CH\text{-}CH{=}CH_2$	1.11
6460.	591-93-5	1	0	0	1,4-Pentadiene	$H_2C{=}CH\text{-}CH_2\text{-}CH{=}CH_2$	1.11
6461.	763-30-4	1	0	0	1,4-Pentadiene, 2-methyl-		1.11
6462.	1115-08-8	1	0	0	1,4-Pentadiene, 3-methyl-		1.11
6463.	21293-29-8 14375-45-2	0	1	0	2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-, [S-(*Z,E*)]- {abscisic acid}		2.5, 3.13, 4.3
6464.	4949-20-6	1	0	0	2,4-Pentadien-1-ol	$H_2C{=}CH\text{-}CH{=}CH\text{-}CH_2OH$	2.5
6465.	110-62-3	1	1	1	Pentanal {valeraldehyde}	$H_3C\text{-}(CH_2)_3\text{-}CH{=}O$	3.12, 24.3, 25.29
6466.		1	0	0	Pentanal, methyl-		3.12
6467.	123-15-9	1	0	0	Pentanal, 2-methyl-	$H_3C\text{-}(CH_2)_2\text{-}CH(CH_3)\text{-}CH{=}O$	3.12
6468.	15877-57-3	1	0	0	Pentanal, 3-methyl-		3.12
6469.	1119-16-0	1	0	0	Pentanal, 4-methyl-	$H_3C\text{-}CH(CH_3)\text{-}(CH_2)_2\text{-}CH{=}O$	3.12
6470.	7332-93-6	1	0	0	Pentanal, 2-oxo-	$H_3C\text{-}(CH_2)_2\text{-}CO\text{-}CH{=}O$	3.12, 3.13
6471.	626-96-0	1	0	0	Pentanal, 4-oxo-	$H_3C\text{-}CO\text{-}(CH_2)_2\text{-}CH{=}O$	3.12, 3.13
6472.	626-97-1	1	0	0	Pentanamide {valeramide}	$H_3C\text{-}(CH_2)_3\text{-}CO\text{-}NH_2$	13.1
6473.	61892-69-1	1	0	0	Pentanamide, 3-methyl-		13.1

(*continued*)

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6474.	1119-29-5	1	0	0	Pentanamide, 4-methyl-		13.1
6475.	54007-33-9	1	0	0	Pentanamide, *N*-ethyl-	H_3C-$(CH_2)_3$-CO-NH-C_2H_5	13.1
6476.	110-58-7	1	1	1	1-Pentanamine	H_3C-$(CH_2)_4$-NH_2	12.2
6477.	688-31-3	1	0	0	1-Pentanamine, 2-ethyl-*N,N*-dimethyl-	H_3C-$(CH_2)_2$-$CH(C_2H_5)$-CH_2-$N(CH_3)_2$	12.2
6478.	625-30-9	1	1	1	2-Pentanamine	H_3C-$(CH_2)_2$-$CH(NH_2)$-CH_3	12.2
6479.	616-24-0	1	0	0	3-Pentanamine	$(H_3C$-$CH_2)_2$=CH-NH_2	12.2
6480.	109-66-0	1	1	1	Pentane	H_3C-$(CH_2)_3$-CH_3	1.10
6481.	1067-20-5	1	0	0	Pentane, 3,3-diethyl-		1.10
6482.	108-08-7	1	0	0	Pentane, 2,4-dimethyl-		1.10
6483.	43133-95-5	1	0	0	Pentane, methyl-		1.10
6484.	107-83-5	1	1	1	Pentane, 2-methyl-	H_3C-$(CH_2)_2$-CH=$(CH_3)_2$	1.10
6485.	96-14-0	1	1	1	Pentane, 3-methyl-	$(H_3C$-$CH_2)_2$=CH-CH_3	1.10
6486.	760-21-4	1	0	0	Pentane, 3-methylene- {2-ethyl-1-butene}	$(H_3C$-$CH_2)_2$=C=CH_2	1.11
6487.	628-05-7	1	0	0	Pentane, 1-nitro-	H_3C-$(CH_2)_3$-CH_2-NO_2	16.1
6488.	4609-89-6	1	0	0	Pentane, 2-nitro-	H_3C-$(CH_2)_2$-$CH(NO_2)$-CH_3	16.1
6489.	25683-11-8	0	1	0	1,5-Pentanediamide, 2-amino- {glutamine amide}	H_2N-OC-$(CH_2)_2$-$CH(NH_2)$-CO-NH_2	12.2, 13.1
6490.	462-94-2	0	1	0	1,5-Pentanediamine {cadaverine}	H_2N-$(CH_2)_5$-NH_2	12.2
6491.	110-94-1	1	1	1	Pentanedioic acid {glutaric acid}	HOOC-$(CH_2)_3$-COOH	4.3
6492.	63892-02-4	0	1	0	Pentanedioic acid, 2-(1-methylethyl)-, (S)-	HOOC-$(CH_2)_2$-$CH[CH(CH_3)_2]$-COOH	4.3
6493.	617-62-9	0	1	0	Pentanedioic acid, 2-methyl-	HOOC-$(CH_2)_2$-$CH(CH_3)$-COOH	4.3
6494.	328-50-7	1	1	1	Pentanedioic acid, 2-oxo- {α-ketoglutaric acid}	HOOC-$(CH_2)_2$-CO-COOH	3.13, 4.3
6495.	626-51-7	1	0	0	Pentanedioic acid, 3-methyl-	HOOC-CH_2-$CH(CH_3)$-CH_2-COOH	4.3
6496.		0	1	0	Pentanedioic acid, 2,3,4-trihydroxy-	HOOC-$(CHOH)_3$-COOH	2.5, 4.3
6497.	3174-67-2	1	0	0	1,3-Pentanediol		2.5
6498.		1	0	0	1,4-Pentanediol, 3-[2-(2-hydroxyethyl)-1,3,3-trimethylcyclohexyl]-		2.5
6499.	107-41-5	1	1	1	2,4-Pentanediol, 2-methyl-		2.5
6500.	52786-29-5	1	0	0	1,4-Pentanedione, 1-(2-furanyl)-		3.13, 10.2
6501.	600-14-6	1	1	1	2,3-Pentanedione	H_3C-CH_2-CO-CO-CH_3	3.13, 24.3, 25.29
6502.	7493-58-5	1	0	0	2,3-Pentanedione, 4-methyl-	H_3C-$CH(CH_3)$-CO-CO-CH_3	3.13
6503.	123-54-6	1	1	1	2,4-Pentanedione	H_3C-CO-CH_2-CO-CH_3	3.13
6504.	110-59-8	1	0	0	Pentanenitrile {valeronitrile}	H_3C-$(CH_2)_3$-CN	11.2
6505.	69975-94-6	1	0	0	Pentanenitrile, 2,4-dimethyl-	H_3C- $CH(CH_3)$-CH_2-$CH(CH_3)$-CN	11.2
6506.		1	0	0	Pentanenitrile, 2-hydroxy-		2.5, 11.2
6507.		1	0	0	Pentanenitrile, 3-hydroxy-4-methyl-		2.5, 11.2
6508.		1	0	0	Pentanenitrile, methyl-		11.2
6509.	6339-13-5	1	0	0	Pentanenitrile, 2-methyl-	H_3C-$(CH_2)_2$-$CH(CH_3)$-CN	11.2
6510.	21101-88-2	1	0	0	Pentanenitrile, 3-methyl-		11.2
6511.	542-54-1	1	0	0	Pentanenitrile, 4-methyl-	$(H_3C)_2$=$CH(CH_2)_2$-CN	11.2
6512.	927-56-0	1	0	0	Pentanenitrile, 4-oxo-	H_3C-CO-$(CH_2)_2$-CN	3.13, 11.2
6513.	110-66-7	1	0	0	1-Pentanethiol	H_3C-$(CH_2)_4$-SH	18.1
6514.		1	0	0	1,2,5-Pentanetriol, 3-methyl-		2.5
6515.	109-52-4	1	1	1	Pentanoic acid {valeric acid}	H_3C-$(CH_2)_3$-COOH	0.4, 4.3, 24.3, 25.29
6516.	63316-29-0	0	1	0	Pentanoic acid, 5-amino-2-hydroxy-, (*R*)-		2.5, 4.3, 12.2
6517.	591-68-4	0	1	0	Pentanoic acid, butyl ester		5.3
6518.	539-82-2	1	1	1	Pentanoic acid, ethyl ester {ethyl valerate}	H_3C-$(CH_2)_3$-COO-C_2H_5	5.3, 24.3, 25.29

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6519.	96937-52-9	1	0	0	Pentanoic acid, hydroxymethyl-		2.5, 4.3
6520.	27936-41-0	0	1	0	Pentanoic acid, methyl-		4.3
6521.	624-24-8	0	1	0	Pentanoic acid, methyl ester {methyl valerate}	H_3C-$(CH_2)_3$-COO-CH_3	5.3
6522.	96937-54-1	1	0	0	Pentanoic acid, methyl-oxo-		3.13, 4.3
6523.	96937-53-0	1	0	0	Pentanoic acid, oxo-		3.13, 4.3
6524.	10361-39-4	0	1	0	Pentanoic acid, phenylmethyl ester		5.3
6525.	6600-40-4	0	1	0	Pentanoic acid, 2-amino-		4.3, 12.2
6526.	1185-39-3	0	1	0	Pentanoic acid, 2,2-dimethyl-		4.3
6527.	20225-24-5	0	1	0	Pentanoic acid, 2-ethyl-		4.3
6528.	617-31-2	0	1	0	Pentanoic acid, 2-hydroxy-		2.5, 4.3
6529.	488-15-3	0	1	0	Pentanoic acid, 2-hydroxy-3-methyl-		2.5, 4.3
6530.	498-36-2	0	1	0	Pentanoic acid, 2-hydroxy-4-methyl-		2.5, 4.3
6531.	54031-97-9	0	1	0	Pentanoic acid, 2-hydroxy-4-oxo-		2.5, 3.13, 4.3
6532.	97-61-0	1	1	1	Pentanoic acid, 2-methyl- {2-methylvaleric acid}		4.3, 24.3, 25.29
6533.	6641-83-4	1	0	0	Pentanoic acid, 2-methyl-4-oxo-		3.13, 4.3
6534.	70340-00-0	0	1	0	Pentanoic acid, 2-methylphenyl ester		5.3
6535.	6376-59-6	1	0	0	Pentanoic acid, 2-oxo-, methyl ester		3.13, 5.3
6536.		1	1	1	Pentanoic acid, 2,5-di-(methylnitrosoamino)-	R-$(CH_2)_3$-CH(R)-COOH where R = H_3C-N(NO)-	4.3, 12.2, 15.8
6537.	150-96-9	0	1	0	Pentanoic acid, 3-hydroxy-3-methyl-		2.5, 4.3
6538.	5980-21-2	0	1	0	Pentanoic acid, 3-hydroxy-4-methyl-		2.5, 4.3
6539.	105-43-1	1	1	1	Pentanoic acid, 3-methyl- {β-methylvaleric acid, 3-methylpentanoic acid}		0.4, 4.3, 24.3, 25.29
6540.	5870-68-8	1	1	1	Pentanoic acid, 3-methyl-, ethyl ester		5.3
6541.	2177-78-8	1	1	1	Pentanoic acid, 3-methyl-, methyl ester		5.3
6542.	6628-79-1	1	0	0	Pentanoic acid, 3-methyl-4-oxo-		3.13, 4.3
6543.	10191-25-0	0	1	0	Pentanoic acid, 3-oxo-		3.13, 4.3
6544.	150-97-0	0	1	0	Pentanoic acid, 3,5-dihydroxy-5-methyl- {mevalonic acid}		2.5, 4.3
6545.	41654-03-9	0	1	0	Pentanoic acid, 4-hydroxy-3-methyl-		2.5, 4.3
6546.	646-07-1	1	1	1	Pentanoic acid, 4-methyl- {isocaproic acid}		4.3, 24.3
6547.	2412-80-8	1	0	0	Pentanoic acid, 4-methyl-, methyl ester		5.3
6548.	123-76-2	1	1	1	Pentanoic acid, 4-oxo- {levulinic acid}	H_3C-CO-$(CH_2)_2$-COOH	3.13, 4.3, 24.3, 25.29
6549.	539-88-8	1	1	1	Pentanoic acid, 4-oxo-, ethyl ester {ethyl levulinate}	H_3C-CO-$(CH_2)_2$-COO-CH_2-CH_3	3.13, 5.3
6550.	624-45-3	1	1	1	Pentanoic acid, 4-oxo-, methyl ester {methyl levulinate}	H_3C-CO-$(CH_2)_2$-COO-CH_3	3.13, 5.3
6551.	67920-51-8	0	1	0	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (±)-		2.5, 4.3, 12.2
6552.	63316-30-3	0	1	0	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (R)-		2.5, 4.3, 12.2
6553.	16814-81-6	0	1	0	Pentanoic acid, 5-amino-2-hydroxy-, (S)-		2.5, 4.3, 12.2
6554.	63316-28-9	0	1	0	Pentanoic acid, 5-amino-3-hydroxy-		2.5, 4.3, 12.2
6555.	106-60-5	0	1	0	Pentanoic acid, 5-amino-4-oxo-	H_2N-CH_2-CO-$(CH_2)_2$-COOH	3.13, 4.3, 12.2
6556.		0	1	0	Pentanoicacid, 5-hydroxy-3-(1-methylethyl)-		2.5, 4.3
6557.	66274-27-9	1	0	0	Pentanoic acid, 5-hydroxy-4-oxo-, methyl ester		2.5, 3.13, 5.3

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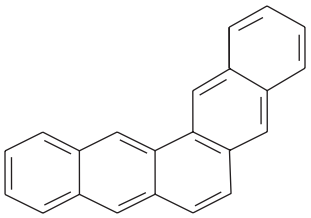
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6558.	526-91-0 D 4172-43-4 4172-44-5 L 17828-56-7 DL	1	0	0	Pentanoic acid, 2,3,4,5-tetrahydroxy-	$HOCH_2$-$(CHOH)_3$-COOH	2.5, 4.3
6559.	71-41-0	1	1	1	1-Pentanol {amyl alcohol}	H_3C-$(CH_2)_3$-CH_2OH	2.5, 24.3
6560.	6570-87-2	0	1	0	1-Pentanol, 3,4-dimethyl-		2.5
6561.	105-30-6	0	1	0	1-Pentanol, 2-methyl-		2.5
6562.	589-35-5	0	1	0	1-Pentanol, 3-methyl-		2.5
6563.	626-89-1	0	1	0	1-Pentanol, 4-methyl-		2.5
6564.	6032-29-7	0	1	0	2-Pentanol		2.5
6565.	590-36-3	0	1	0	2-Pentanol, 2-methyl-		2.5
6566.	565-60-6	0	1	0	2-Pentanol, 3-methyl-		2.5
6567.	108-11-2	1	1	1	2-Pentanol, 4-methyl-		2.5
6568.	584-02-1	0	1	0	3-Pentanol	$(H_3C$-$CH_2)_2$═CHOH	2.5
6569.	565-67-3	1	0	0	3-Pentanol, 2-methyl-		2.5
6570.	77-74-7	1	0	0	3-Pentanol, 3-methyl-		2.5
6571.		1	0	0	3-Pentanol, 1-phenyl-		2.5
6572.	27154-67-2	1	0	0	Pentanone		3.13
6573.	63072-44-6	0	1	0	Pentanone, methyl-		3.13
6574.	1009-14-9	1	0	0	1-Pentanone, 1-phenyl-	H_3C-$(CH_2)_3$-CO-C_6H_5	3.13
6575.	107-87-9	1	1	1	2-Pentanone	H_3C-$(CH_2)_2$-CO-CH_3	3.13, 24.3, 25.29
6576.	64502-89-2	1	0	0	2-Pentanone, 1-hydroxy-	H_3C-$(CH_2)_2$-CO-CH_2OH	2.5, 3.13
6577.	4161-60-8	1	1	1	2-Pentanone, 4-hydroxy-	H_3C-CHOH-CH_2-CO-CH_3	2.5, 3.13
6578.	123-42-2	1	1	1	2-Pentanone, 4-hydroxy-4-methyl- {diacetone alcohol}	$(H_3C)_2$═C(OH)-CH_2-CO-CH_3	2.5, 3.13
6579.	565-61-7	1	1	1	2-Pentanone, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-CO-CH_3	3.13
6580.	108-10-1	1	1	1	2-Pentanone, 4-methyl-	$(H_3C)_2$═CH-CH_2-CO-CH_3	3.13
6581.	5349-62-2	0	1	0	2-Pentanone, 4-methyl-1-phenyl-		3.13
6582.	5185-97-7	1	1	1	2-Pentanone, 5-(acetyloxy)-	H_3C-COO-$(CH_2)_3$-CO-CH_3	3.13, 5.3
6583.	1071-73-4	1	1	1	2-Pentanone, 5-hydroxy-	$HOCH_2$-CH_2-CH_2-CO-CH_3	2.5, 3.13
6584.	1567-93-7	1	0	0	2-Pentanone, 5-hydroxy-3-methyl-	$HOCH_2$-CH_2-$CH(CH_3)$-CO-CH_3	2.5, 3.13
6585.	66309-84-0	1	0	0	2-Pentanone, 5-hydroxy-4-methyl-	$HOCH_2$-$CH(CH_3)$-CH_2-CO-CH_3	2.5, 3.13
6586.	96-22-0	1	1	1	3-Pentanone	H_3C-CH_2-CO-CH_2-CH_3	0.4, 3.13, 25.29
6587.	565-80-0	1	0	0	3-Pentanone, 2,4-dimethyl-	$(H_3C)_2$═CH-CO-CH═$(CH_3)_2$	3.13
6588.	66735-69-***1***	1	0	0	3-Pentanone, 1-(methylthio)-		3.13, 18.1
6589.	565-69-5	1	1	1	3-Pentanone, 2-methyl-	$(H_3C)_2$═CH-CO-CH_2-CH_3	3.13
6590.	222-93-5	1	0	0	Pentaphene {dibenzo[*b,j*] phenanthrene, 2,3,6,7-dibenzophenanethrene}		1.20
6591.	488-31-3	0	1	0	Pentaric acid		4.3
6592.	320-77-4	0	1	0	Pentaric acid, 3-carboxy-2,3-dideoxy-		4.3
6593.	630-07-9	1	1	1	Pentatriacontane	H_3C-$(CH_2)_{33}$-CH_3	1.10, 26.9
6594.	66576-73-6	0	1	0	Pentatriacontane, 2-methyl-	H_3C-$CH(CH_3)$-$(CH_2)_{32}$-CH_3	1.10
6595.	78692-70-3	0	1	0	Pentatriacontane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{31}$-CH_3	1.10
6596.	21978-49-4	1	1	1	5,9,13,17,21,25,29, 33-Pentatriacontaoctaen-2-one, 6,10,14,18,22,26,30,34-octamethyl-, (all-*E*)-		3.13

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6597.	34044-64-9 34786-54-4	0	1	0	1,5,9,13,17,21,25,29,33-Pentatriacontanonaene, 2,6,10, 14,18,22, 26,30,34-nonamethyl- {norsolanesene}		1.11
6598.	34786-54-4	0	1	0	1,5,9,13,17,21,25,29,33-Pentatriacontanonaene, 2,6,10,14,18,22, 26,30,34-nonamethyl- {norsolanesene}		1.11
6599.	31424-04-1	1	0	0	Pentenal		3.12
6600.	764-39-6	1	1	1	2-Pentenal	H_3C-CH_2-CH=CH-CH=O	3.12
6601.	1576-87-0	1	0	0	2-Pentenal, (*E*)-		3.12
6602.		1	0	0	2-Pentenal, 2,3-dimethyl-		3.12
6603.		1	0	0	2-Pentenal, 2,4-dimethyl-		3.12
6604.		1	0	0	2-Pentenal, methyl-		3.12
6605.	623-36-9	1	0	0	2-Pentenal, 2-methyl-		3.12
6606.	5362-56-1	1	1	1	2-Pentenal, 4-methyl-		3.12
6607.	5604-55-7	0	1	0	3-Pentenal		3.12
6608.	53448-06-9	0	1	0	3-Pentenal, (*Z*)-		3.12
6609.	5187-71-3	1	0	0	4-Pentenal, 2-methyl-		3.12
6610.	3973-43-1	1	0	0	4-Pentenal, 4-methyl-		3.12
6611.	15856-96-9	1	0	0	2-Pentenamide	H_3C-CH_2-CH=CH-CO-NH_2	13.1
6612.	61892-67-9	1	0	0	2-Pentenamide, *N*-methyl-		13.1
6613.		1	0	0	3-Pentenamide, *N*-methyl-		13.1
6614.	70265-05-3	1	0	0	3-Pentenamide, 4-methyl-		13.1
6615.	22537-07-1	1	0	0	4-Penten-1-amine	H_2C=CH-$(CH_2)_3$-NH_2	12.2
6616.		1	0	0	1-Penten-1-aminocarbonyl- (1*E*)-{[(1*E*)-1-pent-1-en-1-yl]aminocarbonyl-}	$CH_3(CH_2)_2$-CH=CH-NH-C=O	27.1
6617.	25377-72-4	1	0	0	Pentene		1.11
6618.	37275-41-5	1	0	0	Pentene, methyl-		1.11
6619.	109-67-1	1	0	0	1-Pentene	H_3C-$(CH_2)_2$-CH=CH_2	1.11
6620.	3404-73-7	1	0	0	1-Pentene, 3,3-dimethyl-	H_3C-CH_2-$C(CH_3)_2$-CH=CH_2	1.11
6621.	763-29-1	1	0	0	1-Pentene, 2-methyl-	H_3C-$(CH_2)_2$-$C(CH_3)$=CH_2	1.11
6622.	760-20-3	1	0	0	1-Pentene, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-CH=CH_2	1.11
6623.	691-37-2	1	0	0	1-Pentene, 4-methyl-	$(H_3C)_2$=CH-CH_2-CH=CH_2	1.11
6624.	109-68-2	1	1	1	2-Pentene	H_3C-CH_2-CH=CH-CH_3	1.11
6625.	646-04-8	1	0	0	2-Pentene, (*E*)-		1.11
6626.	627-20-3	1	0	0	2-Pentene, (*Z*)-		1.11
6627.	625-27-4	1	0	0	2-Pentene, 2-methyl-	H_3C-CH_2-CH=C=$(CH_3)_2$	1.11
6628.	922-61-2	1	0	0	2-Pentene, 3-methyl- (*Z*)	H_3C-CH_2-$C(CH_3)$=CH-CH_3	1.11
6629.	616-12-6	1	0	0	2-Pentene, 3-methyl-, (*E*)-		1.11
6630.	4461-48-7	1	0	0	2-Pentene, 4-methyl-	H_3C-$CH(CH_3)$-CH=CH-CH_3	1.11
6631.	674-76-0	1	0	0	2-Pentene, 4-methyl-, (*E*)-		1.11
6632.	691-38-3	1	0	0	2-Pentene, 4-methyl-, (*Z*)-		1.11
6633.	1724-02-3	0	1	0	2-Pentenedioic acid {glutaconic acid}	HOOC-CH_2-CH=CH-COOH	4.3
6634.	5164-76-1	0	1	0	2-Pentenedioic acid, dimethyl ester		5.3
6635.	101758-45-6	0	1	0	2-Pentene-1,4-diol, 5-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-3-methyl-, [1α(3*E*,4S*),2β,4a		2.5
6636.	91238-45-8	1	1	1	4-Pentene-2,3-dione		3.13
6637.	592-51-8	1	0	0	4-Pentenenitrile		11.2
6638.	27516-53-6	1	0	0	Pentenoic acid		4.3
6639.	626-98-2	1	1	1	2-Pentenoic acid	H_3C-CH_2-CH=CH-COOH	4.3

(*continued*)

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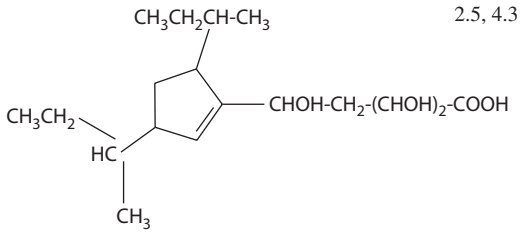
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6640.	3142-72-1	1	1	1	2-Pentenoic acid, 2-methyl-	H_3C-CH_2-CH═C(CH_3)-COOH	4.3
6641.	3675-21-6	0	1	0	2-Pentenoic acid, 3-methyl-	H_3C-CH_2-C(CH_3)═CH-COOH	4.3
6642.		0	1	0	2-Pentenoic acid, 3-methyl-5-(2,6,6-trimethyl-1-cyclohexenyl)-		4.3
6643.	10321-71-8	0	1	0	2-Pentenoic acid, 4-methyl-	H_3C-CH(CH_3)-CH═CH-COOH	4.3
6644.	1617-32-9	1	0	0	3-Pentenoic acid, (*E*)-		4.3
6645.	33698-87-2	1	0	0	3-Pentenoic acid, (*Z*)-		4.3
6646.	16313-37-4	0	1	0	3-Pentenoic acid, 3-methyl-		4.3
6647.	41653-93-4	0	1	0	3-Pentenoic acid, 3-methyl-, (E)-		4.3
6648.	41653-94-5	0	1	0	3-Pentenoic acid, 3-methyl-, (*Z*)		4.3
6649.	504-85-8	0	1	0	3-Pentenoic acid, 4-methyl-		4.3
6650.	591-80-0	1	1	1	4-Pentenoic acid	H_2C═CH-(CH_2)$_2$-COOH	4.3, 24.3
6651.	16386-93-9	0	1	0	4-Pentenoic acid, 2,2-dimethyl-		4.3
6652.	1575-74-2	0	1	0	4-Pentenoic acid, 2-methyl-		4.3
6653.	616-25-1	1	1	1	1-Penten-3-ol		2.5
6654.	2088-07-5	1	1	1	1-Penten-3-ol, 2-methyl-		2.5
6655.	1576-95-0	0	1	0	2-Penten-1-ol, (Z)	H_3C-CH_2-CH═CH-CH_2OH	2.5
6656.	87563-33-5	0	1	0	2-Penten-1-ol, 3-methyl-5-(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1S-[1α(*E*),4aβ,8aα]]-		2.5
6657.	87585-55-5	0	1	0	2-Penten-1-ol, 3-methyl-5-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [4aS-[1(*E*),4aα,8aβ]]-		2.5
6658.	39161-19-8	0	1	0	3-Penten-1-ol		2.5
6659.	763-89-**3**	0	1	0	3-Penten-1-ol, 4-methyl-		2.5
6660.	4325-82-0	1	0	0	3-Penten-2-ol, 4-methyl-		3.12
6661.	60026-13-3	0	1	0	4-Penten-2-ol, 5-(tetrahydro-2-methyl-2-furanyl)-		2.5, 10.2
6662.	1629-58-9	1	1	1	1-Penten-3-one	H_3C-CH_2-CO-CH═CH_2	3.13
6663.	3712-68-8	0	1	0	1-Penten-3-one, 2,4-dimethyl-		3.13
6664.	104-27-8	0	1	0	1-Penten-3-one, 1-(4-methoxyphenyl)-		3.13, 10.2
6665.	25044-01-3	1	0	0	1-Penten-3-one, 2-methyl-	H_3C-CH_2-CO-C(CH_3)═CH_2	3.13
6666.		1	0	0	2-Penten-4-one, 2,3-dimethyl-	(H_3C)$_2$═C═C(CH_3)-CO-CH_3	3.13
6667.	625-33-2	1	1	1	3-Penten-2-one	H_3C-CH═CH-CO-CH_3	3.13
6668.	3102-33-8	0	1	0	3-Penten-2-one, (*E*)		3.13
6669.	1118-66-7	1	0	0	3-Penten-2-one, 4-amino-	H_3C-C(NH_2)═CH-CO-CH_3	3.13, 12.2
6670.	565-62-8	1	0	0	3-Penten-2-one, 3-methyl-	H_3C-CH═C(CH_3)-CO-CH_3	3.13
6671.	141-79-7	1	1	1	3-Penten-2-one, 4-methyl- {mesityl oxide}	(H_3C)$_2$═C═CH-CO-CH_3	3.13, 24.3
6672.	13891-87-7	1	0	0	4-Penten-2-one	H_2C═CH-CH_2-CO-CH_3	3.13
6673.	127-42-4	0	1	0	4-Penten-3-one, 5-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {methyl-α-ionone}		3.13
6674.	72692-98-9	1	0	0	Pentitol, 2,3-dideoxy-3-methyl-		2.5
6675.	61989-60-4	1	0	0	Pentonic acid, 2,3-anhydro-, γ-lactone		2.5, 6.3
6676.	491-14-5	1	0	0	Pentonic acid, 5-C-[3,5-bis(1-methylpropyl)-1-cyclopenten-1-yl]-4-deoxy-		2.5, 4.3

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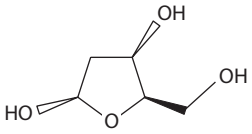
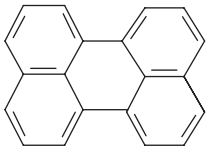
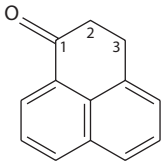
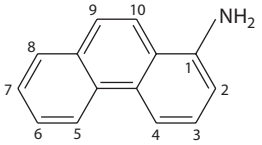
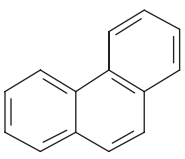
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6677.	9473-19-9	1	1	1	*D*-erythro-Pentonic acid, 3-deoxy-, γ-lactone		2.5, 6.3
6678.	5803-57-6	1	0	0	Pentonic acid, 5-deoxy-, γ-lactone		2.5, 6.3
6679.		0	1	0	Pentosan		0.4, 2.5, 8.3
6680.		0	1	0	Pentose		0.4, 2.5, 8.3
6681.	533-67-5	0	1	0	*D*-erythro-Pentose, 2-deoxy- {deoxyribose}		2.5, 8.3, 10.2
6682.		1	0	0	Pentoxyl radical	$CH_3(CH_2)_4O$	27.1
6683.	488-84-6	0	1	0	*D*-erythro-2-Pentulose = *D*-ribulose {xylulose}	$HOCH_2$-CO-$(CHOH)_2$-CH_2OH	2.5, 3.13, 8.3
6684.	24218-00-6	0	1	0	*D*-erythro-2-Pentulose, 1,5-bis(dihydrogen phosphate)		2.5, 3.13, 8.3
6685.	627-21-4	1	0	0	2-Pentyne	H_3C-C≡C-CH_2-CH_3	1.11
6686.	9031-96-3	0	1	0	Peptidase		22.2
6687.	9055-26-9	0	1	0	Permease, sulfate		22.2
6688.	9003-99-0	0	1	0	Peroxidase		0.4, 22.2
6689.	72906-87-7	0	1	0	Peroxidase, ascorbate		22.2
6690.	9013-66-5 97089-70-8	0	1	0	Peroxidase, glutathione		18.1, 22.2
6691.	198-55-0	1	0	0	Perylene		1.20
6692.		1	0	0	Perylene, alkyl-		1.20
6693.	64760-19-6	1	0	0	Perylene, dimethyl-		1.20
6694.	64031-91-0	1	0	0	Perylene, methyl- {at least two isomers in MSS}		1.20
6695.	24471-47-4	1	0	0	Perylene, 3-methyl-		1.20
6696.	518-85-4	1	0	0	1*H*-Phenalen-1-one, 2,3-dihydro-		3.13
6697.	64849-97-4	1	0	0	Phenanthrenamine		12.2
6698.	4176-53-8	1	0	0	1-Phenanthrenamine		12.2
6699.	3366-65-2	1	0	0	2-Phenanthrenamine		12.2
6700.	1892-54-2	1	0	0	3-Phenanthrenamine		12.2
6701.	17423-48-2	1	0	0	4-Phenanthrenamine		12.2
6702.	947-73-9	1	0	0	9-Phenanthrenamine		12.2
6703.	85-01-8	1	0	0	Phenanthrene		0.4, 1.20, 26.9

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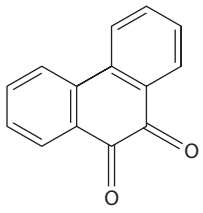
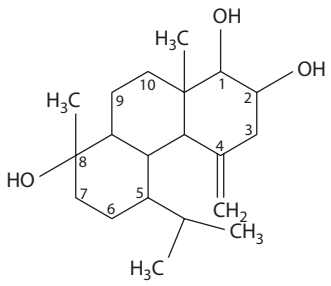
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6704.		1	0	0	Phenanthrene, alkyl-		1.20
6705.	20851-90-5	1	0	0	Phenanthrene, 3,6-dichloro-		18.4
6706.		1	0	0	Phenanthrene, dihydro-		1.20
6707.	776-35-2	1	0	0	Phenanthrene, 9,10-dihydro-		1.20
6708.	71607-56-2	1	0	0	Phenanthrene, dihydrobis(methylene)-		1.20
6709.	29062-98-4	1	0	0	Phenanthrene, dimethyl-		1.20
6710.	20291-72-9	1	0	0	Phenanthrene, 1,2-dimethyl-		1.20
6711.	22349-59-3	1	0	0	Phenanthrene, 1,4-dimethyl-		1.20
6712.	20291-74-1	1	0	0	Phenanthrene, 1,6-dimethyl-		1.20
6713.	483-87-4	1	0	0	Phenanthrene, 1,7-dimethyl-		1.20
6714.	7372-87-4	1	0	0	Phenanthrene, 1,8-dimethyl-		1.20
6715.	3674-66-6	1	0	0	Phenanthrene, 2,5-dimethyl-		1.20
6716.	17980-16-4	1	0	0	Phenanthrene, 2,6-dimethyl-		1.20
6717.	1576-69-8	1	0	0	Phenanthrene, 2,7-dimethyl-		1.20
6718.	1576-67-6	1	0	0	Phenanthrene, 3,6-dimethyl-		1.20
6719.	3674-69-9	1	0	0	Phenanthrene, 4,5-dimethyl-		1.20
6720.	110053-52-6	1	0	0	Phenanthrene, dimethylene-		1.20
6721.	71607-65-3	1	0	0	Phenanthrene, dimethylethyl-		1.20
6722.	30997-38-7	1	0	0	Phenanthrene, ethyl-		1.20
6723.	71607-66-4	1	0	0	Phenanthrene, ethylmethyl-		1.20
6724.	71607-67-5	1	0	0	Phenanthrene, hexamethyl-		1.20
6725.	61128-87-8	1	0	0	Phenanthrene, methoxy-		10.2
6726.	31711-53-2	1	1	1	Phenanthrene, methyl-		1.20
6727.	832-69-9	1	0	0	Phenanthrene, 1-methyl-		1.20
6728.	2531-84-2	1	0	0	Phenanthrene, 2-methyl-		1.20
6729.	832-71-3	1	0	0	Phenanthrene, 3-methyl-		1.20
6730.	832-64-4	1	0	0	Phenanthrene, 4-methyl-		1.20
6731.	883-20-5	1	0	0	Phenanthrene, 9-methyl-		1.20
6732.		1	0	0	Phenanthrene, 1-methyl-5-(1-methylethyl)-		1.20
6733.	71607-68-6	1	0	0	Phenanthrene, pentamethyl-		1.20
6734.	71607-69-7	1	0	0	Phenanthrene, propyl-		1.20
6735.	71607-70-0	1	0	0	Phenanthrene, tetramethyl- {at least five isomers in MSS}		1.20
6736.	30232-26-9	1	0	0	Phenanthrene, trimethyl- {at least three isomers in MSS}		1.20
6737.	84-11-7	1	0	0	9,10-Phenanthrenedione {phenanthrenequinone, phenanthraquinone}		9.24
6738.	111924-41-5	0	1	0	1,2,8-Phenanthrenetriol, tetradecahydro-8,10a-dimethyl-4-methylene-5-(1-methylethyl)-		2.5

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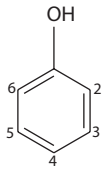
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
6739.	108-95-2	1	1	1	Phenol		0.4, 9.22, 23.5, 25.29, 26.9
6740.		1	0	0	Phenol, C_2-alkyl-		9.22
6741.		1	0	0	Phenol, C_3-alkyl-		9.22
6742.		1	0	0	Phenol, C_4-alkyl-		9.22
6743.		1	0	0	Phenol, C_5-alkyl-		9.22
6744.		1	0	0	Phenol, C_2-alkyl-ethenyl- {two isomers}		9.22
6745.		1	0	0	Phenol, C_4-alkyl-ethenyl-		9.22
6746.		1	0	0	Phenol, C_5-alkyl-ethenyl-		9.22
6747.		1	0	0	Phenol, alkyl-dimethoxy-		9.22, 10.2
6748.		1	0	0	Phenol, diethyl-		9.22
6749.	25155-26-4	1	0	0	Phenol, dimethoxy-		9.22, 10.2
6750.		1	0	0	Phenol, dimethoxy-4-ethenyl-		9.22, 10.2
6751.	1300-71-6	1	1	1	Phenol, dimethyl- {xylenol}		9.22
6752.	73850-14-3	1	0	0	Phenol, dimethylethenyl-		9.22
6753.	73850-04-1	1	0	0	Phenol, dimethyl-4-ethenyl-		9.22
6754.	50984-45-7	1	0	0	Phenol, dimethyl-ethenyl-ethyl-		9.22
6755.		1	0	0	Phenol, dimethyl-ethenyl-2-methoxy-		9.22, 10.2
6756.	85528-07-0	1	0	0	Phenol, dimethylethyl-		9.22
6757.	27178-34-3	1	0	0	Phenol, (1,1-dimethylethyl)-		9.22
6758.	1329-97-1	1	0	0	Phenol, dimethyl-methoxy-		9.22, 10.2
6759.		1	0	0	Phenol, dimethyl-2-methoxy-		9.22, 10.2
6760.		1	0	0	Phenol, dimethyl-4-methoxy-		9.22, 10.2
6761.		1	0	0	Phenol, dimethyl-2-nitro-		9.22, 16.1
6762.	31257-96-2	1	0	0	Phenol, ethenyl-		9.22
6763.	50851-69-9	1	0	0	Phenol, ethenylethyl-		9.22
6764.		1	0	0	Phenol, ethenyl-ethyl-methyl-		9.22
6765.		1	0	0	Phenol, ethenyl-2-methoxy-trimethyl-		9.22, 10.2
6766.	73850-05-2	1	0	0	Phenol, ethenylmethyl-		9.22
6767.	73850-13-2	1	0	0	Phenol, ethenyltrimethyl-		9.22
6768.	25429-37-2	1	0	0	Phenol, ethyl-		9.22
6769.	80652-16-0	1	0	0	Phenol, ethylmethoxy-		9.22, 10.2
6770.		1	0	0	Phenol, ethyl-2-methoxy-		9.22, 10.2
6771.	30230-52-5	1	0	0	Phenol, ethylmethyl-		9.22
6772.		1	0	0	Phenol, ethyl-methyl-nitro-		9.22, 16.1
6773.		1	0	0	Phenol, ethyl-nitro-		9.22, 16.1
6774.	26638-03-9	1	0	0	Phenol, methoxy-		9.22, 10.2
6775.	32391-38-1	1	1	1	Phenol, methoxymethyl-		9.22, 10.2
6776.	1319-77-3	1	1	1	Phenol, methyl- {cresol}		0.4, 9.22
6777.	12167-20-3	1	0	0	Phenol, methyl-nitro-		9.22, 16.1
6778.		1	0	0	Phenol, methylpropylenyl-		9.22
6779.	62744-64-3	1	0	0	Phenol, methylpropyl-		9.22
6780.		1	0	0	Phenol, propenyl-		9.22
6781.		1	0	0	Phenol, propyl-		9.22
6782.	66586-93-4	1	0	0	Phenol, tetramethyl-		9.22
6783.	26998-80-1	1	0	0	Phenol, trimethyl-		9.22
6784.	3180-09-4	1	0	0	Phenol, 2-butyl-		9.22
6785.	95-57-8	1	0	0	Phenol, 2-chloro-		9.22, 18.4

(*continued*)

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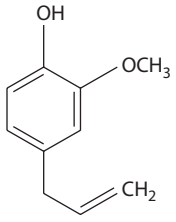
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6786.	3743-22-4	1	0	0	Phenol, 2-(dimethylamino)-		9.22, 12.2
6787.	88-18-6	1	1	1	Phenol, 2-(1,1-dimethylethyl)-		9.22, 26.9
6788.	25013-16-5	1	0	0	Phenol, 2-(1,1-dimethylethyl)-4-methoxy-		9.22, 10.2
6789.	695-84-1	1	0	0	Phenol, 2-ethenyl-		9.22
6790.	120550-69-8	1	0	0	Phenol, 2-ethenyl-6-methoxy-		9.22, 10.2
6791.	135295-09-9	1	0	0	Phenol, 2-ethenyl-6-methyl-		9.22
6792.	94-86-0	0	1	0	Phenol, 2-ethoxy-5-propenyl- {5-propenylguaethol}		9.22, 10.2
6793.	90-00-6	1	0	0	Phenol, 2-ethyl-		9.22
6794.	13391-32-7	1	0	0	Phenol, 2-ethyl-4-methoxy-		9.22, 10.2
6795.	90534-46-6	1	0	0	Phenol, 2-ethyl-6-methoxy-		9.22, 10.2
6796.	6161-62-2	1	0	0	Phenol, 2-ethyl-3-methyl-		9.22
6797.	3855-26-3	1	0	0	Phenol, 2-ethyl-4-methyl-		9.22
6798.	1687-61-2	1	0	0	Phenol, 2-ethyl-5-methyl-		9.22
6799.	1687-64-5	1	0	0	Phenol, 2-ethyl-6-methyl-		9.22
6800.	71607-97-1	1	0	0	Phenol, 2-ethyl-3-nitro-		9.22, 16.1
6801.		1	0	0	Phenol, 2-ethyl-4-nitro-		9.22, 16.1
6802.	90-05-1	1	1	1	Phenol, 2-methoxy- {guaiacol}		0.4, 9.22, 10.2, 24.3, 25.29
6803.	60825-46-9	1	0	0	Phenol-$^{14}C_6$, 2-methoxy- {guaiacol-$^{14}C_6$}		9.22, 10.2
6804.		1	0	0	Phenol, 2-methoxymethyl-		9.22, 10.2
6805.	18102-31-3	1	0	0	Phenol, 2-methoxy-3-methyl-		9.22, 10.2
6806.	53587-16-9	1	0	0	Phenol, 2-methoxy-4-(1-methylethyl)-		9.22, 10.2
6807.	97-54-1	1	1	1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}		0.4, 9.22, 10.2, 25.29
6808.	5932-68-3	1	1	1	Phenol, 2-methoxy-4-(1-propenyl)-, (*E*)- {*trans*-isoeugenol}		9.22, 10.2
6809.	5912-86-7	1	1	1	Phenol, 2-methoxy-4-(1-propenyl)-, (*Z*)- {*cis*-isoeugenol}		9.22, 10.2
6810.	97-53-0	1	1	1	Phenol, 2-methoxy-4-(2-propenyl)- {eugenol}		0.4, 9.22, 10.2
6811.	93-15-2	1	1	1	Phenol, 2-methoxy-methyl-4-(2-propenyl)- {eugenol, methyl-}		9.22, 10.2, 23.5
6812.	93-51-6	1	1	1	Phenol, 2-methoxy-4-methyl- {4-methylguaiacol}		9.22, 10.2, 24.3, 25.29
6813.	2785-87-7	1	1	1	Phenol, 2-methoxy-4-propyl-		9.22, 10.2
6814.	19784-98-6	1	0	0	Phenol, 2-methoxy-5-(1-propenyl)-, (*E*)-		9.22, 10.2
6815.	1195-09-1	1	1	1	Phenol, 2-methoxy-5-methyl-		9.22, 10.2
6816.	58539-27-8	1	0	0	Phenol, 2-methoxy-5-propyl-		9.22, 10.2
6817.	29275-83-0	1	0	0	Phenol, 2-methoxy-6-(1-propenyl)-, (*E*)-		9.22, 10.2
6818.	29275-82-9	1	0	0	Phenol, 2-methoxy-6-(1-propenyl)-, (*Z*)-		9.22, 10.2
6819.	2896-67-5	1	0	0	Phenol, 2-methoxy-6-methyl-		9.22, 10.2
6820.	32073-24-8	1	0	0	Phenol, 2-methoxy-propyl-		9.22, 10.2
6821.	93526-86-4	1	0	0	Phenol, 2-methoxy-trimethyl-		9.22, 10.2

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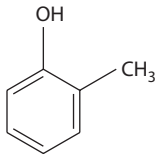
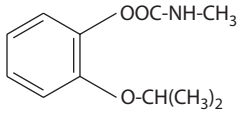
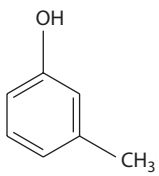
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6822.	95-48-7	1	1	1	Phenol, 2-methyl- {*o*-cresol}		0.4, 9.22
6823.	70-30-4	1	0	0	Phenol, 2,2′-methylenebis [3,4,6-trichloro-		9.22, 18.4
6824.	114-26-1	0	1	0	Phenol, 2-(1-methylethoxy)-, methylcarbamate {Undene®, Propoxur®}		5.3, 10.2, 21.3
6825.	88-69-7	1	1	1	Phenol, 2-(1-methylethyl)- {2-isopropylphenol}		9.22, 24.3
6826.	1740-97-2	1	0	0	Phenol, 2-methyl-4-(1-methylethyl)-		9.22
6827.	499-75-2	1	1	1	Phenol, 2-methyl-5-(1-methylethyl)- {carvacrol}		9.22, 24.3, 25.29
6828.		1	0	0	Phenol, 2-methyl-(2-methylpropyl)-		9.22
6829.	99-53-6	1	0	0	Phenol, 2-methyl-4-nitro-		9.22, 16.1
6830.	73850-08-5	1	0	0	Phenol, (2-methylpropyl)-		9.22
6831.	3520-52-3	1	0	0	Phenol, 2-methyl-6-propyl-		9.22
6832.	89-72-5	1	1	1	Phenol, 2-(1-methylpropyl)-		9.22
6833.	4167-75-3	1	0	0	Phenol, 2-(2-methylpropyl)-		9.22
6834.	88-75-5	1	0	0	Phenol, 2-nitro-		9.22, 16.1
6835.	2417-10-9	1	0	0	Phenol, 2-phenoxy-		9.22, 10.2
6836.	26761-75-1	1	0	0	Phenol, (2-propen-1-yl-)-		9.22
6837.	6380-21-8	1	0	0	Phenol, 2-(1-propen-1-yl)-		9.22
6838.	1745-81-9	1	0	0	Phenol, 2-(2-propenyl)-		9.22
6839.	644-35-9	1	0	0	Phenol, 2-propyl-		9.22, 25.29
6840.	591-27-5	1	0	0	Phenol, 3-amino-		9.22, 12.2
6841.	108-43-0	1	0	0	Phenol, 3-chloro-		9.22, 18.4
6842.	585-34-2	1	0	0	Phenol, 3-(1,1-dimethylethyl)-		9.22
6843.	88-32-4	1	0	0	Phenol, 3-(1,1-dimethyethyl)-4-methoxy-		9.22, 10.2
6844.	618-45-1	1	1	1	Phenol, 3-(1-methylethyl)-		9.22
6845.	79755-53-6	1	0	0	Phenol, 3-(1-propenyl)-		9.22
6846.	620-18-8	1	0	0	Phenol, 3-ethenyl-		9.22
6847.	73850-03-0	1	0	0	Phenol, 3-ethenyl-methyl-		9.22
6848.	66164-30-5	1	0	0	Phenol, 3-ethenyl-4-methyl-		9.22
6849.	73850-06-3	1	0	0	Phenol, 3-ethenyl-2,?,?-trimethyl-		9.22
6850.	621-34-1	1	0	0	Phenol, 3-ethoxy-		9.22, 10.2
6851.	620-17-7	1	1	1	Phenol, 3-ethyl-		9.22
6852.	29760-89-2	1	0	0	Phenol, 3-ethyl-2-methoxy-		9.22, 10.2
6853.	1123-73-5	1	0	0	Phenol, 3-ethyl-2-methyl-		9.22
6854.	6161-67-7	1	0	0	Phenol, 3-ethyl-4-methyl-		9.22
6855.	698-71-5	1	1	1	Phenol, 3-ethyl-5-methyl-		9.22
6856.	150-19-6	1	1	1	Phenol, 3-methoxy-		9.22, 10.2
6857.	5451-83-2	1	0	0	Phenol, 3-methoxy-, acetate		5.3, 10.2
6858.	108-39-4	1	1	1	Phenol, 3-methyl- {*m*-cresol}		0.4, 9.22, 23.5

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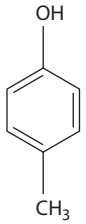
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6859.	4920-77-8	1	0	0	Phenol, 3-methyl-2-nitro-		9.22, 16.1
6860.	2581-34-2	1	0	0	Phenol, 3-methyl-4-nitro-		9.22, 16.1
6861.	554-84-7	1	0	0	Phenol, 3-nitro-		9.22, 16.1
6862.	713-68-8	1	0	0	Phenol, 3-phenoxy-		9.22, 10.2
6863.	621-27-2	1	0	0	Phenol, 3-propyl-		9.22
6864.	98-54-4	1	1	1	Phenol, 4-(1,1-dimethylethyl)-		9.22
6865.	99-89-8	1	1	1	Phenol, 4-(1-methylethyl)-		9.22
6866.	99-71-8	1	1	1	Phenol, 4-(1-methylpropyl)-		9.22
6867.	51-67-2	1	1	1	Phenol, 4-(2-aminoethyl)- {tyramine}		9.22, 12.2
6868.	539-12-8	1	0	0	Phenol, 4-(1-propen-1-yl)-		9.22
6869.	501-92-8	1	1	1	Phenol, 4-(2-propen-1yl)-		9.22
6870.	3690-05-9	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)- {coumaryl alcohol}		2.5, 9.22
6871.	537-33-7	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)-2,6-dimethoxy- {sinapyl alcohol}		2.5, 9.22, 10.2
6872.	458-35-5	1	1	1	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy- {coniferyl alcohol}		2.5, 9.22, 10.2
6873.	32811-40-8	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*E*)-		2.5, 9.22, 10.2
6874.	69056-21-9	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*Z*)-		2.5, 9.22, 10.2
6875.	59832-96-1	1	0	0	Phenol, 4-butyl-2-methoxy-		9.22, 10.2
6876.	2628-17-3	1	1	1	Phenol, 4-ethenyl-		9.22
6877.		1	0	0	Phenol, 4-ethenyl-2-ethyl-		9.22
6878.	7786-61-0	1	1	1	Phenol, 4-ethenyl-2-methoxy- {4-vinylguaiacol}		9.22, 10.2, 24.3, 25.29
6879.	45803-83-6	1	0	0	Phenol, 4-ethenyl-2-methyl-		9.22
6880.	123-07-9	1	1	1	Phenol, 4-ethyl- {*p*-ethylphenol}		9.22, 24.3, 25.29
6881.	2785-89-9	1	1	1	Phenol, 4-ethyl-2-methoxy- {ethylguaiacol}		9.22, 10.2
6882.	120550-71-2	1	0	0	Phenol, 4-ethyl-2-methoxy-5-methyl-		9.22, 10.2
6883.	120550-70-1	1	0	0	Phenol, 4-ethyl-2-methoxy-6-methyl-		9.22, 10.2
6884.	2219-73-0	1	0	0	Phenol, 4-ethyl-2-methyl-		9.22
6885.	1123-94-0	1	0	0	Phenol, 4-ethyl-3-methyl-		9.22
6886.	71607-98-2	1	0	0	Phenol, 4-ethyl-3-nitro-		9.22, 16.1
6887.	150-76-5	1	1	1	Phenol, 4-methoxy-		9.22, 10.2, 26.9
6888.	106-44-5	1	1	1	Phenol, 4-methyl- {*p*-cresol}		9.22, 23.5
6889.	4427-56-9	1	0	0	Phenol, 4-methyl-2-(1-methylethyl)-		9.22
6890.	119-33-5	1	0	0	Phenol, 4-methyl-2-nitro-		9.22, 16.1
6891.	2042-14-0	1	0	0	Phenol, 4-methyl-3-nitro-		9.22, 16.1
6892.	4074-46-8	1	0	0	Phenol, 4-methyl-2-propyl-		9.22
6893.	100-02-7	1	0	0	Phenol, 4-nitro-		9.22, 16.1
6894.	831-82-3	1	0	0	Phenol, 4-phenoxy-		9.22, 10.2
6895.	1988-89-2	0	1	0	Phenol, 4-(1phenylethyl)-		9.22
6896.	101-53-1 7563-63-5	1	0	0	Phenol, 4-phenylmethyl-		9.22

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6897.	85960-81-2	1	0	0	Phenol, 4-propenyl-		9.22
6898.	645-56-7	1	0	0	Phenol, 4-propyl-		9.22
6899.	2785-88-8	1	0	0	Phenol, 5-ethyl-2-methoxy-		9.22, 10.2
6900.	1687-65-6	1	0	0	Phenol, 5-ethyl-2-methyl-		9.22
6901.	71278-12-1	1	0	0	Phenol, 5-ethyl-2-methyl-4-nitro- {phenol, 3-ethyl-6-methyl-4-nitro-}		9.22, 16.1
6902.	89-83-8	1	0	0	Phenol, 5-methyl-2-(1-methylethyl)- {thymol}		9.22, 24.3, 25.29
6903.	5150-42-5	1	1	1	Phenol, 2,3-dimethoxy-		9.22, 10.2
6904.	20578-97-6	1	1	1	Phenol, 2,3-dimethoxy-4-ethyl-		9.22, 10.2
6905.	526-75-0	1	1	1	Phenol, 2,3-dimethyl- {2,3-xylenol}		9.22
6906.	18441-55-9	1	0	0	Phenol, 2,3-dimethyl-6-ethyl-		9.22
6907.	34883-01-7	1	1	1	Phenol, 2,3-dimethyl-5-methoxy-		9.22, 10.2
6908.	6665-95-8	1	0	0	Phenol, 2,3-dimethyl-6-nitro- {phenol, 5,6-dimethyl-2-nitro-}		9.22, 16.1
6909.	105-67-9	1	1	1	Phenol, 2,4-dimethyl- {2,4-xylenol}		9.22
6910.		1	0	0	Phenol, 2,4-dimethyl-6-ethyl-		9.22
6911.	95-87-4	1	1	1	Phenol, 2,5-dimethyl- {2,5-xylenol}		9.22
6912.		1	0	0	Phenol, 2,5-dimethyl-6-nitro-		9.22, 16.1
6913.	1006-59-3	1	0	0	Phenol, 2,6-diethyl-		9.22
6914.	4130-42-1	1	1	1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-		9.22
6915.	128-37-0	1	1	1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl- {BHT}		9.22, 26.9
6916.	91-10-1	1	1	1	Phenol, 2,6-dimethoxy- {syringol}		9.22, 10.2, 24.3, 25.29
6917.		1	0	0	Phenol, 2,6-dimethoxy-ethenyl-		9.22, 10.2
6918.	28343-22-8	1	1	1	Phenol, 2,6-dimethoxy-4-ethenyl-		9.22, 10.2
6919.	14059-92-8	1	1	1	Phenol, 2,6-dimethoxy-4-ethyl-		9.22, 10.2
6920.	6638-05-7	1	1	1	Phenol, 2,6-dimethoxy-4-methyl-		9.22, 10.2
6921.	20675-95-0	1	1	1	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*E*)-		9.22, 10.2
6922.	26624-13-5	1	1	1	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*Z*)-		9.22, 10.2
6923.	6627-88-9	1	1	1	Phenol, 2,6-dimethoxy-4-(2-propenyl)-		9.22, 10.2
6924.	576-26-1	1	1	1	Phenol, 2,6-dimethyl- {2,6-xylenol}		9.22
6925.	71526-64-2	1	0	0	Phenol, 2,6-dimethyl-4-ethenyl-		9.22
6926.	10570-69-1	1	0	0	Phenol, 2,6-dimethyl-4-ethyl-		9.22
6927.		0	1	0	Phenol, 2,6-dimethyl-4-(2-propenyl)-		9.22
6928.	2033-89-8	1	0	0	Phenol, 3,4-dimethoxy-		9.22, 10.2
6929.	95-65-8	1	1	1	Phenol, 3,4-dimethyl- {3,4-xylenol}		9.22, 24.3
6930.	500-99-2	1	1	1	Phenol, 3,5-dimethoxy-		9.22, 10.2
6931.	108-68-9	1	1	1	Phenol, 3,5-dimethyl- {3,5-xylenol}		9.22
6932.	2785-85-5	1	0	0	Phenol, 3,5-dimethyl-2-methoxy-		9.22, 10.2
6933.	71608-10-1	1	0	0	Phenol, 3,6-dimethyl-2-nitro- {phenol, 2,5-dimethyl-6-nitro-}		9.22, 16.1
6934.	72312-07-3	0	1	0	Phenol, 4,5-dimethoxy-2-methyl-		9.22, 10.2
6935.	7771-25-7	1	0	0	Phenol, 4,5-dimethyl-2-methoxy-		9.22, 10.2
6936.	2219-79-6	1	0	0	Phenol, 4,6-dimethyl-2-ethyl-		9.22
6937.	2896-66-4	1	0	0	Phenol, 4,6-dimethyl-2-methoxy-		9.22, 10.2
6938.	123844-48-4	1	0	0	Phenol, 5,6-dimethyl-2-methoxy-		9.22, 10.2
6939.	3238-38-8	1	0	0	Phenol, 2,3,4,6-tetramethyl-		9.22
6940.	527-35-5	1	1	1	Phenol, 2,3,5,6-tetramethyl- {durenol}		9.22
6941.	73850-02-9	1	0	0	Phenol, 2,?,?-trimethyl-		9.22

(*continued*)

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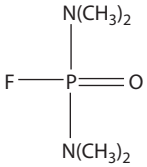
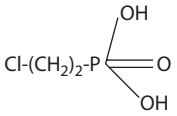
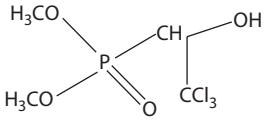
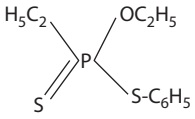
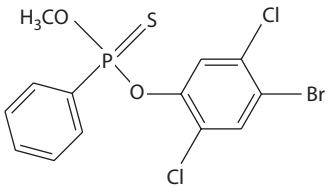
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6942.	526-85-2	1	1	1	Phenol, 2,3,4-trimethyl-		9.22
6943.	697-82-5	1	0	0	Phenol, 2,3,5-trimethyl- {isopseudocumenol}		9.22
6944.	2416-94-6	1	0	0	Phenol, 2,3,6-trimethyl-		9.22
6945.	496-78-6	1	0	0	Phenol, 2,4,5-trimethyl- {pseudocumenol}		9.22
6946.	118-79-6	0	1	0	Phenol, 2,4,6-tribromo-		9.22, 18.4, 21.3
6947.	527-60-6	1	1	1	Phenol, 2,4,6-trimethyl- {mesitol}		9.22
6948.	527-54-8	1	0	0	Phenol, 3,4,5-trimethyl-		9.22
6949.	732-26-3	1	1	1	Phenol, 2,4,6-tris(1,1-dimethylethyl)-		9.22
6950.	**2122-46-5**	1	0	0	Phenoxyl radical	C_6H_5O	27.1
6951.	17374-79-7	1	0	0	Phenoxyl, methyl- radical	CH_3-C_6H_4O	27.1
6952.	63-91-2	1	1	1	*L*-Phenylalanine	C_6H_5-CH_2-$CH(NH_2)$-COOH	0.4, 4.3, 4.10, 12.2, 24.3, 25.29
6953.	31105-03-0	0	1	0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 10.2, 12.2
6954.	51064-37-0	0	1	0	Phenylalanine, ar,ar-dihydroxy-		4.3, 4.10, 9.22, 12.2,
6955.		0	1	0	*Pheophorbide*, hydroxysolanesyl		2.5, 5.3, 17.5
6956.		0	1	0	*Pheophorbide*, solanesyl		5.3, 17.5
6957.		0	1	0	Pheophytin, 10-hydroxy-		2.5, 5.3, 17.5
6958.	24861-47-0	0	1	0	Phorbine		17.5
6959.	20239-99-0	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, [3S-(3α,4β,21β)]-		3.13, 4.3, 17.5
6960.	3147-18-0	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2*E*,7S*,11S*),4β,21β]]- {pheophytin B}		3.13, 5.3, 17.5
6961.	15664-29-6	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18- tetramethyl-20-oxo-, [3S-(3α,4β,21β)]- {*pheophorbide* A}		3.13, 4.3, 5.3, 17.5
6962.	603-17-8	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2*E*,7S*,11S*),4β,21β]]- {pheophytin A}		3.13, 5.3, 17.5
6963.	9013-05-2	0	1	0	Phosphatase		22.2
6964.	122319-88-4	0	1	0	Phosphatase, 2-carboxyarabinitol 1-		22.2
6965.	9001-77-8	0	1	0	Phosphatase, acid		22.2
6966.	9000-83-3	0	1	0	Phosphatase, adenosine tri-		22.2
6967.	134632-85-2	0	1	0	Phosphatase, adenosine tri- (*Petunia hybrida* strain 3704 mitochondria subunit 9)		22.2
6968.	9001-78-9	0	1	0	Phosphatase, alkaline		22.2
6969.	9001-52-9	0	1	0	Phosphatase, fructose di-		22.2
6970.	9001-39-2	0	1	0	Phosphatase, glucose 6-		22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6971.	69669-68-7	0	1	0	Phosphatase, glucose di-		22.2
6972.	9027-69-4	0	1	0	Phosphatase, nucleoside di-		22.2
6973.	9075-51-8	0	1	0	Phosphatase, nucleoside tri-		22.2
6974.	9055-30-5	0	1	0	Phosphatase, phosphoglycerate		22.2
6975.	9025-76-7	0	1	0	Phosphatase, phosphoglycolate		22.2
6976.	52227-92-6	0	1	0	Phosphatase, phosphorylcholine		22.2
6977.	37341-58-5	0	1	0	Phosphatase, phytate		22.2
6978.	9059-33-0	0	1	0	Phosphatase, sucrose		22.2
6979.	14265-44-2	1	1	1	Phosphate	PO_4^{-3}	0.4, 20.5
6980.	300-76-5	0	1	0	Phosphate, 1,2-dibromo-2,2-dichloroethyl dimethyl {Naled®}		18.4, 21.3
6981.	14066-20-7	0	1	0	Phosphate, dihydrogen	$H2PO_4^{-1}$	20.5
6982.		0	1	0	Phosphate, monohydrogen	$H2PO_4^{-2}$	20.5
6983.	20859-73-8	0	1	0	Phosphide, aluminum	Al≡P	20.6, 21.3
6984.	12057-74-8	0	1	0	Phosphide, magnesium	Mg_3P_2	20.6, 21.3
6985.	7803-51-2	1	1	1	Phosphine	PH_3	0.4, 19.5, 20.6, 21.3
6986.	115-26-4	0	1	0	Phosphine oxide, bis(dimethylamino) fluoro- {Dimefox®}		12.2, 18.4, 21.3
6987.	9025-82-5	0	1	0	Phosphodiesterase		22.2
6988.	9036-21-9	0	1	0	Phosphodiesterase, adenosine cyclic 3′,5′-phosphate		22.2
6989.	39434-01-0	0	1	0	Phosphodiesterase, nucleotide		22.2
6990.	12712-31-1	0	1	0	Phosphodoxin		22.2
6991.	9001-81-4	0	1	0	Phosphomutase, glucose		22.2
6992.	16672-87-0	0	1	0	Phosphonic acid, 2-chloroethyl- {Ethephon®, Ethrel®}		18.4, 21.3
6993.	67255-31-6	0	1	0	Phosphonic acid, 2-chloroethyl-, hydrazine salt - {Hydrel®}	H_2PO_3-CH_2CH_2-Cl. H_2N-NH_2	12.2, 18.4
6994.	52-68-6	1	1	1	Phosphonic acid,2,2,2-trichloromethyl-1-hydroxyethyl-, dimethyl ester {Trichlorphon®, Dylox®, Dipterex®}		2.5, 5.3, 18.4, 21.3
6995.	98886-44-3	0	1	0	Phosphonodithioic acid, *O*-ethyl S-(1-methylpropyl) (2-oxo-3-thiazolidinyl)- {Fosthiazate®}		18.1, 21.3
6996.	944-22-9	0	1	0	Phosphonodithioic acid, ethyl-, *O*-ethyl *S*-phenyl ester {Fonofos®}		18.1, 21.3
6997.	21609-90-5	1	1	1	Phosphonothioic acid, phenyl-, *O*-(4-bromo-2,5-dichlorophenyl)-, *O*-methyl ester {Phosvel®}		5.3, 18.1, 18.4, 21.3

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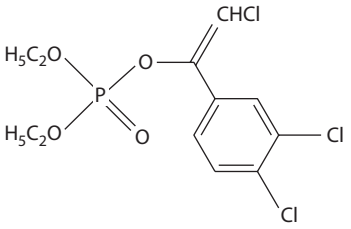
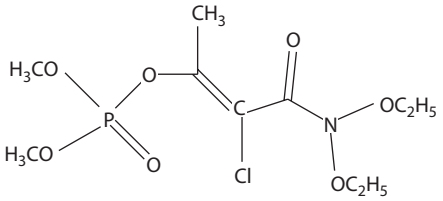
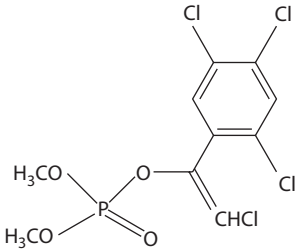
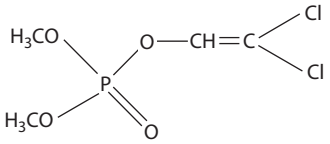
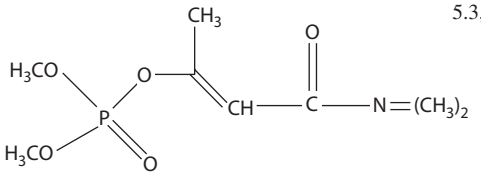
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
6998.	22224-92-6	0	1	0	Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylthio)phenyl ester {Fenamiphos®, Nemacur®}		5.3, 18.1, 21.3
6999.	30560-19-1	0	1	0	Phosphoramidothioic acid, *N*-acetyl-, *O*,S-dimethyl ester {Orthene®, Acephate®}		5.3, 18.1, 21.3
7000.	10265-92-6	0	1	0	Phosphoramidothioic acid *O*,S-dimethyl ester {Methamidophos®}		5.3, 18.1, 21.3
7001.	25311-71-1	0	1	0	Phosphoramidothioic acid, *O*-ethyl *O*-2-(1-methylethyl)carbonylphenyl-, (1-methylethyl) ester {Isofenphos®}		5.3, 18.1, 21.3
7002.	9030-26-6	0	1	0	Phosphoribosyltransferase, nicotinate		22.2
7003.	7664-38-2	0	1	0	Phosphoric acid		20.6
7004.	7757-93-9	0	1	0	Phosphoric acid, calcium salt (1:1)		20.6
7005.	7758-23-8	0	1	0	Phosphoric acid, calcium salt (2:1)		20.6
7006.	470-90-6	0	1	0	Phosphoric acid, 2-chloro-1-(2-dichlorophenyl)ethenyl-, diethyl ester {Chlorfenvinphos®, Birlane®}		5.3, 18.4, 21.3
7007.	13171-21-6	0	1	0	Phosphoric acid, 2-chloro-3-(diethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Phosphamidon®}		5.3, 18.4, 21.3
7008.	22248-79-9	0	1	0	Phosphoric acid, 2-chloro-1-(2,4,5-trichlrophenyl)ethenyl-, dimethyl ester {DDVP, Tetrachlorvinphos®}		5.3, 18.4, 21.3
7009.	7783-28-0	0	1	0	Phosphoric acid, diammonium salt	$(NH_4)_2HPO_4$	20.6
7010.	62-73-7	0	1	0	Phosphoric acid, 2,2,-dichloroethenyl-, dimethyl ester {DDVP, Dichlorvos®}		5.3, 18.4, 21.3
7011.	141-66-2	0	1	0	Phosphoric acid, 3-(dimethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Dicrotophos®}		5.3, 13.1, 21.3
7012.	7558-79-4	1	0	0	Phosphoric acid, disodium salt		20.6
7013.	14298-39-6	0	1	0	Phosphoric acid, holmium salt		20.6

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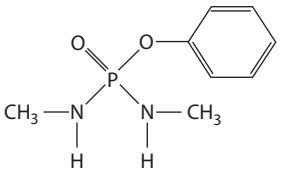
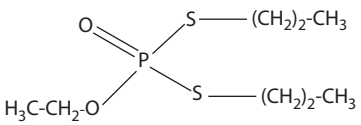
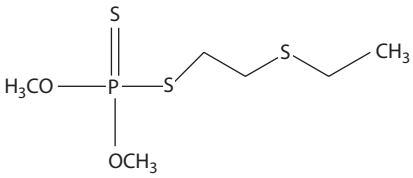
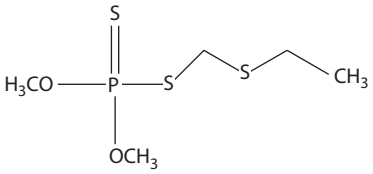
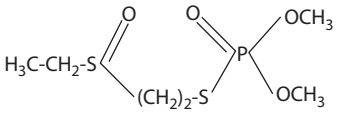
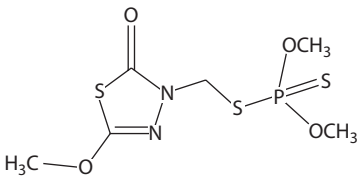
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7014.	7757-86-0	0	1	0	Phosphoric acid, magnesium salt		20.6
7015.	13092-66-5	0	1	0	Phosphoric acid, magnesium salt	$Mg(H_2PO_4)_2$	20.6
7016.	7722-76-1	0	1	0	Phosphoric acid, monoammonium salt		20.6
7017.	7778-77-0	1	1	1	Phosphoric acid, monopotassium salt		20.6
7018.	7558-80-7	1	1	1	Phosphoric acid, monosodium salt		20.6
7019.	7778-53-2	0	1	0	Phosphoric acid, tripotassium salt		20.6
7020.	38527-91-2	1	0	0	Phosphorothioic acid, 2-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester {Ethaphos®}		5.3, 18.1, 18.4, 21.3
7021.	1754-58-1	1	1	1	Phosphorodiamidic acid, *N,N′*-dimethyl-, phenyl ester {Diamidafos®}		5.3, 12.2, 13.1, 21.3
7022.	13194-48-4	0	1	0	Phosphorodithioic acid, *O*-ethyl-S,S, dipropyl ester {Mocap®, Ethoprop®, Prophos®, Rovokil®, Ethoprophos®}		5.3, 18.1, 21.3
7023.	13071-79-9	0	1	0	Phosphorodithioic acid, *O,O*-diethyl S-[(1,1-dimethylethyl)thio]methyl ester {Terbuphos®}		5.3, 18.1, 21.3
7024.	2497-06-5	0	1	0	Phosphorodithioic acid, *O,O*-diethyl S-[2-(ethylsulfonyl)ethyl] ester (Thiodemeton sulfone®)		5.3, 18.1, 21.3
7025.	298-04-4	1	1	1	Phosphorodithioic acid, *O,O*-diethyl S-[2-(ethylthio)ethyl] ester {Disulfoton®}		5.3, 18.1, 21.3
7026.	298-02-2	0	1	0	Phosphorodithioic acid, *O,O*-diethyl S-[2-(ethylthio)methyl] ester {Phorate®}		5.3, 18.1, 21.3
7027.	301-12-2	0	1	0	Phosphorodithioic acid, O,O-dimethyl *S*-[2-(ethylsulfinyl)ethyl] ester {Oxydemeton methyl®}		5.3, 18.1, 21.3
7028.	640-15-3	0	1	0	Phosphorodithioic acid, *O,O*-dimethyl S-[2-(ethylthio)ethyl] ester {Thiometon®}		5.3, 18.1, 21.3
7029.	950-37-8	0	1	0	Phosphorodithioic acid, *O,O*-dimethyl-*S*-2,3-dihydro-5-methoxy-2-oxo-1,3, 4-thiadiazol-3-ylmethyl ester {Supracide®, Methidathion®}		5.3, 18.1, 21.3

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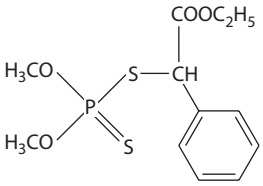
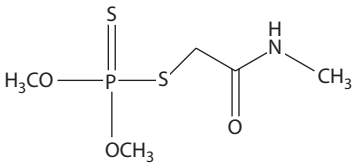
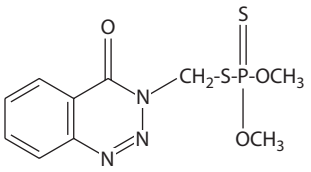
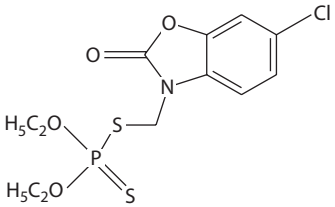
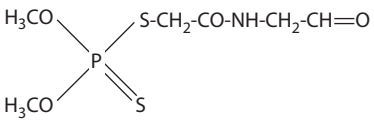
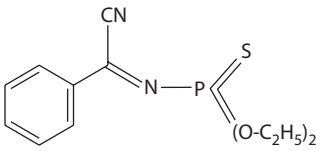
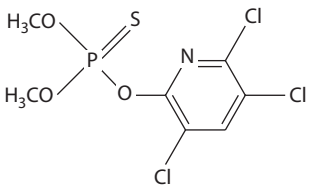
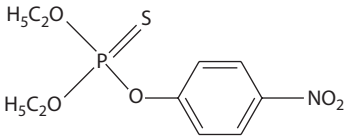
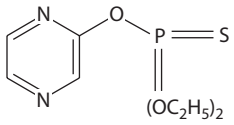
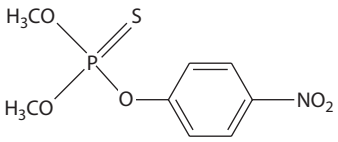
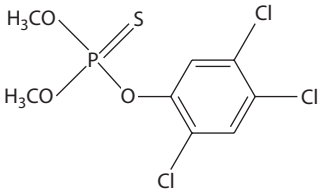
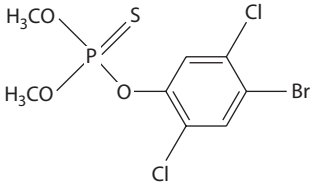
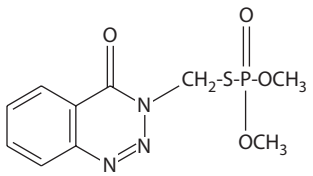
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7030.	2597-03-7	0	1	0	Phosphorodithioic acid, *O,O*-dimethyl-S-(α-ethoxycarbonylbenzyl) ester {Fenthoate®, Phenthoate®}		5.3, 18.1, 21.3
7031.	60-51-5	1	1	1	Phosphorodithioic acid, *O,O*-dimethyl-S-[2-(methylamino)-2-oxoethyl] ester {Dimethoate®}		5.3, 13.1, 18.1, 21.3
7032.	2642-71-9	0	1	0	Phosphorodithioic acid, *O,O*-diethyl S-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Azinphos Ethyl®}		5.3, 18.1, 21.3
7033.	86-50-0	1	1	1	Phosphorodithioic acid, *O,O*-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Guthion®, Azinphos-Methyl®}		5.3, 17.4, 18.1, 21.3
7034.	40626-35-5	1	0	0	Phosphorothioic acid, *O*-ethyl *O*-phenyl S-propyl ester {Heterophos®}		5.3, 18.1, 21.3
7035.	2310-17-0	0	1	0	Phosphorodithioic acid, S-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl) methyl] *O,O*-diethyl ester {Phosalone®}		5.3, 18.1, 18.4, 21.3
7036.	2540-82-1	0	1	0	Phosphorodithioic acid, S-[2-(formylmethylamino)-2-oxoethyl] *O,O*-dimethyl ester {Formothion®}		5.3, 13.1, 18.1, 21.3
7037.	41198-08-7	0	1	0	Phosphorothioic acid, *O*-(4-bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl ester {Profenophos®}		5.3, 18.1, X18.4, 21.3
7038.	14816-18-3	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-(α-cyanobenzylideneamino)- {Phoxim®}		5.3, 11.2, 18.1, 21.3
7039.	2921-88-2	1	1	1	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyrifos®, Chlorpyriphos®, Dursban®}		5.3, 17.7, 18.1, 18.4, 21.3

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7040.	115-90-2	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylsulfinyl)phenyl] ester {Fensulfothion®}		5.3, 18.1, 21.3
7041.	56-38-2	1	1	1	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®}		0.4, 5.3, 16.1, 18.1, 21.3
7042.	297-97-2	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-pyrazinyl ester {Thionazine®, Zinophos®}		5.3, 17.7, 18.1, 21.3
7043.	298-00-0	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-nitrophenyl) ester {Parathion-methyl®}		5.3, 16.1, 18.1, 21.3
7044.	299-84-3	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester {Fenchlorphos®, Phenchlorphos®}		5.3, 18.1, 18.4, 21.3
7045.	2104-96-3	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-bromo-2,5-dichlorophenyl) ester {Bromophos®}		5.3, 18.1, 18.4, 21.3
7046.	333-41-5	1	1	1	Phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester {Diazinon®}		5.3, 17.7, 18.1, 21.3
7047.	24017-47-8	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) ester {Triazophos®}		5.3, 17.4, 18.1, 21.3
7048.	919-86-8	0	1	0	Phosphorothioic acid, *O,O*-dimethyl S-[2-(ethylthio)ethyl] ester {Demeton-S-methyl®}		5.3, 18.1, 21.3
7049.	961-22-8	0	1	0	Phosphorothioic acid, *O,O*-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl) methyl] ester		5.3, 17.4, 18.1, 21.3
7050.	20300-00-9	0	1	0	Phosphorothioic acid, *O,O*-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfinyl]ethyl] ester		5.3, 18.1, 21.3
7051.	2275-23-2	0	1	0	Phosphorothioic acid, *O,O*-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester {Vamidothion®}		5.3, 18.1, 21.3

(*continued*)

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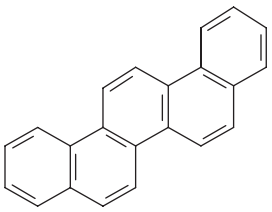
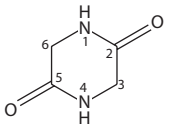
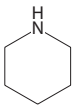
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7052.	70898-34-9	0	1	0	Phosphorothioic acid, *O,* *O* dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfonyl]ethyl] ester		5.3, 18.1, 21.3
7053.	122-14-5	0	1	0	Phosphorothioic acid, *O,* *O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester {Fenitrothion®}		5.3, 16.1, 18.1, 21.3
7054.	55-38-9	0	1	0	Phosphorothioic acid, *O,* *O*-dimethyl *O*-(4-methylthio)-3-methylphenyl ester {Fenthion®}		5.3, 18.1, 21.3
7055.	29232-93-7	0	1	0	Phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O,O*-dimethyl ester {Pirimiphos-methyl®}		5.3, 12.2, 17.7, 18.1, 21.3
7056.	7723-14-0	1	1	1	Phosphorus	P	0.4, 20.5
7057.	1314-56-3	0	1	0	Phosphorus oxide	P_2O_5	20.6
7058.	14596-37-3	0	1	0	Phosphorus, isotope of mass 32	^{32}P	20.5
7059.	9035-74-9	0	1	0	Phosphorylase		22.2
7060.	9032-10-4	0	1	0	Phosphorylase a		22.2
7061.	9030-28-8	0	1	0	Phosphorylase, guanosine		22.2
7062.	9014-12-4	0	1	0	Phosphorylase, polynucleotide {nucleotidyltransferase, polyribonucleotide}		22.2
7063.	71010-49-6	1	1	1	Phytadiene C		1.11
7064.	2437-92-5	0	1	0	Phytodienes		1.11
7065.	37297-20-4	0	1	0	Phytoalexins		22.2
7066.	213-46-7	1	0	0	Picene {benzo[*a*]chrysene}		1.20
7067.	30283-95-5	0	1	0	Picene, methyl-		1.20
7068.	25057-77-6	1	0	0	Piperazine, 1,2-dimethyl-		17.7
7069.	106-58-1	1	0	0	Piperazine, 1,4-dimethyl-		17.7
7070.	106-55-8	1	0	0	Piperazine, 2,5-dimethyl-		17.7
7071.	109-01-3	1	0	0	Piperazine, 1-methyl-		17.7
7072.	109-07-9	1	0	0	Piperazine, 2-methyl-		17.7
7073.	106-57-0	1	0	0	2,5-Piperazinedione		17.7, 17.13
7074.	5076-82-4	1	0	0	2,5-Piperazinedione, *N,N*-dimethyl-		17.7, 17.13
7075.	14771-77-8	1	0	0	2,5-Piperazinedione, 3-(1-methylethyl)-		17.7, 17.13
7076.	61892-78-2	1	0	0	2,5-Piperazinedione, 3-(2-propenyl)-		17.7, 17.13
7077.	5625-46-7	1	0	0	2,5-Piperazinedione, 3,6-dimethyl-		17.7, 17.13
7078.	5625-53-6	1	0	0	2,5-Piperazinedione, 3-methyl-		17.7, 17.13
7079.	4526-77-6	1	0	0	2,5-Piperazinedione, 3-methyl-, (S)-		17.7, 17.13
7080.	110-89-4	1	1	1	Piperidine {azacyclohexane}		0.4, 17.7

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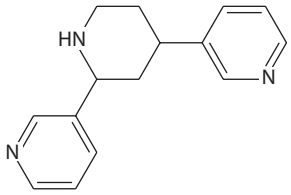
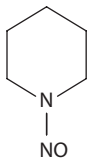
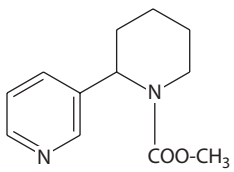
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7081.		1	0	0	Piperidine, C_2-alkyl-		17.7
7082.		1	0	0	Piperidine, C_3-alkyl-		17.7
7083.		1	0	0	Piperidine, C_4-alkyl-		17.7
7084.	3350-86-5	1	1	1	Piperidine, 1-acetyl-2-(3-pyridinyl)-, (S)-		17.11
7085.	5347-68-2	1	0	0	Piperidine, 2,3-dimethyl-		17.7
7086.	23513-39-5	1	0	0	Piperidine, 2,3-dimethyl-, *cis*-		17.7
7087.	6287-19-0	1	1	1	Piperidine, 2,4-dimethyl-		17.7
7088.	19683-91-1	1	0	0	Piperidine, 2,4-dimethyl-, *cis*-		17.7
7089.	504-03-0	1	0	0	Piperidine, 2,6-dimethyl-		17.7
7090.	17721-95-8	1	0	0	Piperidine, 2.6-dimethyl-1-nitroso-		15.8, 17.7
7091.	35794-11-7	1	0	0	Piperidine, 3,5-dimethyl-		17.7
7092.	18793-19-6	1	1	1	Piperidine, 2,4-di(3-pyridinyl)- {pyridine, 3,3′-(2,4-piperidinediyl) bis-, anatalline}		17.11
7093.	766-09-6	1	0	0	Piperidine, 1-ethyl-		17.7
7094.	1484-80-6	1	0	0	Piperidine, 2-ethyl-		17.7
7095.	14300-04-0	1	0	0	Piperidine, 2-ethyl-1-nitroso-		15.8, 17.7
7096.	626-67-5	0	1	0	Piperidine, 1-methyl-		17.7
7097.	109-05-7	1	0	0	Piperidine, 2-methyl-		17.7
7098.	626-56-2	1	0	0	Piperidine, 3-methyl-		17.7
7099.	13603-07-1	1	0	0	Piperidine, 3-methyl-1-nitroso-		15.8, 17.7
7100.	626-58-4	1	0	0	Piperidine, 4-methyl-		17.7
7101.	15104-03-7	1	0	0	Piperidine, 4-methyl-1-nitroso-		15.8, 17.7
7102.	71607-72-2	1	0	0	Piperidine, (1-methylethyl)-		17.7
7103.	100-75-4	1	1	1	Piperidine, 1-nitroso- {NPIP}		15.8, 17.7, 23.5
7104.	62784-01-4	1	0	0	Piperidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-		3.13, 17.11
7105.	96552-69-1	1	0	0	Piperidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-		17.11
7106.	62783-95-3	1	0	0	Piperidine, 1-(1-oxopentyl)-2-(3-pyridinyl)-, (S)-		17.11
7107.	77-10-1	1	0	0	Piperidine, 1-(1-phenylcyclohexyl)-		17.7
7108.		1	0	0	Piperidine, 1-(3-pyridinemethyl)-2-cyano-4,5-didehydro-		11.2, 17.11
7109.		1	0	0	Piperidine, 1-(3-pyridinemethyl)-2-cyano-		11.2, 17.11
7110.	71635-28-4	0	1	0	1-Piperidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)-		3.12, 17.11
7111.	13406-98-9	0	1	0	1-Piperidinecarboxylic acid		4.3, 17.7
7112.	56078-09-2	1	1	1	1-Piperidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)-		5.3, 17.11

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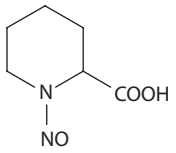
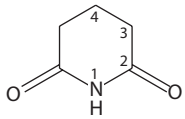
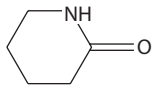
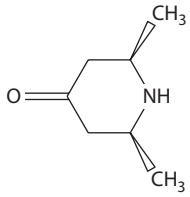
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
7113.		0	1	0	2-Piperidineacetic acid, 1-nitroso- {NPIPAC}		4.3, 15.8, 17.7
7114.	535-75-1	1	1	1	2-Piperidinecarboxylic acid {pipecolic acid}		0.4, 4.3, 17.7
7115.	4515-18-8 30310-81-7	1	1	1	2-Piperidinecarboxylic acid, 1-nitroso- {*N*-nitrosopipecolic acid (NPIC)}		4.3, 15.8, 17.7
7116.	65445-62-7	1	1	1	3-Piperidinecarboxylic acid, 1-nitroso-		4.3, 15.8, 17.7
7117.	6238-69-3	0	1	0	4-Piperidinecarboxylic acid, 1-nitroso-		4.3, 15.8, 17.7
7118.	1121-89-7	1	0	0	2,6-Piperidinedione {glutarimide}		14.1, 17.7
7119.		1	0	0	2,6-Piperidinedione, methoxy-		10.2, 14.1, 17.7
7120.		1	0	0	2,6-Piperidinedione, 3-methoxy-		10.2, 14.1, 17.7
7121.	61892-70-4	1	0	0	2,6-Piperidinedione, 4-methoxy-		10.2, 14.1, 17.7
7122.	72692-70-7	1	0	0	2,6-Piperidinedione, methyl-		14.1, 17.7
7123.	29553-51-3	1	0	0	2,6-Piperidinedione, 3-methyl-		14.1, 17.7
7124.	25077-26-3	1	0	0	2,6-Piperidinedione, 4-methyl-		14.1, 17.7
7125.	27154-43-4	1	0	0	Piperidinone		17.7, 17.13
7126.	675-20-7	1	1	1	2-Piperidinone {5-pentanelactam}		17.7, 17.13
7127.	61891-65-4	1	0	0	2-Piperidinone, methyl-		17.7, 17.13
7128.	931-20-4	1	1	1	2-Piperidinone, 1-methyl-		17.7, 17.13
7129.	4775-98-8	1	0	0	2-Piperidinone, 6-methyl-		17.7, 17.13
7130.	13200-35-6	1	0	0	4-Piperidinone, 2,6-dimethyl-, *cis*-		3.13, 17.7
7131.	69135-98-4	1	0	0	4-Piperidinone, 2,6-dimethyl-, *trans*-		3.13, 17.7
7132.	3311-23-7	1	0	0	4-Piperidinone, 2,2,6-trimethyl-, (R)-		3.13, 17.7
7133.		0	1	0	*Planctomycetes*, *Planctomycetacia*		22.2
7134.	24946-64-3	0	1	0	Plastochromenol {solanachromene isomer}		9.22, 10.2
7135.	3819-09-8	0	1	0	Plastoquinol		9.24
7136.	11005-16-6	0	1	0	Plastoquinone C		9.24
7137.	12778-15-3	0	1	0	Plastoquinone D		9.24
7138.	7440-06-4	0	1	0	Platinum	Pt	20.5
7139.	7647-10-1	0	1	0	Platinum chloride		18.4, 20.6
7140.	13981-16-3	0	1	0	Plutonium, isotope of mass 238	^{238}Pu	20.5
7141.	15117-48-3	1	1	1	Plutonium, isotope of mass 239	^{239}Pu	20.5
7142.	14119-33-6	1	1	1	Plutonium, isotope of mass 240	^{240}Pu	20.5
7143.	7440-08-6	1	1	1	Polonium	Po	20.5
7144.	13981-52-7	1	1	1	Polonium, isotope of mass 210	^{210}Po	20.5, 23.5
7145.	25322-68-3	0	1	0	Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-		2.5
7146.	9032-75-1	0	1	0	Polygalacturonase		22.2

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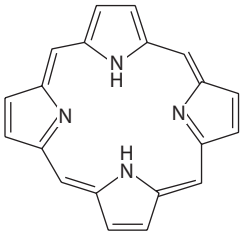
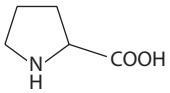
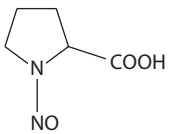
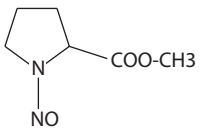
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7147.	152415-56-0	0	1	0	Polygalacturonase (tobacco clone G27.1/G27.2 gene Npg1 precursor reduced)		22.2
7148.	9002-10-2	0	1	0	Polyphenoloxidase {oxygenase, monophenol mono-, tyrosinase}		22.2
7149.		0	1	0	Poly(U)polymerase		22.2
7150.	9030-77-7	0	1	0	Polyprenyltransferase, 4-hydroxybenzoate		22.2
7151.	159965-71-6	0	1	0	Polyubiquitin (*Nicotiana tabacum* clone Ubi.U4 gene Ubi.U4)		22.2
7152.	101-60-0	1	1	1	21*H*,23*H*-Porphine {porphyrin}		17.5
7153.	644-00-8	1	0	0	21*H*,23*H*-Porphine-2-propanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-		4.3, 17.5
7154.	1976-85-8	0	1	0	21*H*,23*H*-Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetrakis (carboxymethyl)-5,10,15,20,22,24-hexahydro-		4.3, 17.5
7155.	9055-40-7	0	1	0	Porphobilinogenase		22.2
7156.	7440-09-7	1	1	1	Potassium	K	0.4, 20.5
7157.	13966-00-2	1	1	1	Potassium, isotope of mass 40	^{40}K	20.5
7158.	14378-21-3	0	1	0	Potassium, isotope of mass 42	^{42}K	20.5
7159.	7447-40-7	1	1	1	Potassium chloride	KCl	18.4, 20.6
7160.	12136-45-7	0	1	0	Potassium oxide	K_2O	20.6
7161.	24203-36-9	1	0	0	Potassium, ion	K^{+1}	20.5
7162.	7w440-10-0	1	1	1	Praseodymium	Pr	20.5
7163.	57-83-0	0	1	0	Pregn-4-ene-3,20-dione		2.7, 3.13
7164.	145-13-1	0	1	0	Pregn-5-en-20-one, 3-hydroxy-, (3β)-		2.5, 2.7, 3.13
7165.	32378-60-2	0	1	0	Pregnan-20-one, 3-[(1-oxohexadecyl) oxy]-, (3β,5α)-		2.7, 3.13
7166.		0	1	0	Proline, hydroxy-		4.3, 4.10
7167.	147-85-3	1	1	1	*L*-Proline		0.4, 4.3, 4.10, 17.4, 24.3, 25.29
7168.		0	1	0	*L*-Proline, *N*-(1-deoxy-*D*-fructos-1-yl)-		1.5, 4.3, 4.10, 17.4, 10.2
7169.	18610-59-8	0	1	0	*L*-Proline, 1-hydroxy-		4.3, 4.10, 17.4, 25.29
7170.	7519-36-0	1	1	1	*L*-Proline, 1-nitroso- {NPRO}		4.3, 4.10, 15.8, 17.4, 25.29
7171.	35909-01-4	1	1	1	*L*-Proline, 1-nitroso-, methyl ester		5.3, 15.8, 17.4

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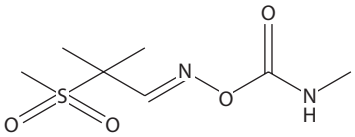
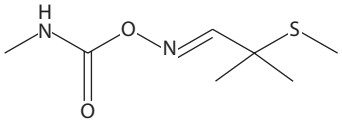
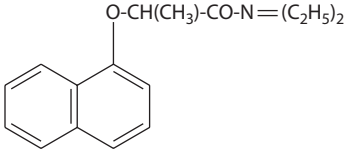
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7172.	147427-29-0	0	1	0	*L*-Proline, 1-[1-[1-(1-*L*-seryl-*L*-prolyl)-*L*-prolyl]-*L*-prolyl]-		4.3, 4.10, 17.4, 17.5
7173.	62137-28-4	0	1	0	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl) oxy]-, *trans*-		2.5, 4.3, 4.10, 8.3, 10.2, 17.4
7174.	62137-29-5	0	1	0	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-		2.5, 4.3, 4.10, 8.3, 10.2, 17.4
7175.	51-35-4	0	1	0	*L*-Proline, 4-hydroxy-, *trans*-		2.5, 4.3, 4.10, 17.4
7176.	30310-80-6	0	1	0	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}		2.5, 4.3, 4.10, 17.4
7177.	463-49-0	1	0	0	1,2-Propadiene {allene}	$H_2C{=}C{=}CH_2$	1.11
7178.	123-38-6	1	1	1	Propanal {propionaldehyde}	$H_3C\text{-}CH_2\text{-}CH{=}O$	3.12, 23.5
7179.	630-19-3	1	0	0	Propanal, 2,2-dimethyl- {pivalaldehyde}	$(H_3C)_3{\equiv}C\text{-}CH{=}O$	3.12
7180.	367-47-5	1	1	1	Propanal, 2,3-dihydroxy- {glyceraldehyde}	$HOCH_2\text{-}CH_2OH\text{-}CH{=}O$	2.5, 3.12
7181.	142-10-9	0	1	0	Propanal, 2,3-dihydroxy-, 3-phosphate		2.5, 5.3, 3.12
7182.	2134-29-4	1	0	0	Propanal, 3-hydroxy-		2.5, 3.12
7183.	78-84-2	1	1	1	Propanal, 2-methyl- {isobutyraldehyde}	$(H_3C)_2{=}CH\text{-}CH{=}O$	3.12, 24.3, 25.29
7184.	1646-87-3	0	1	0	Propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb Sulfoxide®}		18.1, 21.3
7185.	1646-88-4	0	1	0	Propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino)carbonyl]oxime {Aldoxycarb®}		18.1, 21.3, 25.29
7186.	116-06-3	0	1	0	Propanal, 2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb®}		18.1, 21.3, 25.29
7187.	85502-23-4	0	1	0	Propanal, 3-(nitrosomethylamino)-	$H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}CHO$	3.12, 12.2, 15.8
7188.	78-98-8	1	1	1	Propanal, 2-oxo- {pyruvaldehyde, methylglyoxal}	$H_3C\text{-}CO\text{-}CH{=}O$	0.4, 3.12, 3.13
7189.	997-10-4	0	1	0	Propanal, 2-oxo-3-hydroxy- {reductone}	$HOCH_2\text{-}CO\text{-}CH{=}O$	2.5, 3.12, 3.13
7190.	3268-49-3	1	1	1	Propanal, 3-(methylthio)- {methional}		3.12, 18.1 24.3, 25.29
7191.	79-05-0	1	0	0	Propanamide	$H_3C\text{-}CH_2\text{-}CO\text{-}NH_2$	13.1
7192.	7324-05-2	0	1	0	Propanamide, 2-amino-, (S)-	$H_3C\text{-}CH(NH_2)\text{-}CO\text{-}NH_2$	12.2, 13.1
7193.	563-83-7	1	0	0	Propanamide, 2-methyl-	$(H_3C)_2{=}CH\text{-}CO\text{-}NH_2$	13.1
7194.	631-66-3	1	0	0	Propanamide, 2-oxo- {pyruvamide}	$H_3C\text{-}CO\text{-}CO\text{-}NH_2$	3.13, 13.1
7195.	61892-68-0	1	0	0	Propanamide, 3-cyano-	$NC\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}NH_2$	11.2, 13.1
7196.	15299-99-7	0	1	0	Propanamide, diethyl-2-(1-naphthyloxy)- {Devrinol®, Napropamide®}		13.1, 21.3
7197.	2675-88-9	1	0	0	Propanamide, *N*,2-dimethyl-	$H_3C\text{-}CH(CH_3)\text{-}CO\text{-}NH\text{-}CH_3$	13.1

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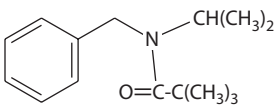
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7198.	35256-85-0	0	1	0	Propanamide, dimethyl-*N*-(1-methylethyl)-*N*-(phenylmethyl) {Butam®}		13.1, 21.3
7199.	5129-72-6	1	0	0	Propanamide, *N*-ethyl-	H_3C-CH_2-CO-NH-CH_2-CH_3	13.1
7200.	1187-58-2	1	0	0	Propanamide, *N*-methyl-	H_3C-CH_2-CO-NH-CH_3	13.1
7201.	25457-49-2	1	0	0	Propanamide, *N*-methyl-*N*-(1-oxopropyl)-		13.1
7202.		1	0	0	Propanamide, *N*-(2-methylpyridyl)-		13.1, 17.7
7203.	107-10-8	1	1	1	1-Propanamine	H_3C-$(CH_2)_2$-NH_2	12.2
7204.	5813-64-9	1	0	0	1-Propanamine, 2,2-dimethyl-	H_3C-$C(CH_3)_2CH_2$-NH_2	12.2
7205.	625-43-4	1	1	1	1-Propanamine, *N*,2-dimethyl-	H_3C-CH(CH3)CH_2-NH-CH_3	12.2
7206.	34419-76-6 2504-18-9	1	1	1	1-Propanamine, *N*,2-dimethyl-*N*-nitroso-	H_3C-$CH(CH_3)CH_2$-N(NO)-CH_3	12.2, 15.8
7207.	20193-20-8	1	1	1	1-Propanamine, *N*-ethyl-		12.2
7208.	71607-99-3	1	1	1	1-Propanamine, *N*-ethyl-2-methyl-*N*-nitroso-	H_3C-$CH(CH_3)CH_2$-N(NO)-CH_2CH_3	12.2, 15.8
7209.	25413-61-0	1	1	1	1-Propanamine, *N*-ethyl-*N*-nitroso-	H_3C-$(CH_2)_2$-N(NO)-CH_2CH_3	12.2, 15.8
7210.	627-35-0	1	1	1	1-Propanamine, *N*-methyl-	H_3C-$(CH_2)_2$-NH-CH_3	12.2
7211.	78-81-9	1	1	1	1-Propanamine, 2-methyl-	$(H_3C)_2$=CH-CH_2-NH_2	12.2
7212.		1	0	0	1-Propanamine, 2-methyl-*N*-butyl-	$(H_3C)_2$=CH-CH_2-NH-$(CH_2)_3$-CH_3	12.2
7213.		1	0	0	1-Propanamine, 2-methyl-, *N*-(2-methylpropyl)-*N*-nitroso-		12.2, 15.8
7214.	22023-64-9	1	0	0	1-Propanamine, *N*-(1-methylethylidene)-	H_3C-$(CH_2)_2$-NH-$C(CH_3)$=CH_2	12.2
7215.	924-46-9	1	1	1	1-Propanamine, *N*-methyl-*N*-nitroso- {NMPA}	H_3C-$(CH_2)_2$-N(NO)-CH_3	12.2, 15.8
7216.	3405-42-3	1	0	0	1-Propanamine, *N*-methyl-*N*-propyl-	$(H_3C$-$CH_2CH_2)_2$=N-CH_3	12.2
7217.	621-64-7	1	1	1	1-Propanamine, *N*-nitroso-*N*-propyl- {NDPA}	$(H_3C$-$CH_2CH_2)_2$=N-NO	12.2, 15.8, 23.5
7218.	142-84-7	1	1	1	1-Propanamine, *N*-propyl-	$(H_3C$-$CH_2CH_2)_2$=NH	12.2
7219.	7239-24-9	0	1	0	1-Propanamine, *N*,*N*,2-trimethyl-	$(H_3C)_2$=CH-CH_2-N=$(CH_3)_2$	12.2
7220.	75-31-0	1	1	1	2-Propanamine	$(H_3C)_2$=CH-NH_2	12.2
7221.	75-64-9	1	1	1	2-Propanamine, 2-methyl-	$(H_3C)_3$≡C-NH_2	12.2
7222.	7515-80-2	1	0	0	2-Propanamine, 2-methyl-*N*-(1-methylethyl)-	$(H_3C)_3$≡C-NH-$CH(CH_3)_2$	12.2
7223.	3376-24-7	1	0	0	2-Propanamine, 2-methyl-*N*-(phenylmethylene)-, *N*-oxide		12.2
7224.		1	0	0	2-Propanamine, *N*-(2,2-dimethylethyl)-		12.2
7225.	4747-21-1	1	1	1	2-Propanamine, *N*-methyl-	$(H_3C)_2$=CH-NH-CH_3	12.2
7226.	16339-04-1	1	0	0	2-Propanamine, *N*-methyl-*N*-nitroso-		12.2, 15.8
7227.	108-18-9	1	0	0	2-Propanamine, *N*-(1-methylethyl)-	$(H_3C)_2$=CH-NH-CH=$(CH_3)_2$	12.2
7228.	601-77-4	1	0	0	2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso-	$[(H_3C)_2$=CH$]_2$-N-NO	12.2, 15.8
7229.	3332-08-9	1	0	0	2-Propanamine, *N*-(1-methylethylidene)-		12.2
7230.		1	0	0	2-Propanamine, *N*-(2-methylpropyl)-		12.2
7231.	21968-17-2	1	1	1	2-Propanamine, *N*-propyl- = 1-propanamine, *N*-(1-methylethyl)-	H_3C-$(CH_2)_2$-NH-CH=$(CH_3)_2$	12.2
7232.	74-98-6	1	0	0	Propane	H_3C-CH_2-CH_3	1.10
7233.	96-12-8	0	1	0	Propane, 1,2-dibromo-3-chloro- {DBCP®}		18.4, 21.3
7234.	78-87-5	0	1	0	Propane, 1,2-dichloro-		18.4, 21.3
7235.	142-28-9	0	1	0	Propane, 1,3-dichloro-		18.4, 21.3
7236.	4110-50-3	1	0	0	Propane, 1-(ethylthio)-	H_3C-$(CH_2)_2$-S-CH_2-CH_3	18.1
7237.	3877-15-4	1	0	0	Propane, 1-(methylthio)-	H_3C-$(CH_2)_2$-S-CH_3	18.1

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7238.	505-84-0	1	0	0	Propane, 1,1′-[methylenebis(oxy)]bis- {dipropoxymethane}	$(C_3H_7O)_2{=}CH_2$	10.2
7239.	76-19-7	0	1	0	Propane, octafluoro- {Freon® 218, Perfluoropropane}	$CF_3CF_2CF_3$	18.4
7240.	111-43-3	1	0	0	Propane, 1,1′-oxybis- {dipropyl ether}	$[H_3C\text{-}(CH_2)_2]_2{=}O$	10.2
7241.	111-47-7	1	0	0	Propane, 1,1′-thiobis- {dipropyl sulfide}	$[H_3C\text{-}(CH_2)_2]_2{=}S$	18.1
7242.	592-65-4	1	0	0	Propane, 1,1′-thiobis[2-methyl- {diisobutyl sulfide}	$[(H_3C)_2{=}(CH)_2]_2{=}S$	18.1
7243.	108-03-2	1	0	0	Propane, 1-nitro-	$H_3C\text{-}(CH_2)_2\text{-}NO_2$	16.1
7244.	7778-85-0	1	0	0	Propane, 1,2-dimethoxy-		10.2
7245.	77-76-9	1	0	0	Propane, 2,2-dimethoxy-		10.2
7246.	75-28-5	1	0	0	Propane, 2-methyl- {isobutane}	$(H_3C)_2{=}CH\text{-}CH_3$	1.10
7247.	79-46-9	1	0	0	Propane, 2-nitro-	$(H_3C)_2{=}CH\text{-}NO_2$	16.1, 23.5
7248.	542-78-9	1	0	0	Propanedial	$H_2C{=}(CH{=}O)_2$	3.12
7249.	4464-20-4	1	0	0	Propanedial, dihydroxy-	$(HO)_2{=}C{=}(CH{=}O)_2$	2.5, 3.12
7250.	497-16-5	1	0	0	Propanedial, oxo-	$O{=}C{=}(CH{=}O)_2$	3.12, 3.13
7251.	56-18-8	1	0	0	1,3-Propanediamine, *N*-(3-aminopropyl)- {norspermidine}		12.2
7252.	141-82-2	1	1	1	Propanedioic acid {malonic acid}	$H_2C{=}(COOH)_2$	0.4, 4.3
7253.	105-53-3	0	1	0	Propanedioic acid, diethyl ester		5.3
7254.	108-59-8	0	1	0	Propanedioic acid, dimethyl ester	$H_2C{=}(COO\text{-}CH_3)_2$	5.3
7255.	80-69-3	1	1	1	Propanedioic acid, hydroxy-	$HO\text{-}CH{=}(COOH)_2$	2.5, 4.3
7256.	516-05-2	0	1	0	Propanedioic acid, methyl-	$H_3C\text{-}CH{=}(COOH)_2$	4.3
7257.	607-81-8	1	0	0	Propanedioic acid, (phenylmethyl)-, diethyl ester		5.3
7258.	57-55-6	1	1	1	1,2-Propanediol {propylene glycol}	$H_3C\text{-}CHOH\text{-}CH_2OH$	2.5, 24.3, 25.29
7259.	627-69-0	1	1	1	1,2-Propanediol, 1-acetate	$H_3C\text{-}CHOH\text{-}CH_2\text{-}OOC\text{-}CH_3$	2.5, 5.3
7260.	6214-01-3	1	1	1	1,2-Propanediol, 2-acetate	$H_3C\text{-}CH(OOC\text{-}CH_3)\text{-}CH_2OH$	2.5, 5.3
7261.	96-24-2	1	0	0	1,2-Propanediol, 3-chloro-	$Cl\text{-}CH_2\text{-}CHOH\text{-}CH_2OH$	2.5, 18.4
7262.	10602-14-9	0	1	0	1,2-Propanediol, 1-(dihydrogen phosphate)		2.5, 5.3
7263.	20390-21-0	1	0	0	1,2-Propanediol, 3-(furfuryloxy)-		2.5, 10.2
7264.	115888-33-0	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8, 8a-octahydro-8,8a-dimethyl- 2-naphthalenyl)-, [2S-[2α(S*),8α,8aβ]]-		2.5
7265.	99694-82-3	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8, 8a-octahydro-8,8a-dimethyl- 2-naphthalenyl)-, [2R-[2α(S*),8β,8aα]]-		2.5
7266.	115788-21-1	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8, 8a-octahydro- 3-hydroxy-8,8a-dimethyl- 2-naphthalenyl)-, [2S-[2α(S*),3α,8β,8aα]]-		2.5
7267.	115788-20-0	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8, 8a-octahydro-5-hydroxy-8, 8a-dimethyl-2-naphthalenyl)-, [2R-[2α(R*),5α,8.		2.5
7268.	54541-18-3	1	0	0	1,2-Propanediol, 2-propanoate		2.5, 5.3
7269.	504-63-2	1	1	1	1,3-Propanediol {trimethylene glycol}	$HOCH_2\text{-}CH_2\text{-}CH_2OH$	2.5
7270.	126-30-7	1	0	0	1,3-Propanediol, 2,2-dimethyl-		2.5
7271.	1438-92-2	1	1	1	1,2-Propanedione, 1-(2-furanyl)-		3.13, 10.2

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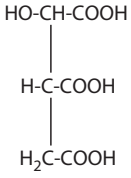
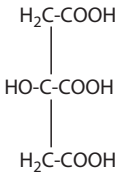
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7272.	2034-60-8	0	1	0	1,2-Propanedione, 1-(4-hydroxy-3-methoxyphenyl)-		3.13, 9.22, 10.2
7273.	1197-20-2	1	1	1	1,2-Propanedione,1-(5-methyl-2-furanyl)-		3.13, 10.2
7274.	579-07-7	1	0	0	1,2-Propanedione, 1-phenyl-		3.13
7275.	107-12-0	1	1	1	Propanenitrile	$H_3C\text{-}CH_2\text{-}CN$	11.2
7276.	78-97-7	1	0	0	Propanenitrile, 2-hydroxy-	$H_3C\text{-}CHOH\text{-}CN$	2.5, 11.2
7277.	75-86-5	1	0	0	Propanenitrile, 2-hydroxy-2-methyl-	$(H_3C)_2{=}COH\text{-}CN$	2.5, 11.2
7278.	78-82-0	1	1	1	Propanenitrile, 2-methyl- {isobutyronitrile}	$(H_3C)_2{=}CH\text{-}CN$	11.2
7279.	78-67-1	0	1	0	Propanenitrile, 2-methyl-, 2,2′-azobis- {Porofor-57®}		11.2
7280.	631-57-2	1	0	0	Propanenitrile, 2-oxo-	$H_3C\text{-}CO\text{-}CN$	3.13, 11.2
7281.	60153-49-3	1	1	1	Propanenitrile, 3-(methylnitrosoamino)- {MNPN}	$H_3C\text{-}N(NO)\text{-}(CH_2)_2\text{-}CN$	11.2, 12.2, 15.8
7282.	1738-25-6	1	0	0	Propanenitrile, 3-(dimethylamino)-		11.2, 12.2
7283.	111-97-7	1	0	0	Propanenitrile, 3,3′-thiobis-		11.2, 18.1
7284.	107-03-9	1	0	0	1-Propanethiol {propyl mercaptan}		18.1
7285.	513-44-0	1	0	0	1-Propanethiol, 2-methyl- {isobutyl mercaptan}		18.1
7286.	75-33-2	1	0	0	2-Propanethiol {isopropyl mercaptan}		18.1
7287.	99-14-3	0	1	0	1,2,3-Propanetricarboxylic acid		4.3
7288.	30810-51-6	0	1	0	1,2,3-Propanetricarboxylicacid,1-hydroxy- {isocitric acid}		2.5, 4.3
7289.	77-92-9	1	1	1	1,2,3-Propanetricarboxylicacid, 2-hydroxy- {citric acid}		0.4, 2.5, 4.3, 24.3, 25.29
7290.	58308-53-5	0	1	0	1,2,3-Propanetricarboxylic-1,3-$^{14}C_2$ acid, 2-hydroxy-, labeled with ^{14}C {citric acid-^{14}C}		2.5, 4.3, 25.29
7291.	813-94-5	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, calcium salt		0.4, 2.5, 20.6
7292.	3609-96-9	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, dipotassium salt		2.5, 20.6
7293.	3344-18-1	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, magnesium salt		0.4, 2.5, 20.6
7294.		1	0	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monomethyl ester		2.5, 5.3
7295.	18996-35-5	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monosodium salt		2.5, 20.6
7296.	68-04-2	1	1	1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, sodium salt		2.5, 20.6
7297.	77-93-0	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester {triethyl citrate}		2.5, 5.3, 24.3, 25.29
7298.	866-84-2	1	1	1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripotassium salt		2.5, 20.6

(*continued*)

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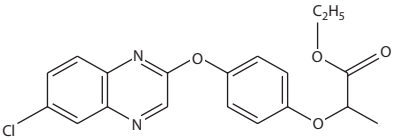
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7299.	6100-05-6	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripotassium salt, monohydrate		0.4, 2.5, 20.6
7300.	56-81-5	1	1	1	1,2,3-Propanetriol {glycerol}	$HOCH_2$-CHOH-CH_2OH	0.4, 2.5, 24.3, 25.29
7301.	63346-81-6	1	1	1	1,2,3-Propanetriol, labeled with ^{13}C {glycerol-^{13}C}		2.5, 25.29
7302.	4254-13-1	1	1	1	1,2,3-Propanetriol, labeled with ^{14}C {glycerol-^{14}C}		2.5, 25.29
7303.	61892-59-9	1	0	0	1,2,3-Propanetriol, 1-acetate 2-formate		2.5, 5.3
7304.	25395-31-7	1	1	1	1,2,3-Propanetriol, diacetate {diacetin}		2.5, 5.3
7305.	29860-16-0	1	1	1	1,2,3-Propanetriol, 1,2-diacetate {1,2-diacetin}		2.5, 5.3
7306.	105-70-4	1	1	1	1,2,3-Propanetriol, 1,3-diacetate {1,3-diacetin}		2.5, 5.3
7307.	57-03-4	0	1	0	1,2,3-Propanetriol, 1-(dihydrogen phosphate)		2.5, 5.3
7308.	927-20-8	0	1	0	1,2,3-Propanetriol, 1-(dihydrogen phosphate), magnesium salt (1:1)		2.5, 5.3, 20.6
7309.	17603-42-8	0	1	0	1,2,3-Propanetriol, 1-(dihydrogen phosphate), sodium salt		2.5, 5.3, 20.6
7310.	1335-34-8	0	1	0	1,2,3-Propanetriol, mono(dihydrogen phosphate), potassium salt		2.5, 5.3, 20.6
7311.	106-61-6 26446-35-5	1	1	1	1,2,3-Propanetriol, monoacetate {monoacetin}		2.5, 5.3
7312.	72692-68-3	1	0	0	1,2,3-Propanetriol, monoformate		2.5, 5.3
7313.		0	1	0	1,2,3-Propanetriol, phosphatidyl-		2.5
7314.	11046-98-3	1	0	0	1,2,3-Propanetriol, propanoate		2.5, 5.3
7315.	62244-24-0	1	0	0	1,2,3-Propanetriol, 1-propanoate, (R)-		2.5, 5.3
7316.	102-76-1	1	1	1	1,2,3-Propanetriol, triacetate {triacetin}		5.3
7317.	555-44-2	0	1	0	1,2,3-Propanetriol, trihexadecanoate {tripalmitin}		5.3
7318.	537-40-6	0	1	0	1,2,3-Propanetriol, tri-9,12-octadecadienoate {trilinolein}		5.3
7319.	68334-00-9	0	1	0	1,2,3-Propanetriol, trioctadecanoate {tristearin}		5.3
7320.	122-32-7	0	1	0	1,2,3-Propanetriol, tri-9-octadecenoate {triolein}		5.3
7321.	139-45-7	1	0	0	1,2,3-Propanetriol, tripropanoate		5.3
7322.	555-45-3	0	1	0	1,2,3-Propanetriol, tritetradecanoate {trimyristin}		5.3
7323.	79-09-4	1	1	1	Propanoic acid {propionic acid}	H_3C-CH_2 OOH	4.3, 24.3, 25.29
7324.	137-40-6	0	1	0	Propanoic acid, sodium salt		20.6
7325.	590-01-2	0	1	0	Propanoic acid, butyl ester		5.3
7326.	62-57-7	0	1	0	Propanoic acid, 2-amino-2-methyl-		4.3, 12.2
7327.	76578-14-8	0	1	0	Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester {Quizalofop-Et®}		5.3, 18.4, 21.3
7328.	75-98-9	0	1	0	Propanoic acid, 2,2-dimethyl- {pivalic acid}	$(H_3C)_3$≡C-COOH	4.3
7329.	473-81-4	1	1	1	Propanoic acid, 2,3-dihydroxy- {glyceric acid}	$HOCH_2$-CHOH-COOH	2.5, 4.3
7330.	6000-40-4	0	1	0	Propanoic acid, 2,3-dihydroxy-, (R)-		2.5, 4.3

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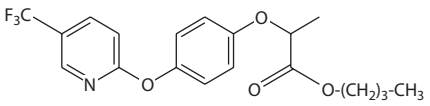
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7331.	65644-56-6	0	1	0	Propanoic acid, 2,3-dihydroxy-, calcium salt		2.5, 20.6
7332.	82546-67-6	1	0	0	Propanoic acid, 3-(ethoxycarbonyl)-3-(1-cyclohexenenyl)-		4.3
7333.	50-21-5 598-82-3	1	1	1	Propanoic acid, 2-hydroxy- {lactic acid}	H_3C-CHOH-COOH	0.4, 2.5, 4.3, 24.3, 25.29
7334.	138-22-7	1	0	0	Propanoic acid, 2-hydroxy-, butyl ester {butyl lactate}		2.5, 5.3
7335.	97-73-4	0	1	0	Propanoic acid, 2-hydroxy-, anhydride		2.5, 7.1
7336.	97-64-3	1	1	1	Propanoic acid, 2-hydroxy-, ethyl ester {ethyl lactate}	H_3C-CHOH-COO-C_2H_5	2.5, 5.3, 24.3, 25.29
7337.	547-64-8	1	0	0	Propanoic acid, 2-hydroxy-, methyl ester	H_3C-CHOH-COO-CH_3	2.5, 5.3
7338.	16595-31-6	0	1	0	Propanoic acid, 2-hydroxy-, sodium salt {sodium lactate}	H_3C-CHOH-COO-Na	2.5, 20.6
7339.	16039-53-5	0	1	0	Propanoic acid, 2-hydroxy-, zinc salt		2.5, 20.6
7340.	594-61-6	0	1	0	Propanoic acid, 2-hydroxy-2-methyl-	$(H_3C)_2$=COH-COOH	2.5, 4.3
7341.	820-11-1	0	1	0	Propanoic acid, 2-hydroxy-3-(phosphonooxy)-		2.5, 4.3
7342.	72-17-3	0	1	0	Propanoic acid, 2-hydroxy-, sodium salt		20.6
7343.	79-31-2	1	1	1	Propanoic acid, 2-methyl- {isobutyric acid}	$(H_3C)_2$=CH-COOH	4.3, 24.3
7344.	97-89-2	0	1	0	Propanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester		5.3
7345.	97-62-1	0	1	0	Propanoic acid, 2-methyl-, ethyl ester		5.3
7346.	37704-28-2	0	1	0	Propanoic acid, 2-methyl-, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-3-cyclohexen-1-yl ester		5.3
7347.	547-63-7	0	1	0	Propanoic acid, 2-methyl-, methyl ester	$(H_3C)_2$=CH-COO-CH_3	5.3
7348.	2445-69-4	0	1	0	Propanoic acid, 2-methyl-, 2-methylbutyl ester		5.3
7349.	2050-01-3	0	1	0	Propanoic acid, 2-methyl-, 3-methylbutyl ester		5.3
7350.	65416-14-0	0	1	0	Propanoic acid, 2-methyl-, 2-methyl-4-oxo-4*H*-pyran-3-yl ester		5.3, 10.2
7351.	103-93-5	0	1	0	Propanoic acid, 2-methyl-, 4-methylphenyl ester {*p*-tolyl isobutyrate}		5.3
7352.	109-15-9	0	1	0	Propanoic acid, 2-methyl-, octyl ester		5.3
7353.	103-48-0	0	1	0	Propanoic acid, 2-methyl-, phenylethyl ester		5.3
7354.	103-28-6	1	1	1	Propanoic acid, 2-methyl-, phenylmethyl ester {benzyl isobutyrate}		5.3, 24.3
7355.	103-59-3	0	1	0	Propanoic acid, 2-methyl-, 3-phenyl-2-propen-1-yl ester		5.3
7356.		0	1	0	Propanoic acid, 2-methylbutyl ester		5.3
7357.	127-17-3	1	1	1	Propanoic acid, 2-oxo- {pyruvic acid}	H_3C-CO-COOH	3.13, 4.3, 24.3
7358.	617-35-6	1	0	0	Propanoic acid, 2-oxo-, ethyl ester	H_3C-CO-COO-C_2H_5	3.13, 5.3
7359.	600-22-6	1	1	1	Propanoic acid, 2-oxo-, methyl ester	H_3C-CO-COO-CH_3	3.13, 5.3
7360.	4151-33-1	0	1	0	Propanoic acid, 2-oxo-, potassium salt		3.13, 20.6
7361.	3913-50-6	0	1	0	Propanoic acid, 2-oxo-3-(phosphonooxy)-		3.13, 4.3
7362.	69806-50-4	0	1	0	Propanoic acid, 2-(4-(5-trifluoromethyl-2-pyridyloxy)phenoxy)-, butyl ester {Fluazifop-butyl®}		10.2, 18.4, 21.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7363.	4272-12-2	1	0	0	Propanoic acid, 3-(acetyloxy)-	H_3C-COO-$(CH_2)_2$-COOH	4.3, 5.3
7364.	503-66-2	1	1	1	Propanoic acid, 3-hydroxy-	HO-$(CH_2)_2$-COOH	2.5, 4.3
7365.	4835-90-9	0	1	0	Propanoic acid, 3-hydroxy-2,2-dimethyl- {hydroxypivalic acid}	HOH_2C-C$(CH_3)_2$-COOH	2.5, 4.3
7366.	80657-57-4	1	0	0	Propanoic acid, 3-hydroxy-2-methyl-, methyl ester		2.5, 5.3
7367.		1	0	0	Propanoic acid, 3-hydroxyphenyl-		4.3, 9.22
7368.	935-13-7	1	0	0	Propanoic acid, 3-(2-furanyl)-		4.3, 10.2
7369.	1456-08-2	1	0	0	Propanoic acid, 3-(5-methyl-2-furanyl)-		4.3, 10.2
7370.		1	0	0	Propanoic acid, 3-hydroxy-, 2-methylamino-, propyl ester		2.5, 5.3, 12.2
7371.	2553-59-5	0	1	0	Propanoic acid, 3-hydroxy-2-(phosphonooxy)-		2.5, 4.3
7372.	1113-60-6	0	1	0	Propanoic acid, 3-hydroxy-2-oxo-	HOH_2C-CO-COOH	2.5, 3.13, 4.3
7373.	2544-06-1	0	1	0	Propanoic acid, 3-methoxy-		4.3, 10.2
7374.	105-68-0	0	1	0	Propanoic acid, 3-methylbutyl ester		5.3
	10478-42-9	0	0	0	Propanoic acid, 3-(methylnitrosoamino)-; see β-alanine, *N*-methyl-*N*-nitroso- {NMPA}	H_3C-N(NO)-$(CH_2)_2$-COOH	4.3, 4.10, 12.2, 15.8, 25.29
7375.	13532-18-8	0	1	0	Propanoic acid, 3-(methylthio)-, methyl ester	H_3C-S-$(CH_2)_2$-COO-CH_3	5.3, 18.1
7376.	103-56-0	1	1	1	Propanoic acid, 3-phenyl-2-propenyl ester {cinnamyl propionate}		5.3
7377.	105-38-4	0	1	0	Propanoic acid, ethenyl ester	H_3C-CH_2-COO-CH═CH_2	5.3
7378.	105-37-3	1	1	1	Propanoic acid, ethyl ester {ethyl propionate}	H_3C-CH_2-COO-C_2H_5	5.3, 24.3, 25.29
7379.	554-12-1	1	1	1	Propanoic acid, methyl ester	H_3C-CH_2-COO-CH_3	5.3
7380.	122-63-4	0	1	0	Propanoic acid, phenylmethyl ester {benzyl propionate}		5.3
7381.	71-23-8	1	1	1	1-Propanol	H_3C-CH_2-CH_2OH	2.5
7382.	110053-58-2	1	0	0	1-Propanol, 2,2-bis(1-hydroxypropoxy)-	$HOCH_2$-C(CH_3)═$(OCH_2CH_2CH_2OH)_2$	2.5, 10.2
7383.	78-83-1	1	1	1	1-Propanol, 2-methyl- {isobutyl alcohol}	$(H_3C)_2$═CH-CH_2OH	2.5, 24.3, 25.29
7384.	108-61-2	1	0	0	1-Propanol, 2,2′-oxybis-		2.5, 10.2
7385.	2396-61-4	1	0	0	1-Propanol, 3,3′-oxybis-		2.5, 10.2
7386.	67-63-0	1	1	1	2-Propanol		2.5
7387.	110053-57-1	1	0	0	2-Propanol, 1,1-bis(2-hydroxypropoxy)-	CH_3-CHOH-CH═$(OCH_2CHOHCH_3)_2$	2.5, 10.2
7388.	110-98-5	1	0	0	2-Propanol, 1,1′-oxybis-	O═$(CH_2$-CHOH-$CH_3)_2$	2.5, 10.2
7389.	127-00-4	1	0	0	2-Propanol, 1-chloro-		2.5, 18.4
7390.		0	1	0	2-Propanol, 2-(2-ethyl-1,3-dimethylcyclopenten-2-yl)-		2.5
7391.	107-98-2	0	1	0	2-Propanol, 1-methoxy-		2.5, 10.2
7392.	75-65-0	1	1	1	2-Propanol, 2-methyl- {*tert*-butanol}	$(H_3C)_3$≡C-OH	2.5, 26.9
7393.		1	0	0	1-Propanone,1-(dimethylhydroxyphenyl)-		3.13, 9.22
7394.		1	0	0	1-Propanone, 1-(3,5-dimethyl-4-hydroxyphenyl)-		3.13, 9.22
7395.	3194-15-8	1	0	0	1-Propanone, 1-(2-furanyl)-		3.13, 10.2
7396.		1	0	0	1-Propanone, 1-(3-furanyl)-		3.13, 10.2
7397.	610-99-1	1	0	0	1-Propanone, 1-(2-hydroxyphenyl)-		3.13, 9.22
7398.		1	0	0	1-Propanone, 1-(3-hydroxyphenyl)-		3.13, 9.22
7399.		1	0	0	1-Propanone, 1-(2-methylphenyl)-		3.13
7400.	51772-30-6	1	0	0	1-Propanone, 1-(3-methylphenyl)-		3.13
7401.	5337-93-9	1	0	0	1-Propanone, 1-(4-methylphenyl)-		3.13
7402.		1	0	0	1-Propanone, 1-(4-methyl-2-pyridinyl)-		3.13, 17.7

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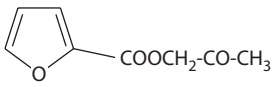
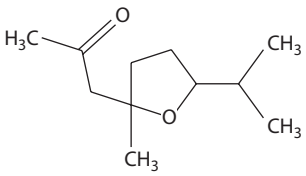
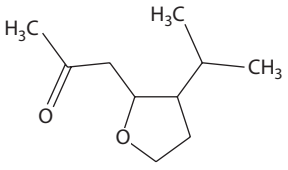
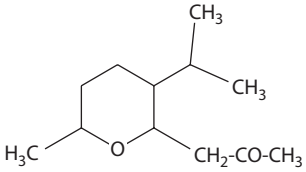
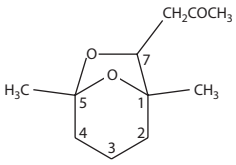
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7403.	93-55-0	1	1	1	1-Propanone, 1-phenyl- {propiophenone}	C_6H_5-CO-CH_2-CH_3	3.13
7404.	1321-48-8	1	0	0	1-Propanone, 1-phenyl-3-hydroxy-		2.5, 3.13
7405.	3238-55-9	1	0	0	1-Propanone, 1-(2-pyridinyl)-		3.13, 17.7
7406.		1	0	0	1-Propanone, 1-(2-pyridinyl)-2-methyl-		3.13, 17.7
7407.	1570-48-5	1	1	1	1-Propanone, 1-(3-pyridinyl)- {pyridyl ethyl ketone}		0.4, 3.13, 17.7
7408.	1701-69-5	1	0	0	1-Propanone, 1-(4-pyridinyl)-		3.13, 17.7
7409.	1073-26-3	1	1	1	1-Propanone, 1-(1*H*-pyrrol-2-yl)-		3.13, 17.4
7410.	80933-75-1	0	1	0	1-Propanone, 1-[2-(3,4,5,6-tetrahydropyridinyl)]-		3.13, 17.7
7411.	67-64-1	1	1	1	2-Propanone {acetone}	H_3C-CO-CH_3	0.4, 3.13, 23.5
7412.	127-06-0	1	0	0	2-Propanone oxime {acetoxime}	$(H_3C)_2$-C═N-OH	16.1
7413.	592-20-1	1	1	1	2-Propanone, 1-(acetyloxy)-	H_3C-CO-CH_2-OOC-CH_3	3.13, 5.3
7414.	298-08-8	1	0	0	2-Propanone, 1-amino-	H_3C-CO-CH_2-NH_2	3.13, 12.2
7415.	78-95-5	1	0	0	2-Propanone, 1-chloro-	H_3C-CO-CH_2-Cl	3.13, 18.4
7416.	10258-70-5	0	1	0	2-Propanone, 1-(formyloxy)-	H_3C-CO-CH_2-OOC-H	3.13, 5.3
7417.	116-09-6	1	1	1	2-Propanone, 1-hydroxy- {acetol}	H_3C-CO-CH_2-OH	2.5, 3.13
7418.		1	0	0	2-Propanone, 1-hydroxy-, 2-furoyl ester		3.13, 5.3, 10.2
7419.	57-04-5	0	1	0	2-Propanone, 1-hydroxy-3-(phosphonooxy)-		2.5, 3.13
7420.	122-84-9	0	1	0	2-Propanone, 1-(4-methoxyphenyl)-		3.13, 10.2
7421.	496-49-1	0	1	0	2-Propanone, 1-(1-methyl-2-pyrrolidinyl)-		3.13, 17.4
7422.	103-79-7	1	1	1	2-Propanone, 1-phenyl-		3.13
7423.	20194-70-1	1	1	1	2-Propanone,1-(tetrahydro-4-methyl-2*H*-pyran-2-yl)-		3.13, 10.2
7424.		0	1	0	2-Propanone, 1-[tetrahydro-(2-methyl-5-methylethyl)-2-furanyl]-		3.13, 10.2
7425.	38713-24-5	0	1	0	2-Propanone, 1-[tetrahydro-3-(1-methylethyl)-2-furanyl]-, *trans*-		3.13, 10.2
7426.	39815-69-5	1	1	1	2-Propanone, 1-[tetrahydro-4-(1-methylethyl)-2-furanyl]-		3.13, 10.2
7427.	39815-68-4	1	1	1	2-Propanone, 1-[tetrahydro-6-methyl-3-(1-methylethyl)-2*H*-pyran-2-yl]- {two isomers reported}		3.13, 10.2
7428.		0	1	0	2-Propanone, 1-[tetrahydro-6-methyl-4-(1-methylethyl)-2*H*-pyran-2-yl]-		3.13, 10.2

(*continued*)

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7429.		0	1	0	2-Propanone, 1-(1,5-dimethyl-6,8-dioxabicyclo[3.2.1]oct-7-yl)-		3.13, 10.2
7430.	6975-60-6	1	1	1	2-Propanone, 1-(2-furanyl)-		3.13, 10.2
7431.		0	1	0	2-Propanone, 1-[2-hydroxy-5-(1-methylethyl)-2-methyl-1-cyclopentyl]-		2.5, 3.13
7432.	13100-05-5	1	0	0	2-Propanone, 1-(2-hydroxyphenyl)-		3.13, 9.22
7433.	5211-62-1	1	0	0	2-Propanone, 1-(2-methoxyphenyl)-		3.13, 10.2
7434.		1	0	0	2-Propanone, 1-(2-tetrahydrofuranyl)-		3.13, 10.2
7435.		1	1	1	2-Propanone, 1-(3-hydroxyphenyl)-		3.13, 9.22
7436.	18826-61-4	1	0	0	2-Propanone, 1-(3-methylphenyl)-		3.13
7437.	6302-03-0	1	1	1	2-Propanone, 1-(3-pyridinyl)-		3.13, 17.7
7438.	96-26-4	1	0	0	2-Propanone, 1,3-dihydroxy-		2.5, 3.13
7439.		0	1	0	2-Propanone, 1-(3,4-dihydro-6-methylpyran-2-yl)-		3.13, 10.2
7440.	19037-58-2	1	1	1	2-Propanone, 1-(3,5-dimethoxy-4-hydroxyphenyl)-		3.13, 9.22, 10.2
7441.	16695-72-0	1	1	1	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (*E*)-		3.13
7442.	16695-73-1	1	1	1	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (*Z*)-		3.13
7443.	2503-46-0	1	1	1	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-		3.13, 9.22, 10.2
7444.	770-39-8	1	0	0	2-Propanone, 1-(4-hydroxyphenyl)-		3.13, 9.22
7445.	6304-16-1	1	0	0	2-Propanone, 1-(4-pyridinyl)-		3.13, 17.7
7446.	13678-74-5	1	1	1	2-Propanone, 1-(5-methyl-2-furanyl)-		3.13, 10.2
7447.	50672-03-2	1	0	0	2-Propanone, 1-[5-(hydroxymethyl)-2-furanyl]-		2.5, 3.13, 10.2
7448.	107-02-8	1	1	1	2-Propenal {acrolein}	$H_2C{=}CH\text{-}CH{=}O$	0.4, 3.12, 23.5
7449.	636-38-4	0	1	0	2-Propenal, 2,3-dihydroxy-	$HOCH{=}CHOH\text{-}CH{=}O$	2.5, 3.12
7450.	78-85-3	1	1	1	2-Propenal, 2-methyl- {methacrolein}	$H_2C{=}C(CH_3)\text{-}CH{=}O$	3.12
7451.	31704-79-7	1	0	0	2-Propenal, 2-methyl-3-(5-methyl-2-furanyl)-		3.12, 10.2
7452.	101-39-3	0	1	0	2-Propenal, 2-methyl-3-phenyl-		3.12
7453.	79407-66-2	0	1	0	2-Propenal, 3-(2,4-dihydroxyphenyl)-		3.12, 9.22
7454.	874-66-8	1	0	0	2-Propenal, 3-(2-furanyl)-2-methyl-		3.12, 10.2
7455.	1504-74-1	0	1	0	2-Propenal, 3-(2-methoxyphenyl)-		3.12, 10.2
7456.	104-55-2	1	1	1	2-Propenal, 3-phenyl- {cinnamaldehyde}		3.12, 24.3, 25.29
7457.	14371-10-9	0	1	0	2-Propenal, 3-phenyl-, (*E*)- {*trans*-cinnamaldehyde}		3.12
7458.	122-40-7	0	1	0	2-Propenal, 3-phenyl-, α-pentyl-		3.12
7459.	79-06-1	1	1	1	2-Propenamide {acrylamide}	$H_2C{=}CH\text{-}CONH_2$	13.1, 23.5
7460.	79-39-0	1	0	0	2-Propenamide, 2-methyl- {methacrylamide}		13.1
7461.	1202-41-1	0	1	0	2-Propenamide, 3-(3,4-dihydroxyphenyl)-		9.22, 13.1
7462.	59001-33-1	0	1	0	2-Propenamide, 3-(3,4-dihydroxyphenyl)-*N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]- {dicaffeoylspermidine}		9.22, 12.2, 13.1

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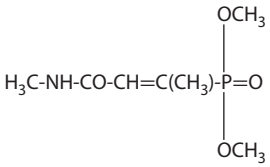
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7463.	59576-98-6	0	1	0	2-Propenamide, 3-(4-hydroxyphenyl)-		9.22, 13.1
7464.	621-79-4	1	0	0	2-Propenamide, 3-phenyl-	C_6H_5-CH=CH-$CONH_2$	13.1
7465.	61892-63-5	1	0	0	2-Propenamide, *N*-(1-oxopropyl)-		13.1
7466.	29554-26-5	0	1	0	2-Propenamide, *N*-(4-aminobutyl)-3-(3,4-dihydroxyphenyl)- {caffeoylputrescine}		9.22, 12.2, 13.1
7467.	501-13-3	0	1	0	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxy-3-methoxyphenyl)-		9.22, 12.2, 13.1
7468.	34136-53-3	0	1	0	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxyphenyl)-		9.22, 12.2, 13.1
7469.	42369-86-8	0	1	0	2-Propenamide, *N,N′*-1,4-butanediylbis [3-(4-hydroxy-3-methoxyphenyl)-		10.2, 9.22, 13.1
7470.	107-11-9	1	0	0	2-Propen-1-amine {allyl amine, acrylamine}	H_2C=CH-CH_2-NH_2	12.2
7471.	2878-14-0	1	0	0	2-Propen-1-amine, 2-methyl-	H_2C=C(CH_3)-CH_2-NH_2	12.2
7472.	115-07-1	1	0	0	1-Propene	H_3C-CH=CH_2	1.11
7473.	115-11-7	1	0	0	1-Propene, 2-methyl- {isobutylene}	H_3C-C(CH_3)=CH_2	1.11
7474.	26952-23-8	0	1	0	1-Propene, 1,2-dichloro- {Telone®}		18.4, 21.3
7475.	542-75-6	0	1	0	1-Propene, 1,3-dichloro- {1,3-*D*}		18.4, 21.3
7476.	2157-98-4	0	1	0	1-Propene, 1-methyl-3-(methylamino)-3-oxo-, dimethyl phosphate {Monocrotophos®}		5.3, 21.3
7477.	557-31-3	1	1	1	1-Propene, 3-ethoxy- {allyl ethyl ether}		10.2
7478.	10152-76-8	1	0	0	1-Propene, 3-(methylthio)-	H_3C-S-CH_2-CH=CH_2	18.1
7479.	27817-67-0	1	0	0	1-Propene, 3-(propylthio)-		18.1
7480.	592-88-1	1	0	0	1-Propene, 3,3′-thiobis-		18.1
7481.	2028-39-9	1	0	0	1-Propene-3-thiol		18.1
7482.	499-12-7	1	1	1	1-Propene-1,2,3-tricarboxylic acid {aconitic acid}		4.3, 26.9
7483.	107-13-1	1	0	0	2-Propenenitrile {acrylonitrile}	H_2C=CH-CN	11.2, 23.5
7484.	126-98-7	1	0	0	2-Propenenitrile, 2-methyl- {methacrylonitrile}	H_2C=C(CH_3)-CN	11.2
7485.	4360-47-8	1	0	0	2-Propenenitrile, 3-phenyl- {cinnamonitrile}		11.2
7486.	54356-27-3	1	0	0	2-Propenenitrile, 3-(3-pyridinyl)-, (*E*)-		11.2, 17.7
7487.	54356-28-4	1	0	0	2-Propenenitrile, 3-(3-pyridinyl)-, (*Z*)-		11.2, 17.7
7488.	870-23-5	1	0	0	2-Propene-1-thiol		18.1
7489.	79-10-7	1	1	1	2-Propenoic acid {acrylic acid}	H_2C=CH-COOH	4.3
7490.	138-08-9	0	1	0	2-Propenoic acid, 2-(phosphonooxy)-		4.3
7491.	79-41-4	1	0	0	2-Propenoic acid, 2-methyl- {methacrylic acid}		4.3
7492.	80-62-6	0	1	0	2-Propenoic acid, 2-methyl-, methyl ester		5.3
7493.		0	1	0	2-Propenoic acid, 3-(2-furanylmethyl)-2-methyl-, ethyl ester		5.3. 10.2
7494.	82826-13-9	0	1	0	2-Propenoic acid, 3-(2-furanyl)-2-methyl-, ethyl ester		5.3. 10.2
7495.	31082-90-3	1	0	0	2-Propenoic acid, 3-(2,3-dihydroxyphenyl)-		4.3, 9.22

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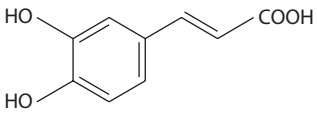
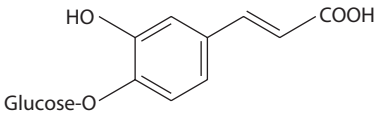
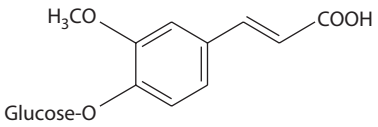
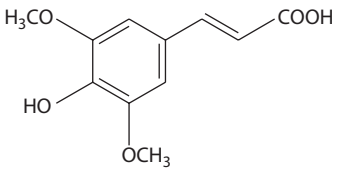
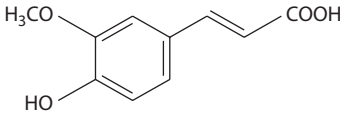
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7496.	331-39-5	1	1	1	2-Propenoicacid,3-(3,4-dihydroxyphenyl)- {caffeic acid}		0.4, 4.3, 9.22, 21.3, 23.5, 25.29, 26.9
7497.	501-16-6	1	1	1	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*E*)- {*trans*-caffeic acid}		4.3, 9.22
7498.	4361-87-9	1	1	1	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*Z*)- {*cis*-caffeic acid}		4.3, 9.22
7499.	58994-15-3	0	1	0	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, monoamide with *N*-(3-aminopropyl)-1, 4-butanediamine {caffeoylspermidine}		9.22, 12.2, 13.1
7500.	2316-26-9	0	1	0	2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-		4.3, 10.2
7501.	17093-82-2	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]- {1-*O*-caffeoylglucose}		2.5, 4.3, 9.22
7502.	7196-71-6 14364-12-6	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-methoxyphenyl]- {1-*O*-feruloylglucose}		2.5, 4.3, 10.2
7503.	14364-05-7	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)phenyl]-		2.5, 4.3, 10.2
7504.	7362-37-0	1	1	1	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*E*)- {*trans*-sinapic acid}		4.3, 9.22, 10.2
7505.	7361-90-2	1	1	1	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*Z*)- {*cis*-sinapic acid}		4.3, 9.22, 10.2
7506.	537-73-5	1	0	0	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-		4.3, 9.22, 10.2
7507.	25522-33-2	1	0	0	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-, (*E*)-		4.3, 9.22, 10.2
7508.	16499-18-6	0	1	0	2-Propenoic acid, 3-(4,5-dihydroxy-3-methoxyphenyl)- {5-hydroxyferulic acid}		4.3, 9.22, 10.2
7509.	530-59-6	1	0	0	2-Propenoic acid, 3-(4-hydroxy-3,5-dimethoxyphenyl)-		4.3, 9.22, 10.2,
7510.	1135-24-6	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, {ferulic acid}		4.3, 9.22, 10.2, 21.3, 26.9
7511.	537-98-4	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid}		4.3, 9.22, 10.2, 21.3, 26.9

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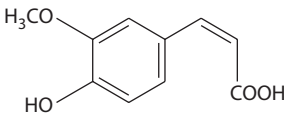
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7512.	1014-83-1	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid}		4.3, 9.22, 10.2, 21.3, 25.29, 26.9
7513.	2309-07-1	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester {ferulic acid, methyl ester}		5.3, 9.22, 10.2
7514.	25429-38-3	1	0	0	2-Propenoic acid, 3-(hydroxyphenyl)-		4.3, 9.22
7515.	539-47-9	1	0	0	2-Propenoic acid, 3-(2-furanyl)-		4.3, 10.2
7516.	583-17-5 614-60-8	1	1	1	2-Propenoic acid, 3-(2-hydroxyphenyl)- {*o*-coumaric acid}		4.3, 9.22, 26.9
7517.	588-30-7	0	1	0	2-Propenoic acid, 3-(3-hydroxyphenyl)-		4.3, 9.22
7518.	14755-02-3	0	1	0	2-Propenoic acid, 3-(3-hydroxyphenyl)-, (*E*)-		4.3, 9.22
7519.	7400-08-0	1	1	1	2-Propenoic acid, 3-(4-hydroxyphenyl)- {coumaric acid}		4.3, 9.22, 21.3
7520.	501-98-4	1	1	1	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*E*)- {*trans*-coumaric acid}		4.3, 9.22
7521.	4501-31-9	1	1	1	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*Z*)- {*cis*-coumaric acid}		4.3, 9.22
7522.	14779-25-0	1	0	0	2-Propenoicacid, 3-(5-methyl-2-furanyl)-		4.3, 10.2
7523.	17570-26-2	1	1	1	2-Propenoic acid, 3-(3-methoxyphenyl)-, (*E*)-		4.3, 10.2
7524.	621-82-9	1	1	1	2-Propenoic acid, 3-phenyl- {cinnamic acid}	C_6H_5-CH=CH-COOH	4.3, 24.3, 25.29, 26.9
7525.	140-10-3	1	1	1	2-Propenoic acid, 3-phenyl-, (*E*)- {*trans*-cinnamic acid}		4.3, 24.3, 25.29
7526.	102-94-3	1	1	1	2-Propenoic acid, 3-phenyl-, (*Z*)- {*cis*-cinnamic acid}		4.3, 24.3
7527.	47018-25-7	1	0	0	2-Propenoic acid, 3-phenyl-, 2-phenylethenyl ester		5.3, 24.3
7528.	122-69-0	1	1	1	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester {cinnamyl cinnamate}		5.3, 24.3, 25.29
7529.	103-36-6	1	1	1	2-Propenoic acid, 3-phenyl-, ethyl ester {ethyl cinnamate}		5.3, 24.3, 25.29
7530.	103-26-4	1	1	1	2-Propenoic acid, 3-phenyl-, methyl ester {methyl cinnamate}	C_6H_5-CH=CH-COO-CH_3	5.3, 24.3, 25.29
7531.	7779-65-9	1	1	1	2-Propenoic acid, 3-phenyl-, 3-methylbutyl ester		5.3, 24.3, 25.29
7532.	122-67-8	0	1	0	2-Propenoic acid, 3-phenyl-, 2-methylpropyl ester		5.3
7533.	103-53-7	0	1	0	2-Propenoic acid, 3-phenyl-, phenylethyl ester		5.3
7534.	103-41-3	1	1	1	2-Propenoic acid, 3-phenyl-, phenylmethyl ester {benzyl cinnamate}		5.3, 24.3, 25.29
7535.	122-68-9	0	1	0	2-Propenoic acid, 3-phenyl-, 3-phenylpropyl ester {3-phenylpropyl cinnamate}		5.3
7536.	96-33-3	1	1	1	2-Propenoic acid, methyl ester	H_2C=CH-COO-CH_3	5.3
7537.	90-50-6	0	1	0	2-Propenoic acid, 3-(3,4,5-trimethoxyphenyl)-		4.3, 10.2
7538.	107-18-6	1	1	1	2-Propen-1-ol {allyl alcohol}	H_2C=CH-CH_2OH	2.5, 21.3

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
7539.	104-54-1	1	1	1	2-Propen-1-ol, 3-phenyl- {cinnamyl alcohol}		2.5, 24.3, 25.29
7540.	4407-36-7	0	1	0	2-Propen-1-ol, 3-phenyl-, (*E*)-		2.5
7541.	21040-45-9	0	1	0	2-Propen-1-ol, 3-phenyl-, acetate, (*E*)-		5.3
7542.	2983-65-5	1	1	1	2-Propen-1-one, 1- (4-hydroxy-3-methoxyphenyl)-		3.13, 9.22, 10.2
7543.	94-41-7	1	0	0	2-Propen-1-one, 1,3-diphenyl- {chalcone}		3.13
7544.	145917-24-4	0	1	0	2-Propen-1-one, 1,3-di-3-pyridinyl-, (*E*)-		3.13, 17.7
7545.		1	0	0	Propoxyl radical	$CH_3(CH_2)_2O$	27.1
7546.	74-99-7	1	0	0	1-Propyne	$H_3C\text{-}C{\equiv}CH$	1.11
7547.	37259-58-8	0	1	0	Protease		0.4, 22.2
7548.		0	1	0	Protease, serine		22.2
7549.		0	1	0	Protease, sulfhydryl		18.1, 22.2
7550.	144419-45-4	0	1	0	Protein (*Arabidopsis thaliana* clone G9.1 gene A9 11.6 kDa reduced)		22.2
7551.	132966-19-9	0	1	0	Protein (tobacco 27.4 kDa RNA-binding precursor reduced)		22.2
7552.	132966-16-6	0	1	0	Protein (tobacco 27.4 kDa RNA-binding)		22.2
7553.	137801-72-0	0	1	0	Protein (tobacco chloroplast clone pTB24 gene psbK)		22.2
7554.	139874-83-2	0	1	0	Protein (tobacco clone.lambda. 18C gene RB7 reduced)		22.2
7555.	139874-82-1	0	1	0	Protein (tobacco clone.lambda. 5A gene RB7 reduced)		22.2
7556.	162572-20-5	0	1	0	Protein (tobacco clone lambda T-FLO 4 gene NFL2)		22.2
7557.	147445-75-8	0	1	0	Protein (tobacco clone pMG15 extensin-like precursor reduced)		22.2
7558.	146591-93-7	0	1	0	Protein (tobacco clone PRP3g12 gene PRP3 pistil-specific proline-rich precursor)		22.2
7559.	162572-19-2	0	1	0	Protein (tobacco clone pTGF220 gene NFL1)		22.2
7560.	145895-79-0	0	1	0	Protein (tobacco flower-associated reduced)		22.2
7561.	155077-18-2	0	1	0	Protein (tobacco gene MST1 hydrogen ion-monosaccharide-cotransporting reduced)		22.2
7562.	160936-45-8	0	1	0	Protein (tobacco leaf curl virus coat)		22.2
7563.	155663-14-2	0	1	0	Protein CPB 20 (tobacco clone cpb20-44 antifungal reduced)		22.2
7564.	155663-12-0	0	1	0	Protein CPB 20 (tobacco clone cpb20-52 antifungal reduced)		22.2
7565.	155663-10-8	0	1	0	Protein CPB 20, prepro- (tobacco clone cpb20-52 antifungal reduced)		22.2
7566.	155663-13-1	0	1	0	Protein CPB 20, pro- (tobacco clone cpb20-44 antifungal reduced)		22.2
7567.	155663-11-9	0	1	0	Protein CPB 20, pro- (tobacco clone cpb20-52 antifungal reduced)		22.2
7568.	144997-83-1	0	1	0	Protein D 2 (*Nicotiana sylvestris* clone yaDC12/yaDC17 gene psaDa precursor)		22.2

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7569.	144997-84-2	0	1	0	Protein D 2 (*Nicotiana sylvestris* clone yaDC12/yaDC17 gene psaDa)		22.2
7570.	146150-25-6	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana plumbaginifolia* clone NeIF-4A2 isoform reduced)		22.2
7571.	146150-27-8	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana plumbaginifolia* clone NeIF-4A3 isoform reduced)		22.2
7572.	162572-22-7	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A9)		22.2
7573.	162572-23-8	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A11)		22.2
7574.	162572-24-9	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A7)		22.2
7575.	162572-25-0	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A15)		22.2
7576.	162572-26-1	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A6)		22.2
7577.	162572-27-2	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A13)		22.2
7578.	162572-28-3	0	1	0	Protein formation initiation factor eIF 4A (*Nicotiana tabacum* clone NeIF-4A14)		22.2
7579.	143514-66-3	0	1	0	Protein formation initiation factor eIF 5A (*Nicotiana plumbaginifolia* clone NeIF-5A1 isoform C-terminal fragment reduced)		22.2
7580.	143514-67-4	0	1	0	Protein formation initiation factor eIF 5A (*Nicotiana plumbaginifolia* clone NeIF-5A2 isoform reduced)		22.2
7581.	143514-68-5	0	1	0	Protein formation initiation factor eIF 5A (*Nicotiana tabacum* samsun clone NeIF-5A3 isoform reduced)		22.2
7582.	152745-97-6	0	1	0	Protein L 17 (tobacco clone TSC81 ribosome reduced)		22.2
7583.	142978-88-9	0	1	0	Protein L 27 (tobacco chloroplast clone L27-1 ribosome precursor reduced)		22.2
7584.	142978-89-0	0	1	0	Protein L 27 (tobacco chloroplast clone L27-1 ribosome reduced)		22.2
7585.	160082-04-2	0	1	0	Protein LTP (tobacco)		22.2
7586.	143513-70-6	0	1	0	Protein OEE 2 (tobacco strain NK326 precursor reduced)		22.2
7587.	9001-92-7	0	1	0	Proteinase		22.2
7588.	37205-61-1	0	1	0	Proteinase inhibitor		22.2
7589.	145090-32-0	0	1	0	Proteinase inhibitor, PI-1		22.2
7590.	150474-41-2	0	1	0	Proteinase inhibitor, prepro-TIMPa (*Nicotiana tabacum* samsun reduced)		22.2
7591.	150474-40-1	0	1	0	Proteinase inhibitor, prepro-TIMPb (*Nicotiana tabacum* samsun reduced)		22.2

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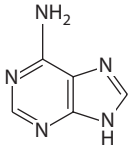
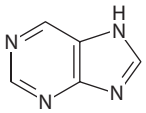
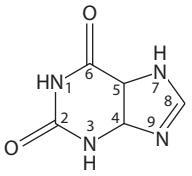
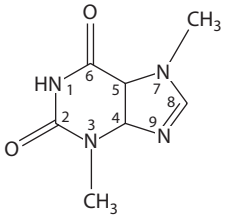
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7592.	150474-44-5	0	1	0	Proteinase inhibitor, pro-TIMPa (*Nicotiana tabacum* samsun reduced)		22.2
7593.	150474-42-3	0	1	0	Proteinase inhibitor, pro-TIMPb (*Nicotiana tabacum* samsun reduced)		22.2
7594.	150474-45-6	0	1	0	Proteinase inhibitor, TIMPa (*Nicotiana tabacum* samsun reduced)		22.2
7595.	150474-43-4	0	1	0	Proteinase inhibitor, TIMPb (*Nicotiana tabacum* samsun reduced)		22.2
7596.		0	1	0	*Proteobacteria*, *Alphaproteobacteria*		22.2
7597.		0	1	0	*Proteobacteria*, *Betaproteobacteria*		22.2
7598.		0	1	0	*Proteobacteria*, *Epsilonproteobacteria*		22.2
7599.		0	1	0	*Proteobacteria*, *Gammaproteobacteria*		22.2
7600.		0	1	0	*Proteobacteria*, *Alphaproteobacteria*		22.2
7601.	9013-10-9	0	1	0	*Proteus* {isomerase, glucosamine phosphate}		22.2
7602.		0	1	0	*Pseudomonas aeruginosa*		22.2
7603.	551-68-8	0	1	0	*D*-Psicose	$HOCH_2$-CO-$(CHOH)_3$-CH_2OH	2.5, 3.13, 8.3
7604.	73-24-5	0	1	0	1*H*-Purin-6-amine {adenine}		0.4, 12.2, 17.23
7605.	525-79-1	0	1	0	1*H*-Purin-6-amine, *N*-(2-furanylmethyl)-		10.2, 12.2, 17.23
7606.	2365-40-4	0	1	0	1*H*-Purin-6-amine, *N*-(3-methyl-2-butenyl)-		12.2, 17.23
7607.	1214-39-7	0	1	0	1*H*-Purin-6-amine, *N*-(phenylmethyl)-		12.2, 17.23
7608.	56159-42-3	0	1	0	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-		2.5, 8.3, 10.2, 12.2, 17.23
7609.	38477-23-5	0	1	0	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-		2.5, 8.3, 10.2, 12.2, 17.23
7610.	54538-20-4	0	1	0	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-		2.5, 8.3, 10.2, 12.2, 17.23
7611.	120-73-0	0	1	0	1*H*-Purine		0.4, 17.21
7612.	69-89-6	0	1	0	1*H*-Purine-2,6-dione, 3,7-dihydro- {xanthine}		14.1, 17.13, 17.23
7613.	58-55-9	0	1	0	1*H*-Purine-2,6-dione, 3,7-dihydro-1, 7-dimethyl-		14.1, 17.13, 17.23
7614.	83-67-0	1	1	1	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- {theobromine}		14.1, 17.13, 17.23, 26.9
7615.	33073-01-7	1	0	0	1*H*-Purine-2,6-dione, 3, 9-dihydro-1,9-dimethyl-		14.1, 17.13, 17.23

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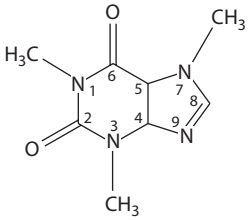
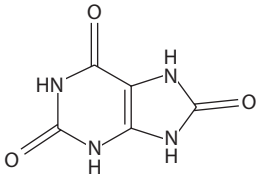
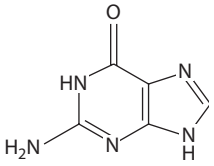
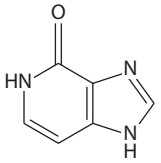
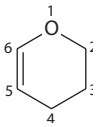
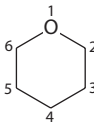
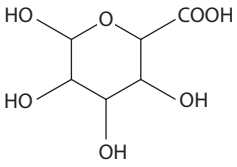
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7616.	58-08-2	1	1	1	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine}		14.1, 17.13, 17.23, 24.3, 26.9
7617.		1	0	0	6*H*-Purine-2,6-dione, 1,7-dihydro-, C_3-alkyl-		14.1, 17.13, 17.23
7618.	69-93-2	1	0	0	1*H*-Purine-2,6,8-trione, 7,9-dihydro- {uric acid}		0.4, 14.1, 17.13, 17.23
7619.	51953-03-8	0	1	0	9*H*-Purine		17.21
7620.	73-40-5	1	1	1	6*H*-Purin-6-one, 2-amino 1,7-dihydro- {guanine}		0.4, 12.2, 17.13, 17.23
7621.	68-94-0	0	1	0	6*H*-Purin-6-one, 1,7-dihydro- {hypoxanthine}		17.13, 17.23
7622.	25512-65-6	1	1	1	2*H*-Pyran, dihydro-		10.2
7623.	110-87-2	1	1	1	2*H*-Pyran, 3,4-dihydro-		10.2
7624.	10141-72-7	0	1	0	2*H*-Pyran, 2-methyltetrahydro-		10.2
7625.	142-68-7	1	1	1	2*H*-Pyran, tetrahydro-		10.2
7626.	16409-43-1	0	1	0	Pyran, tetrahydro-4-methyl-2-(2-methylpropen-1-yl)- {rose oxide}		10.2
7627.	100-73-2	1	1	1	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro- {acrolein dimer}		3.12, 10.2
7628.	70898-35-0	1	1	1	2*H*-Pyran-2-carboxaldehyde, 3, 4-dihydro-6-hydroxy-3-oxo-		2.5, 3.12, 3.13, 10.2
7629.	85373-77-9	1	0	0	4*H*-Pyran-3-carboxylic acid, 5, 6-dihydro-2,6-dimethyl-, methyl ester		5.3, 10.2
7630.	9046-38-2	0	1	0	2-Pyrancarboxylic acid, 3,4,5, 6-tetrahydroxytetrahydro- {oxane-2-carboxylic acid, 3,4,5,6-tetrahydroxy-, *D*-galacturonan}		2.5, 4.3, 10.2

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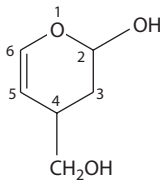
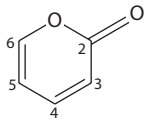
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7631.	112468-46-9	1	1	1	2*H*-Pyran-2,5(6*H*)-dione		3.13, 6.3
7632.		1	0	0	2*H*-Pyran-4-methanol, 3,4-dihydro-2-hydroxy-		2.5, 10.2
7633.	61892-96-4	1	0	0	2*H*-Pyran-6-methanol, 3, 4-dihydro-3-hydroxy-		2.5, 10.2
7634.	19752-84-2	1	0	0	2*H*-Pyran-3-ol, tetrahydro-		2.5, 10.2
7635.	121198-47-8	1	1	1	Pyranone, dimethyl-		3.13, 10.2
7636.	504-31-4	1	0	0	2*H*-Pyran-2-one		6.3
7637.	20357-65-7	1	0	0	2*H*-Pyran-2-one, 6-chloro-		6.3, 18.4
7638.		1	0	0	2*H*-Pyran-2-one, 3,4-dihydro-4-(1-methylethyl)-6-methyl-		6.3
7639.	3393-45-1	0	1	0	2*H*-Pyran-2-one, 5,6-dihydro-		6.3
7640.		1	0	0	2*H*-Pyran-2-one, 5,6-dihydro-4, 5-dimethyl-		6.3
7641.		1	0	0	2*H*-Pyran-2-one, 4,5-dihydro-3-hydroxy-		2.5, 6.3
7642.	55100-07-7	0	1	0	2*H*-Pyran-2-one, 5,6-dihydro-4-hydroxy-		2.5, 6.3
7643.	54657-94-2	1	0	0	2*H*-Pyran-2-one, 3,4-dihydro-5-methyl-		6.3
7644.	2381-87-5	1	1	1	2*H*-Pyran-2-one, 5,6-dihydro-4-methyl-		6.3
7645.	21722-33-8	1	1	1	2*H*-Pyran-2-one, 5, 6-dihydro-4-(1-methylethyl)-		6.3
7646.	6400-69-4	1	0	0	2*H*-Pyran-2-one, 5,6-dihydro-6-propyl-		6.3
7647.	73850-01-8	1	0	0	2*H*-Pyran-2-one, hydroxyethyl-		2.5, 6.3
7648.		1	0	0	2*H*-Pyran-2-one, hydroxymethyl-		2.5, 6.3
7649.	496-64-0	1	1	1	2*H*-Pyran-2-one, 3-hydroxy-		2.5, 6.3
7650.	73692-69-0	0	1	0	2*H*-Pyran-2-one, 3-hydroxy-6-methyl-		2.5, 6.3
7651.	150669-60-6	1	1	1	2*H*-Pyran-2-one, 4-(1-methylethyl)-		6.3
7652.	27593-23-3	0	1	0	2*H*-Pyran-2-one, 6-pentyl- {6-amyl-α-pyrone}		6.3
7653.	542-28-9	1	1	1	2*H*-Pyran-2-one, tetrahydro- {δ-valerolactone}		6.3
7654.		1	0	0	2*H*-Pyran-2-one, tetrahydro-3, 4-epoxy-5-hydroxy-		2.5, 6.3, 10.2
7655.	5058-01-5	1	0	0	2*H*-Pyran-2-one, tetrahydro-3-hydroxy-		2.5, 6.3
7656.		1	0	0	2*H*-Pyran-2-one, tetrahydro-methoxy-		6.3, 10.2
7657.		1	0	0	2*H*-Pyran-2-one, tetrahydro-methyl-		6.3
7658.	32821-70-8	0	1	0	2*H*-Pyran-2-one, tetrahydro-3-(1-methylethyl)-		6.3
7659.	78094-66-3	1	0	0	2*H*-Pyran-2-one, tetrahydro-4,5-dimethyl-, *cis*-(±)-		6.3
7660.	3720-20-5	1	1	1	2*H*-Pyran-2-one, tetrahydro-4,6-dimethyl-		6.3
7661.	710-04-3	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-hexyl- {δ-undecalactone}		6.3
7662.	61892-56-6	1	0	0	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-		2.5, 6.3
7663.	503-48-0 110053-65-1	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-4-methyl-		2.5, 6.3
7664.	1121-84-2	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-methyl-		6.3

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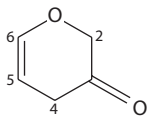
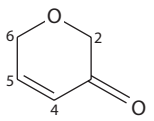
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7665.	96168-15-9	1	0	0	2*H*-Pyran-2-one, tetrahydro-4-methyl-6-(3,7,11-trimethyldodecyl)-		6.3
7666.	56947-55-8	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-		6.3
7667.	21754-22-3	0	1	0	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-, (±)-		6.3
7668.	37147-17-4	0	1	0	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-, (R)		6.3
7669.	10413-18-0 24405-16-1	1	1	1	2*H*-Pyran-2-one, tetrahydro-5,6-dimethyl-		6.3
7670.	33691-73-5	1	0	0	2*H*-Pyran-2-one, tetrahydro-5-hydroxy-		2.5, 6.3
7671.	3301-94-8	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-butyl-{δ-nonalactone}		6.3
7672.	2610-95-9	0	1	0	2*H*-Pyran-2-one, tetrahydro-6,6-dimethyl-		6.3
7673.	59056-32-5	0	1	0	2*H*-Pyran-2-one, tetrahydro-6,6-dimethyl-4-(1-methylethyl)-		6.3
7674.	713-95-1	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-heptyl-{δ-dodecalactone}		6.3
7675.	90-80-2	1	0	0	2*H*-Pyran-2-one, tetrahydro-6-hydroxymethyl, 3,4,5-trihydroxy-{gluconic acid, δ-lactone}		2.5, 6.3
7676.	823-22-3	1	1	1	2*H*-Pyran-2-one, tetrahydro-6-methyl-{δ-hexalactone, δ-caprolactone}		6.3
7677.	21722-34-9	1	1	1	2*H*-Pyran-2-one, tetrahydro-6-methyl-3-(1-methylethyl)-{two isomers indicated}		6.3
7678.		0	1	0	2*H*-Pyran-2-one, tetrahydro-6-methyl-4-(1-methylethyl)-		6.3
7679.	60393-63-7	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-methyl-5-(1-methylethyl)-		6.3
7680.	2721-22-4	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-nonyl-{tetradecalactone}		6.3
7681.	705-86-2	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-pentyl-{δ-decalactone}		6.3
7682.	698-76-0	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-propyl-{δ-octalactone}		6.3, 24.3, 25.29
7683.	28743-04-6	1	1	1	2*H*-Pyran-3(4*H*)-one		3.13, 10.2
7684.	23462-75-1	1	0	0	2*H*-Pyran-3(4*H*)-one, dihydro-		3.13, 10.2
7685.	121197-11-3	1	1	1	2*H*-Pyran-3(4*H*)-one, dihydro-4-(hydroxymethyl)-		2.5, 3.13, 10.2
7686.	65712-87-0	1	0	0	2*H*-Pyran-3(4*H*)-one, dihydro-6-methoxy-		3.13, 10.2
7687.	43152-89-2	1	0	0	2*H*-Pyran-3(4*H*)-one, dihydro-6-methyl-		3.13, 10.2
7688.	98166-23-5	1	1	1	2*H*-Pyran-3(6*H*)-one		3.13, 10.2

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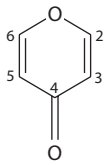
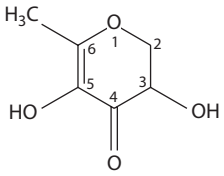
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
7689.	108-97-4	1	0	0	4*H*-Pyran-4-one		3.13, 10.2
7690.	84302-42-1	1	0	0	4*H*-Pyran-4-one, 2,3-dihydro-		3.13, 10.2
7691.	28564-83-2	1	1	1	4*H*-Pyran-4-one, 2,3-dihydro-3, 5-dihydroxy-6-methyl-		2.5, 3.13, 10.2
7692.	6380-97-8	1	1	1	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-2-(hydroxymethyl)-		2.5, 3.13, 10.2
7693.	38877-21-3	1	0	0	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-6-methyl-		2.5, 3.13, 10.2
7694.	131524-09-9	1	0	0	4*H*-Pyran-4-one, 2,6-diethyl-3-hydroxy-		2.5, 3.13, 10.2
7695.	1004-36-0	1	0	0	4*H*-Pyran-4-one, 2,6-dimethyl-		3.13, 10.2
7696.	4940-17-4	1	0	0	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-		2.5, 3.13, 10.2
7697.	131524-16-8	1	0	0	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-6-methyl-		2.5, 3.13, 10.2
7698.	4940-11-8	1	1	1	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-{ethylmaltol}		2.5, 3.13, 10.2, 24.3, 25.29
7699.	131524-08-8	1	0	0	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5,6-dimethyl-		2.5, 3.13, 10.2
7700.	131524-04-4	1	0	0	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5-methyl-		2.5, 3.13, 10.2
7701.	22639-24-3	1	0	0	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-6-methyl-		2.5, 3.13, 10.2
7702.	61892-88-4	1	0	0	4*H*-Pyran-4-one, 2-hydroxy-3-methyl-		2.5, 3.13, 10.2
7703.	61892-87-3	1	0	0	4*H*-Pyran-4-one, 2-hydroxy-5-methyl-		2.5, 3.13, 10.2
7704.		1	0	0	4*H*-Pyran-4-one, 2-hydroxymethyl-3, 5,6-trihydroxy-		2.5, 3.13, 10.2
7705.		1	0	0	4*H*-Pyran-4-one, 2-methyl-3,5,6-trihydroxy-		2.5, 3.13, 10.2
7706.	29943-42-8	1	0	0	4*H*-Pyran-4-one, 2,3,5,6-tetrahydro- = 4*H*-pyran-4-one, tetrahydro-		2.5, 3.13, 10.2
7707.	488-18-6	1	0	0	4*H*-Pyran-4-one, 3,5-dihydroxy-		2.5, 3.13, 10.2
7708.		1	0	0	4*H*-Pyran-4-one, 2,5-dihydroxy-3-methyl-		2.5, 3.13, 10.2
7709.	61892-86-2	1	0	0	4*H*-Pyran-4-one, 3,5-dihydroxy-2,6-dimethyl-		2.5, 3.13, 10.2
7710.	1073-96-7	1	1	1	4*H*-Pyran-4-one, 3,5-dihydroxy-2-methyl- {5-hydroxymaltol}		2.5, 3.13, 10.2
7711.		1	0	0	4*H*-Pyran-4-one, 3,5-dihydroxymethyl-2,6-dimethyl-		2.5, 3.13, 10.2
7712.	496-63-9	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-		2.5, 3.13, 10.2
7713.	40311-00-0	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylethyl)-		2.5, 3.13, 10.2
7714.	4940-18-5	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylpropyl)-		2.5, 3.13, 10.2
7715.	131524-11-3	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylbutyl)-		2.5, 3.13, 10.2
7716.	76015-10-6	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylpropyl)-		2.5, 3.13, 10.2

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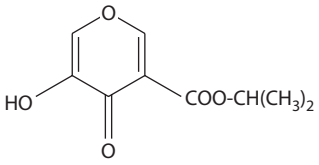
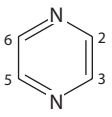
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7717.	131524-12-4	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(3-methylbutyl)-		2.5, 3.13, 10.2
7718.	131524-05-5	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2,5,6-trimethyl-		2.5, 3.13, 10.2
7719.	131524-02-2	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2,5-dimethyl-		2.5, 3.13, 10.2
7720.	2298-99-9	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2,6-dimethyl-		2.5, 3.13, 10.2
7721.		1	0	0	4*H*-Pyran-4-one, 3-hydroxymethyl-		2.5, 3.13, 10.2
7722.	118-71-8	1	1	1	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}		2.5, 3.13, 10.2, 24.3, 25.29
7723.	131524-10-2	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-6-propyl-		2.5, 3.13, 10.2
7724.	131524-13-5	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-pentyl-		2.5, 3.13, 10.2
7725.	4940-16-3	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-propyl-		2.5, 3.13, 10.2
7726.	42508-10-1	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-5-methyl-		2.5, 3.13, 10.2
7727.	131524-07-7	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylethyl)-		2.5, 3.13, 10.2
7728.	131524-14-6	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylpropyl)-		2.5, 3.13, 10.2
7729.	131524-15-7	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(2-methylpropyl)-		2.5, 3.13, 10.2
7730.	40861-87-8	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-propyl-		2.5, 3.13, 10.2
7731.	50671-50-6	1	0	0	4*H*-Pyran-4-one, 3-methyl-		3.13, 10.2
7732.	131524-03-3	1	0	0	4*H*-Pyran-4-one, 5-hydroxy-2,3-dimethyl-		2.5, 3.13, 10.2
7733.	644-46-2	1	0	0	4*H*-Pyran-4-one, 5-hydroxy-2-methyl- = 4*H*-pyran-4-one, 3-hydroxy-6-methyl- {allomaltol}		2.5, 3.13, 10.2
7734.	131524-06-6	1	0	0	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-methyl-		2.5, 3.13, 10.2
7735.	131524-17-9	1	1	1	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-propyl-		2.5, 3.13, 10.2
7736.	499-78-5	1	1	1	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-		2.5, 3.13, 4.3, 10.2
7737.		1	0	0	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-, (1-methylethyl) ester		2.5, 3.13, 5.3, 10.2
7738.	290-37-9	1	1	1	Pyrazine		17.7
7739.		1	1	1	Pyrazine, alkyl-		17.7
7740.	66288-42-4	1	1	1	Pyrazine, butenyl-		17.7
7741.	29460-93-3	1	1	1	Pyrazine, 2-(2-butenyl)-		17.7
7742.	78210-56-7	1	1	1	Pyrazine, 3-butenyl- = pyrazine, 2-butenyl-		17.7
7743.	29460-91-1	1	0	0	Pyrazine, 2-butyl-		17.7
7744.	32184-51-3	1	1	1	Pyrazine, 2-cyclopentyl-6-methyl-		17.7
7745.	15707-24-1	1	1	1	Pyrazine, 2,3-diethyl-		17.7, 24.3, 25.29
7746.	18138-04-0	1	1	1	Pyrazine, 2,3-diethyl-5-methyl-		17.7

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7747.	13238-84-1	1	1	1	Pyrazine, 2,5-diethyl-		17.7, 24.3
7748.	32736-91-7	1	0	0	Pyrazine, 2,5-diethyl-3-methyl-		17.7
7749.	13067-27-1	1	1	1	Pyrazine, 2,6-diethyl-		17.7, 24.3
7750.	18138-05-1	1	0	0	Pyrazine, 2,6-diethyl-3-methyl- = pyrazine, 3,5-diethyl-2-methyl-		17.7
7751.	25704-73-8	1	1	1	Pyrazine, dimethyl-		17.7
7752.	5910-89-4	1	1	1	Pyrazine, 2,3-dimethyl-		17.7, 24.3, 25.29
7753.	15707-34-3	1	0	0	Pyrazine, 2,3-dimethyl-5-ethyl-		17.7
7754.		1	0	0	Pyrazine, 2,3-dimethyl-5-propyl- = pyrazine, 2,3-dimethyl-6-propyl-		17.7
7755.	123-32-0	1	1	1	Pyrazine, 2,5-dimethyl-		17.7, 24.3, 25.29
7756.	80935-98-4	1	0	0	Pyrazine, 2,5-dimethyl-3-ethenyl-		17.7
7757.		0	1	0	Pyrazine, 2,5-dimethyl-3-(1-methylethyl)- = pyrazine, 3,6-dimethyl-2 (1-methylethyl)-		17.7
7758.		1	0	0	Pyrazine, 2,5-dimethyl-6-propyl-		17.7
7759.	108-50-9	1	1	1	Pyrazine, 2,6-dimethyl-		17.7, 24.3, 25.29
7760.		1	0	0	Pyrazine, 2,6-dimethyl-3-ethenyl-		17.7
7761.	71607-73-3	1	1	1	Pyrazine, dimethylethyl-		17.7
7762.	4177-16-6	1	1	1	Pyrazine, 2-ethenyl-		17.7
7763.	13925-08-1	1	1	1	Pyrazine, 2-ethenyl-5-methyl-		17.7
7764.	13925-09-2	1	1	1	Pyrazine, 2-ethenyl-6-methyl-		17.7
7765.	13925-00-3	1	1	1	Pyrazine, ethyl- = pyrazine, 2-ethyl-		17.7
7766.	33504-66-4	1	0	0	Pyrazine, ethylmethyl-		17.7
7767.	13360-65-1	1	1	1	Pyrazine, 2-ethyl-3,6-dimethyl- = pyrazine, 6-ethyl-2,5-dimethyl-		17.7, 24.3, 25.29
7768.	13925-07-0	1	1	1	Pyrazine, 2-ethyl-3,5-dimethyl- = pyrazine, 3-ethyl-2,6-dimethyl-		17.7, 24.3, 25.29
7769.	15707-34-3	1	1	1	Pyrazine, 2-ethyl-5,6-dimethyl- = pyrazine, 5-ethyl-2,3-dimethyl-		17.7
7770.		0	1	0	Pyrazine, 2-ethyl-5-ethylene-		17.7
7771.	25680-58-4	0	1	0	Pyrazine, 2-ethyl-3-methoxy-		10.2, 17.7
7772.		0	1	0	Pyrazine, 2-ethyl-5-methoxy-		10.2, 17.7
7773.	67845-38-9	0	1	0	Pyrazine, 2-ethyl-6-methoxy-		10.2, 17.7
7774.	15707-23-0	1	1	1	Pyrazine, 2-ethyl-3-methyl-		17.7, 24.3, 25.29
7775.	13360-64-0	1	1	1	Pyrazine, 2-ethyl-5-methyl-		17.7
7776.	13925-03-6	1	1	1	Pyrazine, 2-ethyl-6-methyl- = pyrazine, 6-ethyl-2-methyl-		17.7
7777.	17398-16-2	0	1	0	Pyrazine, 2-ethyl-3,5,6-trimethyl-		17.7
7778.	32736-95-1	1	1	1	Pyrazine, 2-furanyl-		10.2, 17.7
7779.	29460-98-8	1	1	1	Pyrazine, 3-furanyl-		10.2, 17.7
7780.	36238-34-3	1	1	1	Pyrazine, 5-(2-furanyl)-2,3-dimethyl- = pyrazine, 2-(2-furanyl)-5,6-dimethyl-		10.2, 17.7
7781.	32737-01-2	1	1	1	Pyrazine, 2-(2-furanyl)-3-methyl-		10.2, 17.7
7782.	27610-38-4	1	1	1	Pyrazine, 2-(2-furanyl)-5-methyl-		10.2, 17.7
7783.	32737-03-4	1	1	1	Pyrazine, 2-(2-furanyl)-6-methyl-		10.2, 17.7
7784.	29461-10-7	1	0	0	Pyrazine, 2-(3-furanyl)-5-methyl-		10.2, 17.7
7785.	3149-28-8	0	1	0	Pyrazine, methoxy-		10.2, 17.7

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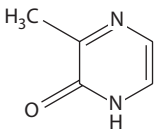
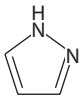
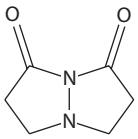
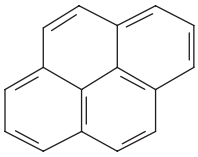
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7786.	2847-30-5	0	1	0	Pyrazine, 3-methoxy-2-methyl- = pyrazine, 2-methoxy-3-methyl-		10.2, 17.7
7787.	2882-22-6	0	1	0	Pyrazine, 5-methoxy-2-methyl-		10.2, 17.7
7788.	2882-21-5	0	1	0	Pyrazine, 6-methoxy-2-methyl-		10.2, 17.7
7789.	24683-00-9	0	1	0	Pyrazine, 2-methoxy-3-methylpropyl-		10.2, 17.7
7790.	109-08-0	1	1	1	Pyrazine, methyl- = pyrazine, 2-methyl-		17.7, 24.3, 25.29
7791.	38713-41-6	1	1	1	Pyrazine, 2-(1-methylethenyl)-		17.7
7792.	29460-90-0	0	1	0	Pyrazine, 2-(1-methylethyl)-		17.7
7793.	34514-52-8	1	0	0	Pyrazine, methyl(1-methylethyl)-		17.7
7794.		1	0	0	Pyrazine, 2-methyl-3-butyl-		17.7
7795.		1	0	0	Pyrazine, 2-methyl-3-(2-methylbutyl)-		17.7
7796.	32737-06-7	1	0	0	Pyrazine, 2-methyl-3-(3-methylbutyl)-		17.7
7797.	15986-81-9	0	1	0	Pyrazine, 2-methyl-3-(1-methylethyl)-		17.7
7798.	13925-05-8	1	0	0	Pyrazine, 2-methyl-5-(1-methylethyl)-		17.7
7799.	13925-06-9	1	0	0	Pyrazine, 2-methyl-3-(2-methylpropyl)-		17.7
7800.	29444-53-9	1	0	0	Pyrazine, 2-methyl-3-phenyl-		17.7
7801.	58861-90-8	1	0	0	Pyrazine, 2-methyl-5-phenyl-		17.7
7802.	74233-03-7	1	0	0	Pyrazine, 2-methyl-6-phenyl-		17.7
7803.	55138-67-5	0	1	0	Pyrazine, 2-methyl-6-(1-propenyl)-		17.7
7804.	36541-30-7	1	0	0	Pyrazine, methylpropyl-		17.7
7805.	29461-03-8	1	0	0	Pyrazine, 2-methyl-5-propyl-		17.7
7806.	29444-46-0	1	0	0	Pyrazine, 2-methyl-6-propyl-		17.7
7807.	67952-65-2	0	1	0	Pyrazine, 3 (5 or 6)-methyl-2-methylthio-		17.7, 18.1
7808.	6303-75-9	1	0	0	Pyrazine, 2-pentyl-		17.7
7809.	29460-97-7	1	1	1	Pyrazine, 2-phenyl-		17.7
7810.	28217-95-0	1	0	0	Pyrazine, 2-phenylmethyl-		17.7
7811.		1	0	0	Pyrazine, 2-(1-propenyl)-		17.7
7812.	18138-03-9	1	0	0	Pyrazine, 2-propyl-		17.7
7813.	1124-11-4	1	1	1	Pyrazine, tetramethyl-		17.7, 24.3, 25.29
7814.	14667-55-1	1	1	1	Pyrazine, trimethyl-		17.7, 24.3, 25.29
7815.	61892-91-9	1	0	0	Pyrazinebutanol, 3-methyl-		2.5, 17.7
7816.	5780-66-5	1	0	0	Pyrazinecarboxaldehyde		3.12, 17.7
7817.		0	1	0	Pyrazinecarboxaldehyde, 5-(2-furanyl)-3-methyl-		3.12, 10.2, 17.7
7818.	6705-63-9	1	1	1	Pyrazineethanol		2.5, 17.7
7819.	61892-92-0	1	1	1	Pyrazineethanol, 3-methyl-		2.5, 17.7
7820.	61892-93-1	1	1	1	Pyrazineethanol, 6-methyl-		2.5, 17.7
7821.	6705-33-5	1	0	0	Pyrazinemethanol		2.5, 17.7
7822.	61892-95-3	1	1	1	Pyrazinemethanol, 5-methyl-		2.5, 17.7
7823.		0	1	0	Pyrazinepentanol		2.5, 17.7
7824.	6270-63-9	1	0	0	2(1*H*)-Pyrazinone = 2-pyrazinol		17.7, 17.13
7825.	78210-68-1	1	0	0	2(1*H*)-Pyrazinone, 1-methyl-3-(1-methylethyl)-		17.7, 17.13
7826.	19838-07-4	1	1	1	2(1*H*)-Pyrazinone, 3-methyl-		17.7, 17.13
7827.	20721-17-9	1	0	0	2(1*H*)-Pyrazinone, 5-methyl-		17.7, 17.13

(*continued*)

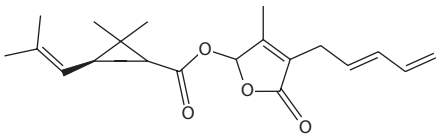
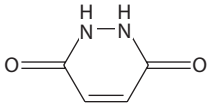
(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7828.	20721-18-0	1	0	0	2(1*H*)-Pyrazinone, 6-methyl-		17.7, 17.13
7829.	288-13-1	1	1	1	1*H*-Pyrazole		17.4
7830.		1	0	0	1*H*-Pyrazole, C_2-alkyl-		17.4
7831.	13808-64-5	1	0	0	1*H*-Pyrazole, 4-bromo-3-methyl-		17.4, 18.4
7832.	67771-72-6	1	0	0	1*H*-Pyrazole, dimethyl-		17.4
7833.	2820-37-3	1	0	0	1*H*-Pyrazole, 3,4-dimethyl-		17.4
7834.	67-51-6	1	0	0	1*H*-Pyrazole, 3,5-dimethyl-		17.4
7835.	1131-16-4	1	0	0	1*H*-Pyrazole, 3,5-dimethyl-1-phenyl-		17.4
7836.	66719-08-2	1	0	0	1*H*-Pyrazole, methyl-		17.4
7837.	930-36-9	1	0	0	1*H*-Pyrazole, 1-methyl-		17.4
7838.	1453-58-3	1	0	0	1*H*-Pyrazole, 3-methyl-		17.4
7839.	3347-62-4	0	1	0	1*H*-Pyrazole, 3-methyl-5-phenyl-		17.4
7840.	7554-65-6	1	0	0	1*H*-Pyrazole, 4-methyl-		17.4
7841.	1072-91-9	1	0	0	1*H*-Pyrazole, 1,3,5-trimethyl-		17.4
7842.	5519-42-6	1	0	0	1*H*-Pyrazole, 3,4,5-trimethyl-		17.4
7843.	61892-79-3	1	0	0	1*H*,7*H*-Pyrazolo[1,2-*a*]pyrazole-1, 7-dione, tetrahydro-		17.13, 17.23
7844.	33986-27-5	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methyl-2-butenyl)-		12.2, 17.23
7845.	33698-49-6	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methylbutyl)-		12.2, 17.23
7846.	34232-31-0	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methyl-2-butenyl)-		12.2, 17.23
7847.	33986-28-6	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methylbutyl)-		12.2, 17.23
7848.	64990-23-4	1	0	0	Pyrenamine		12.2
7849.	64828-53-1	1	0	0	Pyrenamine, *N*-methyl-		12.2
7850.	1606-67-3	1	0	0	1-Pyreneamine		12.2
7851.	129-00-0	1	1	1	Pyrene {benzo[*def*]phenanthrene}		0.4, 1.20, 25.29, 26.9
7852.		1	0	0	Pyrene, alkyl-		1.20
7853.	35980-18-8	1	0	0	Pyrene, 1-butyl-		1.20
7854.	55682-90-1	1	0	0	Pyrene, 1-decyl-		1.20
7855.	28779-32-0	1	0	0	Pyrene, dihydro-		1.20
7856.	14927-67-4	1	0	0	Pyrene, 1,2-dihydro-		1.20
7857.	30582-03-7	1	0	0	Pyrene, dimethyl- {at least three isomers in MSS}		1.20
7858.	64401-21-4	1	0	0	Pyrene, 1,3-dimethyl-		1.20
7859.	42397-64-8	1	0	0	Pyrene, 1,6-dinitro-		16.1
7860.	42397-65-9	1	0	0	Pyrene, 1,8-dinitro-		16.1
7861.		1	0	0	Pyrene, ethyl-		1.20
7862.	56142-12-2	1	0	0	Pyrene, 1-ethyl-		1.20

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7863.	71607-74-4	1	0	0	Pyrene, ethylmethyl-		1.20
7864.	71607-75-5	1	0	0	Pyrene, hexamethyl-		1.20
7865.	72692-89-8	1	0	0	Pyrene, 1-hexyl-		1.20
7866.	27577-90-8	1	0	0	Pyrene, methyl- {several isomers in MSS}		1.20
7867.	2381-21-7	1	1	1	Pyrene, 1-methyl-		1.20
7868.	3442-78-2	1	0	0	Pyrene, 2-methyl-		1.20
7869.	3353-12-6	1	0	0	Pyrene, 4-methyl-		1.20
7870.	5522-43-0	1	0	0	Pyrene, 1-nitro-		16.1
7871.	57835-92-4	1	0	0	Pyrene, 4-nitro-		16.1
7872.	71608-00-9	1	0	0	Pyrene, 1-octyl-		1.20
7873.	71607-76-6	1	0	0	Pyrene, pentamethyl- {at least three isomers in MSS}		1.20
7874.	56142-09-7	1	0	0	Pyrene, propyl-		1.20
7875.	71630-71-2	1	0	0	Pyrene, 1-tetradecyl-		1.20
7876.	66161-17-9	1	0	0	Pyrene, tetrahydro-		1.20
7877.	57633-59-7	1	0	0	Pyrene, 1,2,6,7-tetrahydro-		1.20
7878.	60826-75-7	1	0	0	Pyrene, tetramethyl- {at least four isomers in MSS}		1.20
7879.	41637-88-1	1	0	0	Pyrene, trimethyl- {at least three isomers in MSS}		1.20
7880.		1	0	0	Pyrenol		9.22
7881.	121-21-1 4466-14-2 25402-06-6 121-21-9 1171-63-0 121-29-9 121-20-0	0	1	0	Pyrethrins (natural)		5.3, 21.3
7882.	289-80-5	1	0	0	Pyridazine		17.7
7883.	123-33-1	1	1	1	3,6-Pyridazinedione, 1,2-dihydro- {maleic hydrazide, MH, MH-30®}		17.7, 17.13, 21.3, 25.29
7884.	5716-15-4	0	1	0	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt		2.5, 12.2, 17.7, 17.13
7885.	51542-52-0	0	1	0	3,6-Pyridazinedione, 1, 2-dihydro-, potassium salt		17.7, 17.13
7886.		1	0	0	(2*H*)-Pyridazinone, 1-methyl-3-propyl-		17.7
7887.	26445-05-6	1	0	0	Pyridinamine		12.2, 17.7
7888.	71607-77-7	1	0	0	Pyridinamine, *N*-methyl-		12.2, 17.7
7889.	504-29-0	1	1	1	2-Pyridinamine		12.2, 17.7
7890.	1603-40-3	1	0	0	2-Pyridinamine, 3-methyl-		12.2, 17.7
7891.	695-34-1	1	0	0	2-Pyridinamine, 4-methyl- {2-amino-4-picoline}		12.2, 17.7
7892.	1603-41-4	1	0	0	2-Pyridinamine, 5-methyl-		12.2, 17.7
7893.	1824-81-3	1	0	0	2-Pyridinamine, 6-methyl-		12.2, 17.7
7894.	30315-34-5	0	1	0	2-Pyridinamine, 5-(1-methyl-2-pyrrolidinyl)-, (S)-		12.2, 17.9
7895.	1202-34-2	1	0	0	2-Pyridinamine, *N*-2-pyridinyl-		12.2, 17.11
7896.	462-08-8	1	0	0	3-Pyridinamine		12.2, 17.7

(*continued*)

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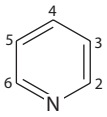
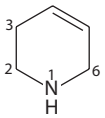
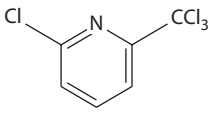
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7897.	61771-67-3	1	0	0	3-Pyridinamine, 6-methoxy-*N*-methyl-		10.2, 12.2, 17.7
7898.	3430-10-2	1	0	0	3-Pyridinamine, 2-methyl-		12.2, 17.7
7899.	3430-27-1	1	0	0	3-Pyridinamine, 4-methyl-		12.2, 17.7
7900.	18364-47-1	1	0	0	3-Pyridinamine, *N*-methyl-		12.2, 17.7
7901.	504-24-5	1	0	0	4-Pyridinamine		12.2, 17.7
7902.	110-86-1	1	1	1	Pyridine		0.4, 17.7, 23.5, 24.3, 25.29
7903.		1	0	0	Pyridine, (C_5-alkenyl)-		17.7
7904.		1	0	0	Pyridine, alkyl-		17.7
7905.		1	0	0	Pyridine, C_3-alkyl-		17.7
7906.		1	0	0	Pyridine, (C_3-alkylphenyl)- {two isomers detected}		17.7
7907.	65375-18-0	1	0	0	Pyridine, butenyl- {three isomers}		17.7
7908.	31388-09-7	1	0	0	Pyridine, butyl-		17.7
7909.	27175-64-0	1	1	1	Pyridine, dimethyl- {lutidine}		0.4, 17.7
7910.	29011-62-9	1	0	0	Pyridine, dimethylethenyl-		17.7
7911.		0	1	0	Pyridine, dimethylethyl- {three isomers detected}		17.7
7912.		1	0	0	Pyridine, dimethyl-2-(1-methylethyl)-		17.7
7913.		1	0	0	Pyridine, dimethylphenyl-		17.7
7914.	56842-43-4	1	0	0	Pyridine, diphenyl-		17.7
7915.	1337-81-1	1	0	0	Pyridine, ethenyl-		17.7
7916.	25638-00-0	1	0	0	Pyridine, ethenylmethyl-		17.7
7917.		1	0	0	Pyridine, ethenyltrimethyl-		17.7
7918.	28631-77-8	1	0	0	Pyridine, ethyl-		17.7
7919.	27987-10-6	1	1	1	Pyridine, ethyl methyl- {four isomers}		17.7
7920.	64849-96-3	1	0	0	Pyridine, ethylphenyl-		17.7
7921.	1333-41-1	1	1	1	Pyridine, methyl- {picoline}		0.4, 17.7
7922.	64828-54-2	1	0	0	Pyridine, methylphenyl-		17.7
7923.	65307-85-9	1	0	0	Pyridine, pentyl-		17.7
7924.	64828-55-3	1	0	0	Pyridine, phenylpropyl-		17.7
7925.		1	0	0	Pyridine, phenyltrimethyl-		17.7
7926.	65375-17-9	1	0	0	Pyridine, propenyl-		17.7
7927.	65307-84-8	1	0	0	Pyridine, propyl-		17.7
7928.		1	0	0	Pyridine, tetramethyl-		17.7
7929.	29611-84-5	1	1	1	Pyridine, trimethyl- {collidine}		0.4, 17.7
7930.	6972-40-3	1	0	0	Pyridine, 1-ethyl-1,2,3,6-tetrahydro-		17.7
7931.	694-05-3	1	1	1	Pyridine, 1,2,3,6-tetrahydro- {Δ^3-piperidine}		17.7
7932.		0	1	0	Pyridine, 1-methyl-6-(2-pyridinyl)- 1,2,5,6-tetrahydro-		17.11
7933.		1	0	0	Pyridine, 2-(C_3-alkylphenyl)- {two isomers detected}		17.7
7934.	5058-19-5	1	0	0	Pyridine, 2-butyl-		17.7
7935.	1929-82-4	0	1	0	Pyridine, 2-chloro-6-(trichloromethyl)- {Nitrapyrin®}		17.7, 18.4, 21.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7936.	100-69-6	1	1	1	Pyridine, 2-ethenyl-		17.7
7937.	22382-94-1	1	0	0	Pyridine, 2-ethenyl-3-methyl-		17.7
7938.	3883-39-4	1	0	0	Pyridine, 2-ethenyl-5-methyl-		17.7
7939.	1122-70-9	1	0	0	Pyridine, 2-ethenyl-6-methyl-		17.7
7940.	14529-53-4	1	0	0	Pyridine, 2-ethoxy-		10.2, 17.7
7941.	100-71-0	1	1	1	Pyridine, 2-ethyl-		17.7
7942.	1123-96-2	1	0	0	Pyridine, 2-ethyl-3,5-dimethyl- = pyridine, 2,4-dimethyl-6-ethyl-		17.7
7943.	1124-35-2	1	0	0	Pyridine, 2-ethyl-4,6-dimethyl-		17.7
7944.	56986-88-0	1	0	0	Pyridine, 2-ethyl-3-methyl-		17.7
7945.	2150-18-7	1	0	0	Pyridine, 2-ethyl-4-methyl-		17.7
7946.	18113-81-0	1	0	0	Pyridine, 2-ethyl-5-methyl-		17.7
7947.	1122-69-6	1	0	0	Pyridine, 2-ethyl-6-methyl-		17.7
7948.	59239-12-2	1	0	0	Pyridine, 2-ethyl-6-phenyl-		17.7
7949.		1	0	0	Pyridine, 2-(1-hydroxy-1-pentyl)-		2.5, 17.7
7950.	1628-89-3	1	0	0	Pyridine, 2-methoxy-		10.2, 17.7
7951.	109-06-8	1	1	1	Pyridine, 2-methyl- {2-picoline}		0.4, 17.7, 25.29
7952.		1	0	0	Pyridine, 2-methyl-3-(1-methylethyl)-		17.7
7953.	64114-31-4	1	1	1	Pyridine, 2-methyl-3-(1-methyl-2-pyrrolidinyl)- {2-methylnicotine}		17.9
7954.	78210-48-7	1	0	0	Pyridine, 2-methyl-3-(1-propenyl)-		17.7
7955.	15032-21-0	1	0	0	Pyridine, 2-methyl-4-phenyl-		17.7
7956.	56057-93-3	1	1	1	Pyridine, 2-methyl-5-(1-methylethenyl)-		17.7
7957.	20194-71-2	1	1	1	Pyridine, 2-methyl-5-(1-methylethyl)-		17.7
7958.	56057-96-6	1	0	0	Pyridine, 2-methyl-5-(1-propenyl)-		17.7
7959.		1	0	0	Pyridine, 2-methyl-6-(3-methylbutyl)-		17.7
7960.	2294-76-0	1	1	1	Pyridine, 2-pentyl-		17.7, 24.3
7961.	1008-89-5	1	0	0	Pyridine, 2-phenyl-		17.7
7962.		1	0	0	Pyridine, 2-propenyl-		17.7
7963.	622-39-9	1	0	0	Pyridine, 2-propyl-		17.7
7964.	101-82-6	1	0	0	Pyridine, 2-(phenylmethyl)-		17.7
7965.	64389-08-8	1	0	0	Pyridine, 2-(1,5-dimethyl-1*H*-pyrrol-2-yl)-		17.9
7966.	7399-50-0	1	0	0	Pyridine, 2-(1-ethylpropyl)-		17.7
7967.	59409-91-5	1	0	0	Pyridine, 2-(1-methyl-3-butenyl)-		17.7
7968.	6515-13-5	1	0	0	Pyridine, 2-(1-methylethenyl)-		17.7
7969.	644-98-4	1	0	0	Pyridine, 2-(1-methylethyl)-		17.7
7970.	525-75-7	1	1	1	Pyridine, 2-(1-methyl-1*H*-pyrrol-2-yl)- {α-nicotyrine}		17.9
7971.	17618-94-9	1	0	0	Pyridine, 2-(1-propenyl)-		17.7
7972.	78210-51-2	1	0	0	Pyridine, 2-(1*H*-pyrrol-1-ylmethyl)-		17.9
7973.	21606-61-1	1	0	0	Pyridine, 2-(2-butenyl)-		17.7
7974.	114-91-0	1	0	0	Pyridine, 2-(2-methoxyethyl)-		10.2, 17.7
7975.		1	0	0	Pyridine, 2-(2-methylbutyl)-		17.7
7976.	6304-24-1	1	0	0	Pyridine, 2-(2-methylpropyl)-		17.7
7977.	583-61-9	1	1	1	Pyridine, 2,3-dimethyl- {2,3-lutidine}		17.7
7978.	78210-40-9	1	0	0	Pyridine, 2-(3-ethylphenyl)-		17.7
7979.	6973-66-6	1	0	0	Pyridine, 2-(3-methylbutyl)-		17.7
7980.	68258-35-5	0	1	0	Pyridine-2-^{13}C-3-^{14}C, 3-fluoro-5-(2-piperidinyl)-, (±)-, labeled with ^{13}C and ^{14}C		17.11, 18.4
7981.	2233-29-6	1	0	0	Pyridine, 2,3,4-trimethyl- {2,3,4-collidine}		17.7

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
7982.	695-98-7	1	1	1	Pyridine, 2,3,5-trimethyl- {2,3,5-collidine}		17.7
7983.	1462-84-6	1	1	1	Pyridine, 2,3,6-trimethyl- {2,3,6-collidine}		17.7
7984.	108-47-4	1	1	1	Pyridine, 2,4-dimethyl- {2,4-lutidine}		17.7
7985.	1122-45-8	1	0	0	Pyridine, 2,4-dimethyl-, 1-oxide		17.7
7986.	36238-36-5	1	0	0	Pyridine, 2,4-dimethyl-5-(1-methylethyl)-		17.7
7987.	1122-39-0	1	0	0	Pyridine, 2,4,5-trimethyl- {2,4,5-collidine}		17.7
7988.	108-75-8	1	1	1	Pyridine, 2,4,6-trimethyl- {2,4,6-collidine}		0.4, 17.7
7989.	589-93-5	1	1	1	Pyridine, 2,5-dimethyl- {2,5-lutidine}		17.7
7990.	15827-72-2	0	1	0	Pyridine, 2,5-diphenyl-		17.7
7991.	108-48-5	1	1	1	Pyridine, 2,6-dimethyl- {2,6-lutidine}		0.4, 17.7
7992.	23580-52-1	0	1	0	Pyridine, 2,6-dimethyl-3-ethyl-		17.7
7993.	36917-36-9	1	0	0	Pyridine, 2,6-dimethyl-4-ethyl-		17.7
7994.	1463-03-2	1	0	0	Pyridine, 2,6-dimethyl-3-phenyl-		17.7
7995.	3558-69-8	1	0	0	Pyridine, 2,6-diphenyl-		17.7
7996.	3731-52-0	1	1	1	Pyridine, 3-(aminomethyl)-		12.2, 17.7
7997.	539-32-2	1	1	1	Pyridine, 3-butyl-		17.7
7998.	6760-12-9	1	0	0	Pyridine, 3-butyl-2,6-dimethyl-		17.7
7999.	1121-55-7	1	1	1	Pyridine, 3-ethenyl-		17.7
8000.	51961-51-4	1	0	0	Pyridine, 3-ethenyl-5-methyl-		17.7
8001.	536-78-7	1	1	1	Pyridine, 3-ethyl-		17.7, 24.3
8002.	529-21-5	1	0	0	Pyridine, 3-ethyl-4-methyl-		17.7
8003.	3999-78-8	1	0	0	Pyridine, 3-ethyl-5-methyl-		17.7
8004.	7295-76-3	1	1	1	Pyridine, 3-methoxy-		10.2, 17.7
8005.	78210-42-1	1	0	0	Pyridine, 3-methoxy-5-methyl-		10.2, 17.7
8006.	108-99-6	1	1	1	Pyridine, 3-methyl- {3-picoline}		17.7, 25.29
8007.	1003-73-2	1	0	0	Pyridine, 3-methyl-1-oxide		17.7
8008.		1	0	0	Pyridine, 3-methyl-2-(2-methylbutyl)-		17.7
8009.		1	0	0	Pyridine, 3-methyl-2-(3-methylbutyl)-		17.7
8010.	72693-04-0	1	0	0	Pyridine, 3-methyl-2-(1-methylethyl)-		17.7
8011.	18368-73-5	1	0	0	Pyridine, 3-methyl-2-nitro-		16.1, 17.7
8012.	10273-90-2	1	0	0	Pyridine, 3-methyl-2-phenyl-		17.7
8013.	10477-94-8	1	0	0	Pyridine, 3-methyl-5-phenyl-		17.7
8014.	1802-20-6	1	1	1	Pyridine, 3-pentyl-		17.7
8015.	1008-88-4	1	0	0	Pyridine, 3-phenyl-		17.7
8016.	4673-31-8	1	0	0	Pyridine, 3-propyl-		17.7
8017.		1	1	1	Pyridine, 3-propenyl-		17.7
8018.	78210-50-1	1	0	0	Pyridine, 3-(tetrahydro-2-furanyl)-		10.2, 17.9
8019.		1	0	0	Pyridine, 3-(1-butyl-2-pyrrolidinyl)-		17.9
8020.	73952-98-4	1	0	0	Pyridine, 3-(dimethyl-1*H*-pyrrolyl)-		17.9
8021.	78210-38-5	1	0	0	Pyridine, 3-(1,3-dimethyl-1*H*-pyrrol-2-yl)-		17.9
8022.	27293-93-2	0	1	0	Pyridine, 3-(1,3-dimethyl-2-pyrrolidinyl)-		17.9
8023.	65734-44-3	1	0	0	Pyridine,3-(1,5-dimethyl-1*H*-pyrrol-2-yl)-		17.9
8024.	78210-88-5	1	0	0	Pyridine, 3-[1-(5-ethyl-2-furanyl)-1*H*-pyrrol-2-yl]-		10.2, 17.9
8025.	68245-76-1	1	1	1	Pyridine, 3-(1-ethyl-2-piperidinyl)-, (S)-		17.11
8026.	91429-66-2	1	0	0	Pyridine, 3-(1-ethyl-2-pyrrolidinyl)-		17.9
8027.	5979-92-0	1	0	0	Pyridine, 3-(1-ethyl-2-pyrrolidinyl)-, (S)-		17.9
8028.	78210-87-4	1	0	0	Pyridine, 3-[1-[2-(2-furanyl)ethyl]-2-pyrrolidinyl]-, (S)-		10.2, 17.9

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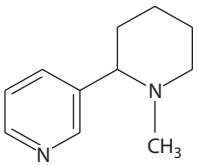
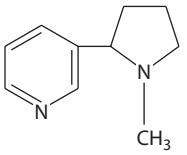
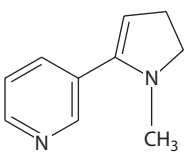
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8029.	78210-85-2	1	0	0	Pyridine, 3-[1-(2-furanylmethyl)-2-pyrrolidinyl]-, (S)-		10.2, 17.9
8030.	4754-27-2	1	0	0	Pyridine, 3-(1-hydroxyethyl)-		2.5, 17.7
8031.	123676-95-9	0	1	0	Pyridine, 3-[1-[(hydroxy-1-oxooctyl)oxy]-2-pyrrolidinyl]-		2.5, 17.9
8032.		1	0	0	Pyridine, 3-(1-methyl-3-butenyl)-		17.7
8033.	72461-69-9	0	1	0	Pyridine, 3-[1-(1-methylethyl)-2-pyrrolidinyl]-, (S)-		17.9
8034.	15825-89-5	1	0	0	Pyridine, 3-(1-methylethenyl)-		17.7
8035.	88111-63-1	1	0	0	Pyridine, 3-(1-methylethoxy)-		10.2, 17.7
8036.		1	0	0	Pyridine, 3-(1-methylethyl)-		17.7
8037.	78210-86-3	1	0	0	Pyridine, 3-[1-[(5-methyl-2-furanyl)methyl]-2-pyrrolidinyl]-, (S)-		10.2, 17.9
8038.	78210-84-1	1	0	0	Pyridine, 3-[1-methyl-2-(1-methylethyl)-1*H*-imidazol-5-yl]-		17.9
8039.	24380-92-5 19730-04-2	1	1	1	Pyridine, 3-(1-methyl-2-piperidinyl)-, (S)- {*N*-methylanabasine}		0.4, 17.11
8040.	22083-74-5	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (±)-		17.9
8041.	25162-00-9	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (R)- {*d*-nicotine}		17.9
8042.	54-11-5	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine}		0.4, 17.9, 21.3, 23.5, 25.29, 26.9
8043.	65-30-5	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate (2:1)		17.9, 18.1, 20.6, 21.3
8044.	6505-86-8	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate		17.9, 18.1, 20.6, 21.3
8045.	2820-55-5	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, 1-oxide, (S)- {nicotine *N*-oxide}		0.4, 17.9
8046.	2820-51-1	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, hydrochloride, (S)-		17.9, 18.4, 20.6
8047.	16586-18-8	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, labeled with ^{14}C, (S)-		17.9
8048.	25429-24-7	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, monohydroxy derivative, (*S*)-		2.5, 17.9
8049.	2055-29-0	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, *N*,1-dioxide, (S)-		17.9
8050.	491-26-9	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, *N*-oxide, (2S)-		17.9
8051.	6912-85-2	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolinyl)- {2,3-dehydronicotine}		17.9
8052.	101540-79-8	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolinyl)-6-methyl-		17.9

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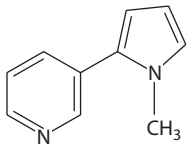
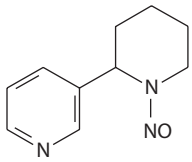
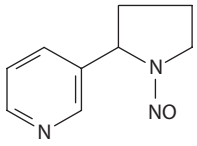
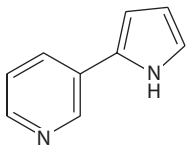
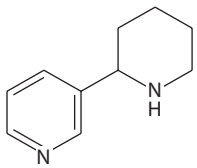
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8053.	487-19-4	1	1	1	Pyridine, 3-(1-methyl-1*H*-pyrrol-2-yl)- {nicotyrine}		0.4, 17.9
8054.	1133-64-8 37620-20-5	1	1	1	Pyridine, 3-(1-nitroso-2-piperidinyl)-, (S)- {NAB}		15.8, 17.11, 23.5
8055.	16543-55-8	1	1	1	Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-, (S)- {NNN}		15.8, 17.9, 23.5
8056.	53844-45-4	1	1	1	Pyridine, 3-(1-nitroso-2-pyrrolidinyl-2-^{14}C)-, (S)-, label with ^{14}C		15.8, 17.9
8057.		1	0	0	Pyridine, 3-(1-pentyl-2-piperidinyl)-,		17.11
8058.		1	0	0	Pyridine, 3-(1-pentyl-2-pyrrolidinyl)-		17.9
8059.	15376-62-2	1	1	1	Pyridine, 3-(1-propenyl)-		17.7
8060.	78210-89-6	1	0	0	Pyridine, 3-[1-(5-propyl-2-furanyl)-1*H*-pyrrol-2-yl]-		10.2, 17.9
8061.	72692-99-0 50966-74-0	1	0	0	Pyridine, 3-(1*H*-pyrrol-1-yl)-		17.9
8062.	494-98-4	1	1	1	Pyridine, 3-(1*H*-pyrrol-2-yl)- {nornicotyrine}		0.4, 17.9
8063.	80866-95-1	1	0	0	Pyridine, 3-(1*H*-pyrrol-1-ylmethyl)-		17.9
8064.	36127-43-2	1	0	0	Pyridine, 3-(1,3,3-trimethyl-2-pyrrolidinyl)-		17.9
8065.	78210-90-9	1	0	0	Pyridine, 3-(2-butenyl)-		17.7
8066.		1	0	0	Pyridine, 3-(2-ethylphenyl)-		17.7
8067.	78210-49-8	1	0	0	Pyridine, 3-(2-methyl-1*H*-pyrrol-1-yl)-		17.9
8068.	6312-09-0	1	0	0	Pyridine, 3-(2-phenylethyl)-		17.7
8069.	13078-04-1	1	0	0	Pyridine, 3-(2-piperidinyl)-		17.11
8070.	34366-21-7	1	0	0	Pyridine, 3-(2-piperidinyl)-, (R)- {*d*-anabasine}		17.11
8071.	494-52-0	1	1	1	Pyridine, 3-(2-piperidinyl)-, (S)- {*l*-anabasine}		0.4, 17.11, 25.29
8072.		0	1	0	Pyridine, 3-(2-piperidinyl)- 6-oxo- {6-oxoanabasine}		17.11
8073.	7300-28-9	1	0	0	Pyridine, 3-(2-propenyl)-		17.7
8074.	69698-09-5	1	1	1	Pyridine, 3-(1-pyrrolidinyl)-		17.9
8075.	5746-86-1	1	0	0	Pyridine, 3-(2-pyrrolidinyl)-		17.9
8076.	7076-23-5	1	1	1	Pyridine, 3-(2-pyrrolidinyl)-, (R)- {*d*-nornicotine}		17.9

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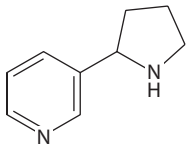
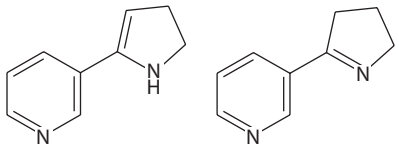
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
8077.	494-97-3	1	1	1	Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine}		0.4, 17.9, 25.29, 26.9
8078.	53844-44-3	1	1	1	Pyridine, 3-(2-pyrrolidinyl-2-^{14}C)-, (S)-, labeled with ^{14}C		17.9
8079.	71532-24-6	1	0	0	Pyridine, 3-(3-butenyl)-		17.7
8080.		1	0	0	Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)- {*d*-myosmine}		17.9
8081.	532-12-7	1	1	1	Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)- {*l*-myosmine}		0.4, 17.9
8082.	525-74-6	1	1	1	Pyridine, 3-(3,4-dihydro-1-methyl-2*H*-pyrrol-5-yl)- {*N*-methylmyosmine}		0.4, 17.9
8083.	65719-03-1	1	0	0	Pyridine, 3-(3,4-dihydro-2-methyl-2*H*-pyrrol-5-yl)-		17.9
8084.	78249-81-7	1	0	0	Pyridine, 3-(3,4-dihydro-3-methyl-2*H*-pyrrol-5-yl)-		17.9
8085.	78210-37-4	1	0	0	Pyridine, 3-(3,4-dihydro-4-methyl-2*H*-pyrrol-5-yl)-		17.9
8086.	24950-44-5	1	0	0	Pyridine, 3,3′-(1,2-ethenediyl)bis-		17.7
8087.	78210-39-6	1	0	0	Pyridine, 3-(3-ethyl-3,4-dihydro-2*H*-pyrrol-5-yl)-		17.9
8088.	78210-43-2	1	0	0	Pyridine, 3,3′-methylenebis-		17.7
8089.		1	0	0	Pyridine, 3,4′-methylenebis		17.7
8090.	4385-67-5	1	0	0	Pyridine, 3-(3-methylphenyl)-		17.7
8091.		1	0	0	Pyridine, 3-(3-penten-2-yl)-		17.7
8092.	64811-57-0	1	0	0	Pyridine, dihydro-3-(1-methyl-I*H*-pyrrol-2-yl)-		17.9
8093.	525-74-6	0	1	0	Pyridine, 3-(4,5-dihydro-1-methyl-1*H*-pyrrol-2-yl)-		17.9
8094.	583-58-4	1	1	1	Pyridine, 3,4-dimethyl- {3,4-lutidine}		17.7
8095.		1	0	0	Pyridine, 3,4-diphenyl-		17.7
8096.		1	0	0	Pyridine, 3-(4-butenyl)-		17.7
8097.	78210-41-0	1	0	0	Pyridine, 3-(4-ethylphenyl)-		17.7
8098.	2057-39-8	1	0	0	Pyridine, 3-(4-methyl-3-pentenyl)-		17.7
8099.	72692-97-8	1	0	0	Pyridine, 3-(4-methylpentyl)-		17.7
8100.	78210-44-3	1	0	0	Pyridine, 3-(4-pyridinylmethyl)-		17.11
8101.	78210-45-4	1	0	0	Pyridine, 3-[2,5-dihydro-1-[(5-methyl-2-furanyl)methyl]-1*H*-pyrrol-2-yl]-		17.9
8102.	591-22-0	1	1	1	Pyridine, 3,5-dimethyl- {3,5-lutidine}		17.7
8103.	92-07-9	1	0	0	Pyridine, 3,5-diphenyl-		17.7
8104.	78210-46-5	1	0	0	Pyridine, 3-[(5-methyl-2-furanyl) methyl]-		10.2, 17.7
8105.	5335-75-1	1	0	0	Pyridine, 4-butyl-		17.7
8106.	100-43-6	1	1	1	Pyridine, 4-ethenyl-		17.7
8107.	536-75-4	1	1	1	Pyridine, 4-ethyl-		17.7
8108.	70199-60-9	1	0	0	Pyridine, 4-(methoxymethyl)-		10.2, 17.7
8109.	108-89-4	1	1	1	Pyridine, 4-methyl- {4-picoline}		17.7, 25.29
8110.		1	0	0	Pyridine, 4-methyl-2-(2-methylbutyl)-		17.7

(*continued*)

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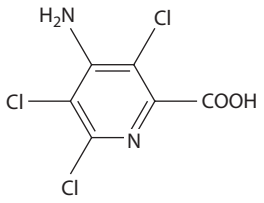
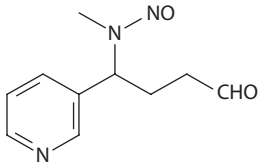
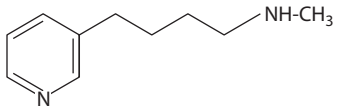
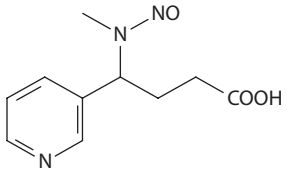
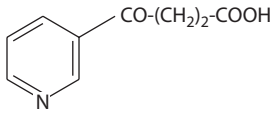
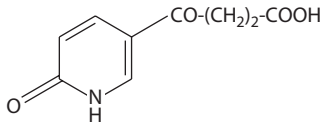
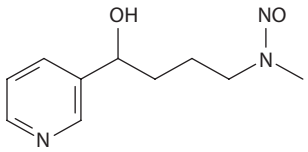
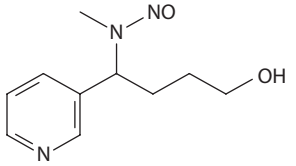
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8111.	78210-47-6	1	0	0	Pyridine, 4-methyl-2-(3-methylbutyl)-		17.7
8112.		1	0	0	Pyridine, 4-methyl-2-(2-methylpropyl)-		17.7
8113.	84625-54-7	1	0	0	Pyridine, 4-methyl-2-pentyl-		17.7
8114.	30256-45-2	1	0	0	Pyridine, 4-methyl-2-propyl-		17.7
8115.	75835-01-7	1	0	0	Pyridine, 4-methyl-2-(2-phenylethyl)-		17.7
8116.	3475-21-6 19352-29-5	1	1	1	Pyridine, 4-methyl-3-phenyl-		17.7
8117.	939-23-1	1	1	1	Pyridine, 4-phenyl-		17.7
8118.	2116-65-6	0	1	0	Pyridine, 4-(phenylmethyl)-		17.7
8119.	78210-91-0	1	0	0	Pyridine, 4-(1-butenyl)-		17.7
8120.	3978-81-2	1	1	1	Pyridine, 4-(1,1-dimethylethyl)- {4-*tert*-butylpyridine}		17.7
8121.	696-30-0	1	0	0	Pyridine, 4-(1-methylethyl)-		17.7
8122.	22241-38-9	1	0	0	Pyridine, 4-(4-methylpentyl)-		17.7
8123.		1	0	0	Pyridine, 4-(2-phenylpropyll)-		17.7
8124.	17618-95-0	1	0	0	Pyridine, 4-(1-propenyl)-		17.7
8125.	140-76-1	1	0	0	Pyridine, 5-ethenyl-2-methyl-		17.7
8126.	104-90-5	1	1	1	Pyridine, 5-ethyl-2-methyl-		17.7
8127.	34137-26-3	0	1	0	Pyridine, 5-fluoro-3-(1-methyl-2-pyrrolidinyl)-, (S)-		17.9, 18.4
8128.	55270-47-8	1	0	0	Pyridine, 5-methoxy-2-methyl-		10.2, 17.7
8129.		1	0	0	Pyridine, 5-methyl-2-(2-methylbutyl)-		17.7
8130.	6343-58-4	1	0	0	Pyridine, 5-methyl-2-(1-methylethyl)-		17.7
8131.		1	0	0	Pyridine, 5-methyl-2-(2-methylpropyl)-		17.7
8132.		1	0	0	Pyridine, 5-methyl-2-pentyl-		17.7
8133.		1	0	0	Pyridine, 5-methyl-2-propyl-		17.7
8134.		1	0	0	Pyridine, 6-methyl-3-(1-methyl-2-pyrrolinyl)-		17.9
8135.	36541-27-2	1	0	0	Pyridinecarbonitrile, dimethyl-		11.2, 17.7
8136.	36541-26-1	1	0	0	Pyridinecarbonitrile, methyl-		11.2, 17.7
8137.	55738-21-1	1	0	0	Pyridinedicarbonitrile		11.2, 17.7
8138.	17945-79-8	1	0	0	2-Pyridinebutanol		2.5, 17.7
8139.	100-70-9	1	0	0	2-Pyridinecarbonitrile		11.2, 17.7
8140.	20970-75-6	1	0	0	2-Pyridinecarbonitrile, 3-methyl-		11.2, 17.7
8141.	1620-76-4	1	0	0	2-Pyridinecarbonitrile, 4-methyl-		11.2, 17.7
8142.	1121-60-4	1	0	0	2-Pyridinecarboxaldehyde		3.12, 17.7
8143.	1452-77-3	1	0	0	2-Pyridinecarboxamide		13.1, 17.7
8144.	72693-02-8	1	0	0	2-Pyridinecarboxamide, 4,6-dimethyl-		13.1, 17.7
8145.	32743-35-4	1	0	0	2-Pyridinecarboxamide, 4-ethyl-		13.1, 17.7
8146.	13509-17-6	1	0	0	2-Pyridinecarboxamide, 5-ethyl-		13.1, 17.7
8147.	78210-61-4	1	0	0	2-Pyridinecarboxamide, 6-ethyl-		13.1, 17.7
8148.	20970-77-8	1	0	0	2-Pyridinecarboxamide, 5-methyl-		13.1, 17.7
8149.	63668-37-1	1	0	0	2-Pyridinecarboxamide, 6-methyl-		13.1, 17.7
8150.	1918-02-1	0	1	0	2-Pyridinecarboxylic acid, 4-amino-3,5,6-trichloro- {Picloram®}		4.3, 12.2, 17.7, 18.4, 21.3
8151.	103-74-2	1	0	0	2-Pyridinemethanol		2.5, 17.7
8152.	35549-47-4	1	0	0	2-Pyridinepropanenitrile		11.2, 17.7
8153.	42545-63-1	1	0	0	3-Pyridineacetaldehyde		3.12, 17.7
8154.	70898-37-2	0	1	0	3-Pyridinebutanal, γ-(methylamino)-		3.12, 12.2, 17.7

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8155.	64091-90-3	1	1	1	3-Pyridinebutanal, γ-(methylnitrosoamino)- {NNA}		3.12, 12.2, 15.8, 17.7
8156.	64142-45-6	1	1	1	3-Pyridinebutanal, γ-(methylnitrosoamino)-, (*Z*)-		3.12, 12.2, 15.8, 17.7
8157.	76014-80-7	0	1	0	3-Pyridinebutanal, γ-oxo-		3.12, 3.13, 17.7
8158.		1	0	0	3-Pyridinebutanamide, *N*-methyl-		13.1, 17.7
8159.	6021-23-4	0	1	0	3-Pyridinebutanamine		12.2, 17.7
8160.	3000-74-6	1	1	1	3-Pyridinebutanamine, *N*-methyl- {dihydrometanicotine}		12.2, 17.7
8161.	17270-48-3	0	1	0	3-Pyridinebutanoic acid, γ-(methylamino)-, (±)-		4.3, 12.2, 17.7
8162.	152720-16-6	0	1	0	3-Pyridinebutanoic acid, γ-(methylnitroamino)-		4.3, 12.2, 15.8, 16.1, 17.7
8163.	123743-84-0 133201-36-2	1	1	1	3-Pyridinebutanoic acid, γ-(methylnitrosoamino)- {iso-NNAC}		4.3, 12.2, 15.8, 17.7
8164.	4192-31-8	0	1	0	3-Pyridinebutanoic acid, γ-oxo-		3.13, 4.3, 17.7
8165.	15873-27-5	1	1	1	3-Pyridinebutanoic acid, 1,6-dihydro-γ,6-dioxo-		3.13, 4.3, 17.7, 17.13
8166.	59578-66-4 76014-81-8	1	1	1	3-Pyridinebutanol, δ-(methylnitrosoamino)- {NNAL} {1-butanol, 4-(*N*-methylnitrosoamino)-1-(3-pyridinyl)-, 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-}		2.5, 12.2, 15.8, 17.7
8167.	133201-37-3	1	1	1	3-Pyridinebutanol, δ-(methylnitrosoamino)- {iso-NNAL} {1-butanol, 4-(*N*-methylnitrosoamino)-4-(3-pyridinyl)-}		2.5, 12.2, 15.8, 17.7
8168.	70898-36-1	0	1	0	3-Pyridinebutanol, δ-amino-		2.5, 12.2, 17.7
8169.	36541-27-2	1	1	1	Pyridinecarbonitrile, dimethyl-		11.2, 17.7
8170.	36541-26-1	1	0	0	Pyridinecarbonitrile, methyl-		11.2, 17.7
8171.	100-54-9	1	1	1	3-Pyridinecarbonitrile {nicotinonitrile}		0.4, 11.2, 17.7
8172.	38076-78-7	1	0	0	3-Pyridinecarbonitrile, 2-amino-5-methyl-		11.2, 12.2, 17.7
8173.	71607-63-1	1	0	0	3-Pyridinecarbonitrile, dimethyl-		11.2, 17.7

(*continued*)

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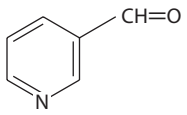
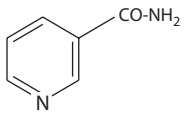
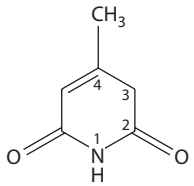
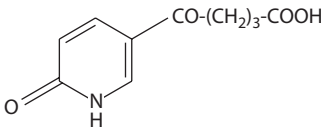
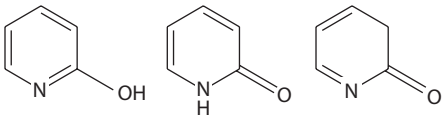
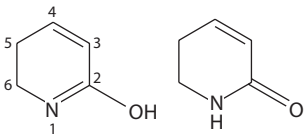
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8174.	61391-07-9	1	0	0	3-Pyridinecarbonitrile, 5-ethyl-		11.2, 17.7
8175.	3222-52-4 32214-82-7	1	0	0	3-Pyridinecarbonitrile, 6-ethyl- = 5-pyridinecarbonitrile, 2-ethyl-		11.2, 17.7
8176.	5444-01-9	1	0	0	3-Pyridinecarbonitrile, 4-methyl-		11.2, 17.7
8177.	42885-14-3	1	0	0	3-Pyridinecarbonitrile, 5-methyl-		11.2, 17.7
8178.	500-22-1	1	1	1	3-Pyridinecarboxaldehyde {nicotinaldehyde, 3-formylpyridine}		3.12, 17.7
8179.	98-92-0	1	1	1	3-Pyridinecarboxamide {nicotinamide}		0.4, 13.1, 17.7
8180.	72692-96-7	1	0	0	3-Pyridinecarboxamide, 2,4-dimethyl-		13.1, 17.7
8181.	10131-48-3	1	0	0	3-Pyridinecarboxamide, 2,6-dimethyl-		13.1, 17.7
8182.	58539-65-4	1	0	0	3-Pyridinecarboxamide, 2-methyl-		13.1, 17.7
8183.	78210-59-0	1	0	0	3-Pyridinecarboxamide, 4-ethyl-		13.1, 17.7
8184.	78210-60-3	1	0	0	3-Pyridinecarboxamide, 6-ethyl-		13.1, 17.7
8185.	6960-22-1	1	0	0	3-Pyridinecarboxamide, 6-methyl-		13.1, 17.7
8186.	4314-66-3	1	0	0	3-Pyridinecarboxamide, *N*-ethyl-		13.1, 17.7
8187.	114-33-0	1	1	1	3-Pyridinecarboxamide, *N*-methyl-		13.1, 17.7
8188.	59-67-6	1	1	1	3-Pyridinecarboxylic acid {nicotinic acid}		0.4, 4.3, 17.7
8189.	5006-66-6	0	1	0	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-		3.13, 4.3, 17.7
8190.	614-18-6	1	1	1	3-Pyridinecarboxylic acid, ethyl ester		5.3, 17.7
8191.	93-60-7	1	1	1	3-Pyridinecarboxylic acid, methyl ester {methyl nicotinate}		5.3, 17.7, 24.3
8192.	55557-02-3	0	1	0	3-Pyridinecarboxylic acid, 1,2,5,6- tetrahydro-1-nitroso-, methyl ester		5.3, 15.8, 17.7
8193.	89-00-9	0	1	0	2,3-Pyridinedicarboxylic acid {quinolinic acid}		4.3, 17.7
8194.	58-56-0	0	1	0	3,4-Pyridinedimethanol, 5-hydroxy- 6-methyl-, hydrochloride		2.5, 17.7, 18.4, 20.6
8195.	13121-99-8	1	0	0	4-Pyridineacetonitrile		11.2, 17.7
8196.	5264-15-3	1	0	0	4-Pyridinebutanol		2.5, 17.7
8197.	100-48-1	1	0	0	4-Pyridinecarbonitrile		11.2, 17.7
8198.	1453-82-3	0	1	0	4-Pyridinecarboxamide {isonicotinamide}		13.1, 17.7
8199.	70898-25-8	1	1	1	2,6(1*H*,3*H*)-Pyridinedione, 3,5-dimethyl-		14.1, 17.7
8200.	72692-95-6	1	0	0	2,6(1*H*,3*H*)-Pyridinedione, 4-methyl-		14.1, 17.7
8201.	72692-94-5	1	0	0	2,6(1*H*,3*H*)-Pyridinedione, 5-methyl-		14.1, 17.7
8202.		1	0	0	3-Pyridinemethanamine, ethyl-		12.2, 17.7
8203.	3000-75-7	1	0	0	3-Pyridinemethanamine, *N*-ethyl-		12.2, 17.7

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8204.	100-55-0	0	1	0	3-Pyridinemethanol		2.5, 17.7
8205.	85352-99-4	0	1	0	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-, 1-oxide		2.5, 12.2, 15.8, 17.7
8206.	71608-01-0	0	1	0	3-Pyridinepentanoic acid, 1, 6-dihydro-δ,6-dioxo-		3.13, 4.3, 17.7, 17.13
8207.	60655-87-0	0	1	0	Pyridinium, 1-α-*L*-arabinopyranosyl-3-carboxy-		2.5, 10.2, 17.7
8208.	35323-45-6	0	1	0	Pyridinium, 3-carboxy-1-β-*D*-glucopyranosyl-, hydroxide {trigonelline}		2.5, 10.2, 17.7
8209.	535-83-1	0	1	0	Pyridinium, 3-carboxy-1-methyl-, hydroxide, inner salt		2.5, 17.7
8210.	27341-45-3	1	0	0	Pyridinol {pyridinone}		2.5, 17.7
8211.	51025-25-3	1	0	0	Pyridinol, dimethyl- {pyridinone, dimethyl-}		2.5, 17.7
8212.		1	1	1	Pyridinol, methyl- {pyridinone, methyl-}		2.5, 17.7
8213.	142-08-5 72762-00-6	1	1	1	2-Pyridinol {2(1*H*)-pyridinone}		2.5, 17.7, 17.13
8214.	61892-76-0	1	0	0	2-Pyridinol, 5-acetyl-3,4-dihydro- {2(1*H*)-pyridinone, 5-acetyl-3,4-dihydro-}		3.13, 17.7, 17.13
8215.	57147-25-8	1	0	0	2-Pyridinol, 3,4-dihydro- {2(1*H*)-pyridinone, 3,4-dihydro-}		2.5, 17.7, 17.13
8216.	61892-77-1	1	0	0	2-Pyridinol, 3,6-dihydro- {2(1*H*)-pyridinone, 3,6-dihydro-}		2.5, 17.7, 17.13
8217.	6052-73-9	1	1	1	2-Pyridinol, 5,6-dihydro- {2(1*H*)-pyridinone, 5,6-dihydro-, 2-piperidone, 3,4-dehydro-}		2.5, 17.7, 17.13
8218.		0	1	0	2-Pyridinol, 5,6-dihydro-3,6,6-trimethyl- {2(1*H*)-pyridinone, 5,6-dihydro-3,6,6-trimethyl-}		2.5, 17.7, 17.13
8219.	72692-83-2	1	0	0	2-Pyridinol, dimethyl- {2(1*H*)-pyridinone, dimethyl-}		2.5, 17.7, 17.13
8220.	6456-92-4	1	0	0	2-Pyridinol, 1,3-dimethyl- {2(1*H*)-pyridinone, 1,3-dimethyl-}		2.5, 17.7, 17.13
8221.	36330-90-2 95907-02-1	1	0	0	2-Pyridinol, 3,4-dimethyl- {2(1*H*)-pyridinone, 3,4-dimethyl-}		2.5, 17.7, 17.13
8222.	3718-67-0	1	0	0	2-Pyridinol, 3,5-dimethyl- {2(1*H*)-pyridinone, 3,5-dimethyl-}		2.5, 17.7, 17.13
8223.	53428-02-7	1	0	0	2-Pyridinol, 3,6-dimethyl- {2(1*H*)-pyridinone, 3,6-dimethyl-}		2.5, 17.7, 17.13
8224.	16115-08-5	1	0	0	2-Pyridinol, 4,6-dimethyl- {2(1*H*)-pyridinone, 4,6-dimethyl-}		2.5, 17.7, 17.13
8225.	27992-31-0	1	0	0	2-Pyridinol, 5,6-dimethyl-		2.5, 17.7

(*continued*)

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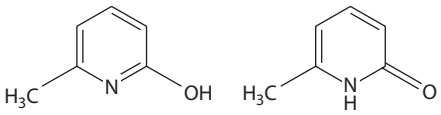
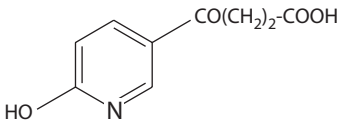
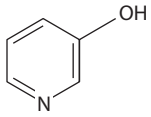
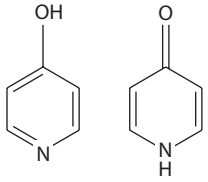
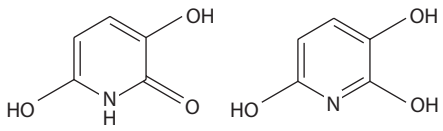
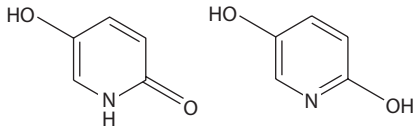
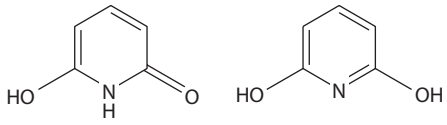
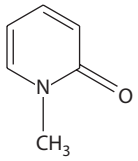
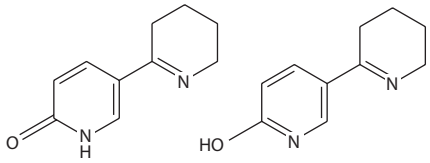
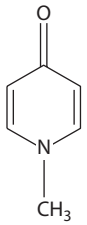
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8226.		1	0	0	2-Pyridinol, 3-ethyl- {2(1*H*)-pyridinone, 3-ethyl-}		2.5, 17.7, 17.13
8227.	62003-48-9	1	0	0	2-Pyridinol, 5-ethyl- {2(1*H*)-pyridinone, 5-ethyl-}		2.5, 17.7, 17.13
8228.	61892-99-7	1	0	0	2-Pyridinol, 6-ethyl- {2(1*H*)-pyridinone, 6-ethyl-}		2.5, 17.7, 17.13
8229.	1003-56-1 91914-04-4	1	0	0	2-Pyridinol, 3-methyl- {2(1*H*)-pyridinone, 3-methyl-}		2.5, 17.7, 17.13
8230.	91914-05-5	1	0	0	2-Pyridinol, 4-methyl- {2(1*H*)-pyridinone, 4-methyl-}		2.5, 17.7, 17.13
8231.	1003-68-5 91914-06-6	1	0	0	2-Pyridinol, 5-methyl- {2(1*H*)-pyridinone, 5-methyl-}		2.5, 17.7, 17.13
8232.	3279-76-3	1	0	0	2-Pyridinol, 6-methyl- {2(1*H*)-pyridinone, 6-methyl-}		2.5, 17.7, 17.13
8233.	19006-81-6	1	1	1	2-Pyridinol, 4-phenyl- {2(1*H*)-pyridinone, 4-phenyl-}		2.5, 17.7, 17.13
8234.		0	1	0	2-Pyridinol-5-butanoic acid, γ-oxo- {2(1*H*)-pyridinone-5-butanoic acid, γ-oxo-}		2.5, 3.13, 4.3, 17.7, 17.13
8235.		0	1	0	2-Pyridinol-5-pentanoic acid, δ-oxo- {2(1*H*)-pyridinone-5-pentanoic acid, δ-oxo-}		2.5, 3.13, 4.3, 17.7, 17.13
8236.	109-00-2 52536-09-1 58064-43-0	1	1	1	3-Pyridinol		2.5, 17.7
8237.	17747-43-2	1	0	0	3-Pyridinol, acetate (ester)		5.3, 17.7
8238.		1	0	0	3-Pyridinol, alkyl-		2.5, 17.7
8239.	27296-76-0	1	0	0	3-Pyridinol, 2,4-dimethyl-		2.5, 17.7
8240.	1122-43-6	1	0	0	3-Pyridinol, 2,6-dimethyl-		2.5, 17.7
8241.	27296-77-1	1	0	0	3-Pyridinol, 4,6-dimethyl-		2.5, 17.7
8242.	61893-00-3	1	0	0	3-Pyridinol, 5,6-dimethyl-		2.5, 17.7
8243.	61893-02-5	1	1	1	3-Pyridinol, 2-ethyl-		2.5, 17.7
8244.	62003-48-9	1	0	0	3-Pyridinol, 5-ethyl-		2.5, 17.7
8245.	51834-96-9	1	0	0	3-Pyridinol, 6-ethyl-		2.5, 17.7
8246.	42451-07-0	1	0	0	3-Pyridinol, 6-ethyl-2-methyl-		2.5, 17.7
8247.	61893-01-4	1	0	0	3-Pyridinol, 6-ethyl-4-methyl-		2.5, 17.7
8248.	40222-77-3	1	0	0	3-Pyridinol, 6-hydroxymethyl- {2-pyridinemethanol, 5-hydroxy-}		2.5, 17.7
8249.	91491-14-4	1	0	0	3-Pyridinol, methyl-		2.5, 17.7
8250.	1121-25-1	1	1	1	3-Pyridinol, 2-methyl-		2.5, 17.7
8251.	1121-19-3	1	0	0	3-Pyridinol, 4-methyl-		2.5, 17.7
8252.	42732-49-0	1	0	0	3-Pyridinol, 5-methyl-		2.5, 17.7
8253.	1121-78-4	1	0	0	3-Pyridinol, 6-methyl-		2.5, 17.7
8254.	14159-68-3	1	0	0	3-Pyridinol, 2-propyl-		2.5, 17.7
8255.	61893-03-6	1	0	0	3-Pyridinol, 4-propyl-		2.5, 17.7
8256.	61893-04-7	1	0	0	3-Pyridinol, 5-propyl-		2.5, 17.7 17.7, 17.13

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8257.	108-96-3 626-64-2	1	0	0	4-Pyridinol {4(1*H*)-pyridinone}		2.5, 3.13, 17.7
8258.	70969-38-9	0	1	0	2(1*H*)-Pyridinone, 5-(3,4-dihydro-2*H*-pyrrol-5-yl)- 2-Pyridinol, 5-(3,4-dihydro-2*H*-pyrrol-5-yl)-		17.9, 17.13
8259.	39954-19-3	0	1	0	2(1*H*)-Pyridinone, 3,6-dihydroxy-{2,3,6-pyridinetriol}		2.5, 17.7, 17.13
8260.	5154-01-8	0	1	0	2(1*H*)-Pyridinone, 5-hydroxy-{2,5-pyridinediol}		2.5, 17.7, 17.13
8261.	626-06-2	0	1	0	2(1*H*)-Pyridinone, 6-hydroxy-{2,6-pyridinediol}		2.5, 17.7, 17.13
8262.	694-85-9	1	1	1	2(1*H*)-Pyridinone, 1-methyl-		17.7, 17.13
8263.	40316-88-9	1	1	1	2(1*H*)-Pyridinone, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {2-pyridinol, 3-(1-methyl-2-pyrrolidinyl)-} - {nicotone}		17.9, 17.13
8264.	10516-09-3	0	1	0	2(1*H*)-Pyridinone, 5-(1-methyl-2-pyrrolidinyl)-, (S)- {2-pyridinol,5-(1-methyl-2-pyrrolidinyl)-}		17.9, 17.13
8265.		0	1	0	2(1*H*)-Pyridinone, 5-(2,3,4,5-tetrahydropyridinyl)- {2-pyridinol, 5-(2,3,4,5-tetrahydropyridinyl)-}		2.5, 17.11, 17.13
8266.	1445-73-4	1	1	1	4(1*H*)-Pyridinone, 1-methyl-		17.7, 17.13

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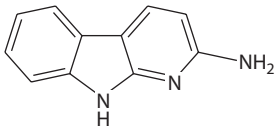
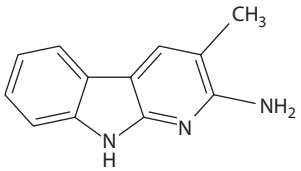
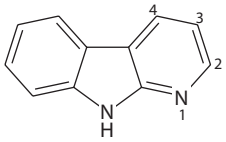
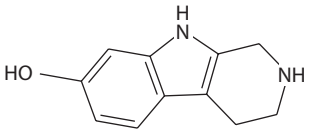
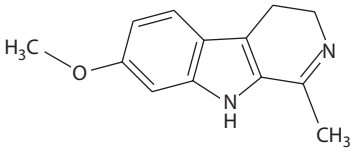
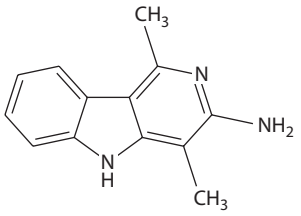
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8267.	26148-68-5	1	0	0	9*H*-Pyrido[2,3-*b*]indol-2-amine {AαC}		12.2, 17.31, 23.5
8268.	68006-83-7	1	0	0	9*H*-Pyrido[2,3-*b*]indol-2-amine, 3-methyl- {MeAαC}		12.2, 17.31, 23.5
8269.		1	0	0	Pyridoindole		17.21
8270.		1	0	0	Pyridoindole, butyl-		17.21
8271.		1	0	0	Pyridoindole, C_3-alkyl-		17.21
8272.	80700-46-5	1	0	0	Pyridoindole, *N*-methyl-		17.21
8273.	245-08-9	1	0	0	5*H*-Pyrido[3,2-*b*]indole		17.21
8274.	244-76-8	1	0	0	9*H*-Pyrido[2,3-*b*]indole		17.21
8275.		1	0	0	9*H*-Pyrido[2,3-*a*]indole, 2-acyl-		3.13, 17.21
8276.	72693-00-6	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 1-butyl-		17.21
8277.	61893-11-6	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 2-ethyl-		17.21
8278.	17276-85-6	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 2-methyl-		17.21
8279.	76162-60-2	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 3-methyl-		17.21
8280.	78210-54-5	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-		17.21
8281.	78210-53-4	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 2-pentyl-		17.21
8282.	42438-90-4	1	0	0	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-, (S)-		4.3, 17.23
8283.	40678-46-4	1	0	0	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-1-methyl-, (1S-*cis*)-		4.3, 17.23
8284.	83177-17-7	0	1	0	3*H*-Pyrido[3,4-*b*]indol-7-ol, 1,2-dihydro- {1,2-dihydro-1-demethylharmalol}		17.23
8285.	3589-73-9	1	0	0	3*H*-Pyrido[3,4-*b*]indole, 4,9-dihydro-6-methoxy-1-methyl-		10.2
8286.	304-21-2	1	0	0	3*H*-Pyrido[3,4-*b*]indole, 4,9-dihydro-7-methoxy-1-methyl- {harmaline}		10.2
8287.	62450-06-0	1	0	0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1,4-dimethyl- {Trp-P-1}		12.2, 17.31, 23.5

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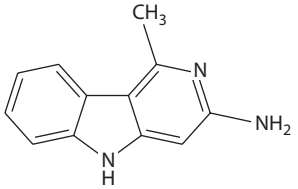
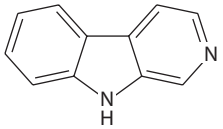
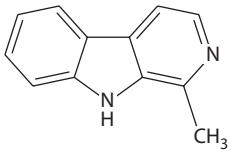
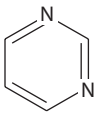
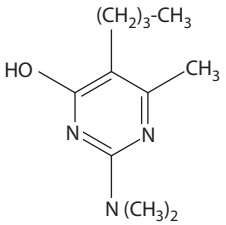
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8288.	62450-07-1	1	0	0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1-methyl- {Trp-P-2}		12.2, 17.31, 23.5
8289.	244-69-9	1	0	0	5*H*-Pyrido[4,3-*b*]indole		17.21
8290.	244-63-3 8001-81-8	1	1	1	9*H*-Pyrido[3,4-*b*]indole {norharman = β-carboline = 2-azacarbazole}		17.21
8291.	10371-85-4	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 1-butyl-		17.21
8292.	20127-61-1	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 1-ethyl-		17.21
8293.	3589-72-8	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 6-methoxy-1-methyl-		10.2
8294.	442-51-3	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 7-methoxy-1-methyl- {harmine}		10.2
8295.	5667-11-8	1	0	0	9*H*-Pyrido[3,4-*b*]indole, methyl- {?-methylnorharman}		17.21
8296.	486-84-0	1	1	1	9*H*-Pyrido[3,4-*b*]indole, 1-methyl- {harman}		17.21
8297.	78210-55-6	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 1-(1-propenyl)-		17.21
8298.	78538-74-6	1	0	0	9*H*-Pyrido[3,4-*b*]indole-3-carboxamide, *N*-methyl-		13.1, 17.23
8299.	50609-61-5	1	0	0	4*H*-Pyrido[1,2-*a*]pyrimidine-3-acetic acid, 9-hydroxy-4-oxo-, ethyl ester		2.5, 5.3, 17.23
8300.	3303-26-2	0	1	0	Pyrido[3,2-*d*]pyrimidin-4-ol, 2-methyl-		2.5, 17.23
8301.	289-95-2	0	1	0	Pyrimidine {1,3-diazine}		0.4, 17.7
8302.	5221-53-4	0	1	0	Pyrimidine, 5-butyl-2-dimethylamino-4-hydroxy-6-methyl- {Dimetherimol®}		2.5, 12.2, 17.7, 21.3
8303.	72692-81-0	1	0	0	Pyrimidine, dimethyl-		17.7
8304.	14331-54-5	1	0	0	Pyrimidine, 2,4-dimethyl-		17.7
8305.	22868-76-4	1	0	0	Pyrimidine, 2,5-dimethyl-		17.7
8306.		1	0	0	Pyrimidine, 2,5-dimethyl-6-hydroxy-		2.5, 17.7
8307.	694-81-5	1	0	0	Pyrimidine, 4,5-dimethyl-		17.7
8308.	1558-17-4	1	0	0	Pyrimidine, 4,6-dimethyl-		17.7
8309.	88070-43-3	1	0	0	Pyrimidine, 5-hydroxy-4-phenyl-		2.5, 17.7

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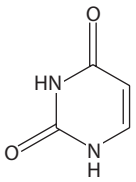
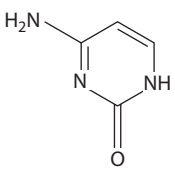
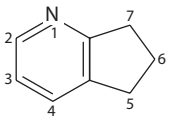
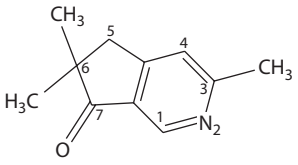
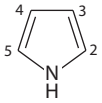
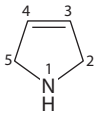
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8310.	3438-46-8	1	0	0	Pyrimidine, 4-methyl-		17.7
8311.		1	0	0	Pyrimidine, methylethyl- {two isomers}		17.7
8312.	66-22-8	0	1	0	2,4(1*H*,3*H*)-Pyrimidinedione {uracil}		14.1, 17.7
8313.	4160-77-4	1	0	0	2,4(1*H*,3*H*)-Pyrimidinedione, 3,5-dimethyl-		14.1, 17.7
8314.	61893-13-8	1	0	0	2,4(1*H*,3*H*)-Pyrimidinedione, 3-ethyldihydro-5-methyl-		14.1, 17.7
8315.	608-34-4	1	0	0	2,4(1*H*,3*H*)-Pyrimidinedione, 3-methyl-		14.1, 17.7
8316.	65-71-4	1	1	1	2,4(1*H*,3*H*)-Pyrimidinedione, 5-methyl- {thymine}		14.1, 17.7
8317.	50-06-6	0	1	0	2,4,6(1*H*,3*H*, 5*H*)-Pyrimidinetrione, 5-ethyl-5-phenyl- {phenobarbital}		14.1, 17.7
8318.	67383-34-0 3059-71-0	1	0	0	4-Pyrimidinol, 2,5-dimethyl- 4(1*H*)-pyrimidinone, 2,5-dimethyl-		2.5, 17.7, 17.13
8319.	71-30-7	1	1	1	2(1*H*)-Pyrimidinone, 4-amino- {cytosine}		12.2, 17.7, 17.13
8320.	34939-17-8	1	0	0	2(1*H*)-Pyrimidinone, 4,5-dimethyl- = 2-pyrimidinol, 4,5-dimethyl-		2.5, 17.7, 17.13
8321.		1	0	0	4(1*H*)-Pyrimidinone, 2,3-dimethyl-6-phenyl-3,4,5,6-tetrahydro-		17.7
8322.	3059-71-0 67383-34-0	1	0	0	4(1*H*)-Pyrimidinone, 2,5-dimethyl- = 4-pyrimidinol, 2,5-dimethyl-		2.5, 17.7, 17.13
8323.	6622-92-0	1	0	0	4(1*H*)-Pyrimidinone, 2,6-dimethyl- = 4-pyrimidinol, 2,6-dimethyl-		2.5, 17.7, 17.13
8324.	34916-78-4	1	0	0	4(1*H*)-Pyrimidinone, 5,6-dimethyl- = 4-pyrimidinol, 5,6-dimethyl-		2.5, 17.7, 17.13
8325.	16858-16-5	1	0	0	4(1*H*)-Pyrimidinone, 6-methyl-2-propyl- = 4-pyrimidinol, 6-methyl-2-propyl-		2.5, 17.7, 17.13
8326.	533-37-9	1	0	0	5*H*-1-Pyrindine, 6,7-dihydro-		17.21
8327.	55713-43-4	0	1	0	7*H*-2-Pyrindin-7-one, 5,6-dihydro-3,6,6-trimethyl-		3.13, 17.23
8328.	9033-44-7	0	1	0	Pyrophosphatase		22.2
8329.	9024-82-2	0	1	0	Pyrophosphatase, inorganic		22.2
8330.	37289-33-1	0	1	0	Pyrophosphatase, nicotinamide adenine dinucleotide		22.2
8331.	9032-64-8	0	1	0	Pyrophosphatase, nucleotide		22.2
8332.	9038-53-3	0	1	0	Pyrophosphatase, thiamin		18.1, 22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8333.	107-49-3	0	1	0	Pyrophosphoric acid, tetraethyl ester {TEPP}	$[(H_3C\text{-}CH_2\text{-}O)_2\text{-}P{=}O]_2{=}O$	0.4, 5.3, 20.6
8334.	68858-66-2	0	1	0	Pyrophosphorylase		22.2
8335.	37277-74-0	0	1	0	Pyrophosphorylase, nicotinate mononucleotide (carboxylating) {phosphoribosyltransferase, quinolinate}		22.2
8336.	106398-69-0	1	0	0	Pyrrole, butyl-		17.4
8337.	71607-59-5	1	0	0	Pyrrole, dihydromethyl-		17.4
8338.		1	0	0	Pyrrole, hydroxymethyl-		2.5, 17.4
8339.	109-97-7	1	1	1	1*H*-Pyrrole {azole}		0.4, 17.4, 24.3, 25.29
8340.	609-41-6	1	0	0	1*H*-Pyrrole, 1-acetyl-		13.1, 17.4
8341.	23105-58-0	1	0	0	1*H*-Pyrrole, 1-acetyl-2,3-dihydro-		13.1, 17.4
8342.	38207-11-3	1	1	1	1*H*-Pyrrole, 1-acetyl-2-methyl-		13.1, 17.4
8343.		1	1	1	1*H*-Pyrrole, 1-acetyl-3-methyl-		13.1, 17.4
8344.	589-33-3	1	0	0	1*H*-Pyrrole, 1-butyl-		17.4
8345.	50691-30-0	1	0	0	1*H*-Pyrrole, 1-butyl-2-methyl-		17.4
8346.	62672-96-2	1	0	0	1*H*-Pyrrole, 1-(1-cyclohexen-1-yl)-		17.4
8347.	28350-87-0	1	0	0	1*H*-Pyrrole, dihydro- {pyrroline}		17.4
8348.	638-31-3	1	0	0	1*H*-Pyrrole, 2,3-dihydro- {2-pyrroline}		17.4
8349.	109-96-6	1	1	1	1*H*-Pyrrole, 2,5-dihydro- {3-pyrroline}		17.4
8350.	554-15-4	1	1	1	1*H*-Pyrrole, 2,5-dihydro-1-methyl-		17.4
8351.	5724-81-2	1	0	0	1*H*-Pyrrole, 3,4-dihydro- {1-pyrroline}		17.4
8352.		1	0	0	1*H*-Pyrrole, dimethyl-		17.4
8353.	600-28-2	1	0	0	1*H*-Pyrrole, 2,3-dimethyl-		17.4
8354.	625-82-1	1	1	1	1*H*-Pyrrole, 2,4-dimethyl-		17.4
8355.	625-84-3	1	1	1	1*H*-Pyrrole, 2,5-dimethyl-		17.4
8356.	822-51-5	1	0	0	1*H*-Pyrrole, 3,4-dimethyl-		17.4
8357.	2433-66-1	0	1	0	1*H*-Pyrrole, 2-ethenyl-		17.4
8358.		1	0	0	1*H*-Pyrrole, ethyl-		17.4
8359.	617-92-5	1	1	1	1*H*-Pyrrole, 1-ethyl-		17.4
8360.	19983-83-6	1	0	0	1*H*-Pyrrole, 1-ethyl-2-methyl-		17.4
8361.	1551-16-***2***	1	0	0	1*H*-Pyrrole, 2-ethyl-		17.4
8362.	488-92-6	1	0	0	1*H*-Pyrrole, 3-ethyl-4-methyl-		17.4
8363.		1	0	0	1*H*-Pyrrole, 3-ethyl-1-phenyl-		17.4
8364.		0	1	0	1*H*-Pyrrole, 4-ethyl-3-methyl-		17.4
8365.		1	0	0	1*H*-Pyrrole, 1-(2-furanyl)-		10.2, 17.4
8366.	1438-94-4	1	1	1	1*H*-Pyrrole, 1-(2-furanylmethyl)-		10.2, 17.4
8367.	27417-39-6	1	0	0	1*H*-Pyrrole, methyl-		17.4
8368.	96-54-8	1	1	1	1*H*-Pyrrole, 1-methyl-		17.4
8369.	636-41-9	1	1	1	1*H*-Pyrrole, 2-methyl-		17.4
8370.		1	0	0	1*H*-Pyrrole, 2-methyl-1-phenyl-		17.4
8371.	616-43-3	1	0	0	1*H*-Pyrrole, 3-methyl-		17.4
8372.		1	0	0	1*H*-Pyrrole, 3-methyl-1-phenyl-		17.4

(*continued*)

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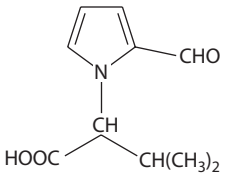
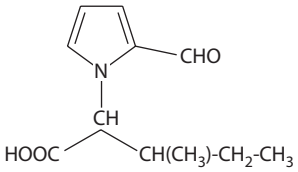
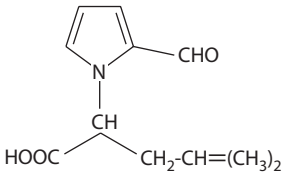
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8373.	13679-79-3	1	1	1	1*H*-Pyrrole, 1-(3-methylbutyl)-		17.4
8374.	66309-87-3	1	0	0	1*H*-Pyrrole, 1-(2-methyl-1-cyclohexen-1-yl)-		17.4
8375.	7057-97-8	1	0	0	1*H*-Pyrrole, 1-(1-methylethyl)-		17.4
8376.	13678-52-9	1	0	0	1*H*-Pyrrole, 1-[(5-methyl-2-furanyl)methyl]-		10.2, 17.4
8377.	78075-83-9	1	0	0	1*H*-Pyrrole, 2-methyl-1-(phenylmethyl)-		17.4
8378.	20884-13-3	1	1	1	1*H*-Pyrrole, 1-(2-methylpropyl)-		17.4
8379.	61480-97-5	1	0	0	1*H*-Pyrrole, 1-(1-oxobutyl)-		17.4
8380.	699-22-9 1551-12-8	1	1	1	1*H*-Pyrrole, 1-pentyl-		17.4
8381.	635-90-5	1	0	0	1*H*-Pyrrole, 1-phenyl-		17.4
8382.	50691-29-7	1	0	0	1*H*-Pyrrole, 1-(2-phenylethyl)-		17.4
8383.	5145-64-2	1	0	0	1*H*-Pyrrole, 1-propyl-		17.4
8384.	1551-08-2	0	1	0	1*H*-Pyrrole, 2-propyl-		17.4
8385.	71646-51-0	1	0	0	1*H*-Pyrrolecarbonitrile, methyl-		11.2, 17.4
8386.	89145-04-0	0	1	0	1*H*-Pyrrolecarboxaldehyde		3.12, 17.4
8387.	72692-79-6	1	0	0	1*H*-Pyrrolecarboxylic acid, ethyl ester		5.3, 17.4
8388.	84499-92-3	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-(ethoxymethyl)-5-formyl-		4.3, 10.2, 17.4
8389.	61837-43-2	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-ethyl-5-formyl-α-(2-methylpropyl)-		4.3, 17.4
8390.	60026-07-5	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylethyl)-		4.3, 17.4
8391.	60026-08-6	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylpropyl)-		4.3, 17.4
8392.	60026-09-7	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(2-methylpropyl)-		4.3, 17.4
8393.		1	0	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-5-hydroxymethyl-α-(2-methylpropyl)-		2.5, 4.3, 17.4
8394.	61837-42-1	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α,5-dimethyl-		4.3, 17.4
8395.	61837-35-2	0	1	0	1*H*-Pyrrole-1-aceticacid, 2-formyl-α-hexyl-		4.3, 17.4
8396.	60026-30-4	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-methyl-		4.3, 17.4
8397.	61837-38-5	0	1	0	1*H*-Pyrrole-1-butanoic acid, 2-formyl-		4.3, 17.4
8398.	61837-39-6	0	1	0	1*H*-Pyrrole-1-butanoic acid, 2-formyl-γ-methyl-		4.3, 17.4
8399.	61837-44-3	0	1	0	1*H*-Pyrrole-1-butanoic acid, 2-formyl-5-methyl-		4.3, 17.4
8400.	78249-88-4	1	0	0	1*H*-Pyrrole-1-carboxaldehyde, 1-methyl-		3.12, 17.4
8401.	61837-40-9	0	1	0	1*H*-Pyrrole-1-hexanoic acid, 2-formyl-		4.3, 17.4
8402.	61837-41-0	0	1	0	1*H*-Pyrrole-1-octanoic acid, 2-formyl-		4.3, 17.4

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8403.	70898-32-7	0	1	0	1*H*-Pyrrole-1-octanoic acid, 2-formyl-5-methyl-		4.3, 17.4
8404.	61837-37-4	0	1	0	1*H*-Pyrrole-1-propanoic acid, β-ethyl-2-formyl-		4.3, 17.4
8405.	61837-36-3	0	1	0	1*H*-Pyrrole-1-propanoic acid, 2-formyl-β-methyl-		4.3, 17.4
8406.		1	0	0	1*H*-Pyrrole-2-acetaldehyde, α-hydroxy-		2.5, 3.12, 17.4
8407.	72693-01-7	1	0	0	1*H*-Pyrrole-2-acetaldehyde, α-oxo-		3.12, 3.13, 17.4
8408.	4513-94-4	1	0	0	1*H*-Pyrrole-2-carbonitrile		11.2, 17.4
8409.	133829-71-7	1	0	0	1*H*-Pyrrole-2-carbonitrile, methyl- {two isomers}		11.2, 17.4
8410.	26173-92-2	1	0	0	1*H*-Pyrrole-2-carbonitrile, 5-methyl-		11.2, 17.4
8411.	1003-29-8	1	1	1	1*H*-Pyrrole-2-carboxaldehyde		3.12, 17.4
8412.	13788-32-4	0	1	0	1*H*-Pyrrole-2-carboxaldehyde, 1-(2-furanylmethyl)-		3.12, 10.2, 17.4
8413.	13678-79-0	0	1	0	1*H*-Pyrrole-2-carboxaldehyde, 1-(3-methylbutyl)-		3.12, 17.4
8414.		1	0	0	1*H*-Pyrrole-2-carboxaldehyde, ethyl-		3.12, 17.4
8415.	2167-14-8	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 1-ethyl-		3.12, 17.4
8416.		1	1	1	1*H*-Pyrrole-2-carboxaldehyde, methyl-		3.12, 17.4
8417.	1192-58-1	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 1-methyl-		3.12, 17.4
8418.	29813-44-3	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 5-(hydroxymethyl)-1-methyl-		2.5, 3.12, 17.4
8419.	52115-69-2	0	1	0	1*H*-Pyrrole-2-carboxaldehyde, 5-[(acetyloxy)methyl]-		3.12, 5.3, 17.4
8420.	1192-79-6	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 5-methyl-		3.12, 17.4
8421.	4551-72-8	1	0	0	1*H*-Pyrrole-2-carboxamide		13.1, 17.4
8422.	634-97-9	1	0	0	1*H*-Pyrrole-2-carboxylic acid		4.3, 17.4
8423.	3220-74-4	0	1	0	1*H*-Pyrrole-2-carboxylic acid, 2,5-dihydro-		4.3, 17.4
8424.	3757-53-7	1	0	0	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-		4.3, 17.4
8425.	3284-51-3	1	0	0	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, ethyl ester		5.3, 17.4
8426.	1194-97-4	1	0	0	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, methyl ester		5.3, 17.4
8427.	1193-62-0	1	1	1	1*H*-Pyrrole-2-carboxylic acid, methyl ester		5.3, 17.4
8428.		1	0	0	1*H*-Pyrrole-3-acetonitrile		11.2, 17.4
8429.	7126-38-7	1	0	0	1*H*-Pyrrole-3-carbonitrile		11.2, 17.4
8430.	17619-39-5	1	1	1	1*H*-Pyrrole-3-carboxaldehyde, 2-methyl-		3.12, 17.4
8431.	103002-58-0	0	1	0	1*H*-Pyrrole-3-carboxaldehyde, 4,5-dihydro-2-methyl-		3.12, 17.4
8432.	78210-62-5	1	0	0	1*H*-Pyrrole-3-carboxaldehyde, 5-ethyl-		3.12, 17.4
8433.	936-12-9	1	0	0	1*H*-Pyrrole-3-carboxylic acid, 2-methyl-, ethyl ester		5.3, 17.4
8434.	487-90-1	0	1	0	1*H*-Pyrrole-3-propanoic acid, 5-(aminomethyl)-4-(carboxymethyl)-		4.3, 12.2, 17.4
8435.	541-59-3	1	1	1	1*H*-Pyrrole-2,5-dione {maleimide}		14.1, 17.4
8436.	29720-92-1	1	1	1	1*H*-Pyrrole-2,5-dione, ethylmethyl-		14.1, 17.4
8437.	128-53-0	1	0	0	1*H*-Pyrrole-2,5-dione, 1-ethyl-		14.1, 17.4
8438.		1	0	0	1*H*-Pyrrole-2,5-dione, 1,3-dimethyl-4-ethyl-		14.1, 17.4
8439.	5997-61-5	1	0	0	1*H*-Pyrrole-2,5-dione, 3-ethyl-		14.1, 17.4
8440.	15542-97-9	1	0	0	1*H*-Pyrrole-2,5-dione, 3-ethyl-1-methyl-		14.1, 17.4
8441.	61892-73-7	1	0	0	1*H*-Pyrrole-2,5-dione, 3-(hydroxymethyl)-		2.5, 14.1, 17.4

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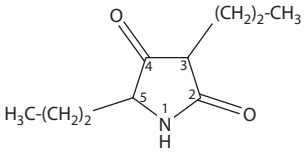
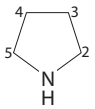
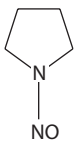
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8442.	61892-71-5	1	1	1	1*H*-Pyrrole-2,5-dione, 3,4-bis(hydroxymethyl)-1-methyl-		2.5, 14.1, 17.4
8443.	17825-86-4	1	1	1	1*H*-Pyrrole-2,5-dione, 3,4-dimethyl-		14.1, 17.4
8444.	61892-72-6	1	1	1	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-(hydroxymethyl)-		2.5, 14.1, 17.4
8445.	20189-42-8	1	1	1	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-methyl-		14.1, 17.4
8446.	1072-87-3	1	0	0	1*H*-Pyrrole-2,5-dione, 3-methyl-		14.1, 17.4
8447.	60026-19-9	0	1	0	1*H*-Pyrrole-2,5-dione, 3-propyl-		14.1, 17.4
8448.	3317-61-1	1	0	0	2*H*-Pyrrole, 3,4-dihydro-2,2-dimethyl-, 1-oxide		17.4
8449.	121197-26-0	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-(2-methylpropyl)-		17.2, 17.13
8450.	121197-16-8	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-propyl-		17.2, 17.13
8451.	121197-27-1	1	0	0	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-bis(2-methylpropyl)-		17.2, 17.13
8452.	121197-23-7	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dibutyl-		17.2, 17.13
8453.	121197-14-6	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dipropyl-		17.2, 17.13
8454.	121197-21-5	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-(2-methylpropyl)-3-propyl-		17.2, 17.13
8455.	121197-24-8	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-(2-methylpropyl)-		17.2, 17.13
8456.	121213-26-1	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-propyl-		17.2, 17.13
8457.	72692-82-1	1	0	0	1*H*-Pyrrolemethanol		2.5, 17.4
8458.	123-75-1	1	1	1	Pyrrolidine		0.4, 17.4
8459.	71607-78-8	1	0	0	Pyrrolidine, diethyl-		17.4
8460.	71607-79-9	1	0	0	Pyrrolidine, dimethyl-		17.4
8461.		1	0	0	Pyrrolidine, 2,5-dimethyl-, 1-nitroso-		15.8, 17.4
8462.	71607-80-2	1	0	0	Pyrrolidine, ethyl-		17.4
8463.	4030-18-6	1	1	1	Pyrrolidine, 1-acetyl-		13.1, 17.4
8464.	5979-94-2	1	1	1	Pyrrolidine, 1-acetyl-2-(3-pyridinyl)-, (S)- {*N*′-acetylnornicotine}		13.1, 17.9, 21.3
8465.	767-10-2	1	0	0	Pyrrolidine, 1-butyl-		17.4
8466.	7335-06-0	1	0	0	Pyrrolidine, 1-ethyl-		17.4
8467.	86900-39-2	0	1	0	Pyrrolidine, 1-ethyl-2-(3-pyridinyl)- {*N*′-ethylnornicotine}		17.9, 21.3
8468.		1	0	0	Pyrrolidine, methyl-		17.4
8469.	120-94-5	1	1	1	Pyrrolidine, 1-methyl-		0.4, 17.4
8470.	930-55-2	1	1	1	Pyrrolidine, 1-nitroso- {NPYR}		15.8, 17.4, 23.5
8471.	7335-07-1	1	0	0	Pyrrolidine, 1-propyl-		17.4
8472.	91907-45-8	0	1	0	Pyrrolidine, 1-propyl-2-(3-pyridinyl)- {*N*′-propylnornicotine}		17.9, 21.3

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8473.	117642-93-0	0	1	0	Pyrrolidine,1-(10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		13.1, 17.9
8474.	120376-92-3	0	1	0	Pyrrolidine,1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		13.1, 17.9
8475.	117642-94-1	0	1	0	Pyrrolidine,1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8476.	120042-36-6	0	1	0	Pyrrolidine,1-(11-methyl-1-oxododecyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8477.	120376-93-4	0	1	0	Pyrrolidine,1-(12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		13.1, 17.9
8478.	33527-93-4	1	0	0	Pyrrolidine, 1-(1-oxobutyl)-		13.1, 17.4
8479.	69730-91-2	1	1	1	Pyrrolidine, 1-(1-oxobutyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8480.	115849-75-7	0	1	0	Pyrrolidine, 1-(1-oxododecyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8481.	74173-71-0	1	0	0	Pyrrolidine, 1-(1-oxoheptyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8482.	38854-09-0	1	1	1	Pyrrolidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8483.		1	0	0	Pyrrolidine, 1-(1-oxo-?-octenyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8484.		1	0	0	Pyrrolidine, 1-(1-oxo-5-octenyl)-2-(3-pyridinyl)-		13.1, 17.9
8485.		1	0	0	Pyrrolidine, 1-(1-oxo-6-octenyl)-2-(3-pyridinyl)-		13.1, 17.9
8486.		1	0	0	Pyrrolidine, 1-(1-oxo-7-octenyl)-2-(3-pyridinyl)-		13.1, 17.9
8487.	38854-10-3	1	1	1	Pyrrolidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8488.	120042-35-5	0	1	0	Pyrrolidine, 1-(1-oxotridecyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8489.	61893-12-7	1	0	0	Pyrrolidine, 1-(2-furanylmethyl)-		10.2, 17.4
8490.	78504-05-9	1	0	0	Pyrrolidine, 1-(2-furoyl)-		3.13, 10.2, 17.4
8491.		1	0	0	Pyrrolidine, 1-(2-furoyl-5-methyl-)-		3.13, 10.2, 17.4
8492.	115849-82-6	0	1	0	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxododecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8493.	115849-79-1	0	1	0	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8494.	116353-95-8	0	1	0	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotetradecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8495.	115849-84-8	0	1	0	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8496.	120042-33-3	0	1	0	Pyrrolidine, 1-(3-hydroxy-14-methyl-1-oxopentadecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8497.	115849-80-4	0	1	0	Pyrrolidine,1-(3-hydroxy-1-oxododecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8498.	120042-32-2	0	1	0	Pyrrolidine,1-(3-hydroxy-1-oxohexadecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8499.	120042-34-4	0	1	0	Pyrrolidine,1-(3-hydroxy-1-oxopentadecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8500.	115849-85-9	0	1	0	Pyrrolidine,1-(3-hydroxy-1-oxotetradecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8501.	115849-83-7	0	1	0	Pyrrolidine,1-(3-hydroxy-1-oxotridecyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9

(*continued*)

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8502.	60026-17-7	0	1	0	Pyrrolidine, 1-(3-methyl-1-oxobutyl)-		13.1, 17.4
8503.		1	0	0	Pyrrolidine, 1-(3-pyridinemethyl)-2-cyano-		11.2, 17.4
8504.	96552-73-7	1	0	0	Pyrrolidine, 1-(4-methyl-1-oxohexyl)-2-(3-pyridinyl)-		13.1, 17.9
8505.	77829-17-5	0	1	0	Pyrrolidine, 1-(6-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8506.	96574-02-6	1	0	0	Pyrrolidine, 1-(6-methyl-1-oxoheptyl)-2-(3-pyridinyl)-, (S)-		13.1, 17.9
8507.	77829-18-6	0	1	0	Pyrrolidine, 1-(7-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-		2.5, 13.1, 17.9
8508.	61480-99-7	1	0	0	Pyrrolidine, 1-[(5-methyl-2-furanyl)methyl]-		10.2, 17.4
8509.	69730-92-3	0	1	0	Pyrrolidine, 1-[4-(dimethylamino)-1-oxobutyl]-2-(3-pyridinyl)-, (S)-		12.2, 13.1, 17.9
8510.		1	0	0	Pyrrolidine, 2-acetyloxy-methyl-		5.3, 17.4
8511.	13603-04-8	1	0	0	Pyrrolidine, 2,4-dimethyl-		17.4
8512.	3378-71-0	1	0	0	Pyrrolidine, 2,5-dimethyl-		17.4
8513.	1003-28-7	1	1	1	Pyrrolidine, 2-ethyl-		17.4
8514.		1	0	0	Pyrrolidine, 2-ethyl-1-methyl-		17.4
8515.	765-38-8	1	0	0	Pyrrolidine, 2-methyl-		17.4
8516.	34375-89-8	1	0	0	Pyrrolidine, 3-methyl-		17.4
8517.	28882-68-0	1	0	0	Pyrrolidinecarboxylic acid		4.3, 17.4
8518.	32389-40-5	0	1	0	Pyrrolidinecarboxylic acid, oxo-, (S)-		3.13, 4.3, 17.4
8519.	29134-29-0	1	0	0	1-Pyrrolidineacetonitrile		11.2, 17.4
8520.	35543-25-0	1	0	0	1-Pyrrolidinebuyronitrile		11.2, 17.4
8521.	1530-88-7	1	0	0	1-Pyrrolidinecarbonitrile		11.2, 17.4
8522.	3760-54-1	1	1	1	1-Pyrrolidinecarboxaldehyde		3.12, 13.1, 17.4
8523.	78914-62-2	1	0	0	1-Pyrrolidinecarboxaldehyde, 2-methyl-, (R)-		3.12, 13.1, 17.4
8524.	38840-03-8 3000-81-5	1	1	1	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)- {*N*′-formylnornicotine}		3.12, 13.1, 17.9, 21.3
8525.	69730-90-1	0	1	0	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, ethyl ester, (S)-		5.3, 17.9
8526.	56078-08-1	1	1	1	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)-		5.3, 17.9
8527.	56879-46-0	0	1	0	2-Pyrrolidineacetic acid		4.3, 17.4
8528.		0	1	0	2-Pyrrolidineacetic acid, 1-nitroso-		4.3, 15.8, 17.4
8529.	61480-98-6	0	1	0	2-Pyrrolidinecarboxaldehyde		3.12, 17.4
8530.	28115-37-9	1	0	0	2-Pyrrolidinemethanol, 5-methyl-, *cis*-		2.5, 17.4
8531.	14498-44-3	1	0	0	2-Pyrrolidinepropanol, 1-methyl-		2.5, 17.4
8532.	60026-15-5	0	1	0	3-Pyrrolidinecarboxaldehyde, 2-methyl-		3.12, 17.4
8533.	121197-25-9	1	1	1	2,4-Pyrrolidinedione, 3-butyl-5-propylidene-		3.13, 17.4, 17.13
8534.	121197-20-4	1	1	1	2,4-Pyrrolidinedione, 5-butyl-3-propylidene-		3.13, 17.4, 17.13
8535.	121197-28-2	1	1	1	2,4-Pyrrolidinedione, 3-butylidene-5-(2-methylpropyl)-		3.13, 17.4, 17.13
8536.	121197-18-0	1	1	1	2,4-Pyrrolidinedione, 3-butylidene-5-propyl-		3.13, 17.4, 17.13
8537.	121197-17-9	1	1	1	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-(2-methylpropylidene)-		3.13, 17.4, 17.13

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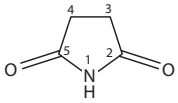
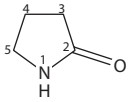
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8538.	121197-22-6	1	1	1	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-propylidene-		3.13, 17.4, 17.13
8539.	121197-19-1	1	1	1	2,4-Pyrrolidinedione, 3-(2-methylpropylidene)-5-propyl-		3.13, 17.4, 17.13
8540.	121197-15-7	1	1	1	2,4-Pyrrolidinedione, 5-propyl-3-propylidene-		3.13, 17.4, 17.13
8541.	123-56-8	1	1	1	2,5-Pyrrolidinedione {succinimide}		14.1, 17.4
8542.	15542-96-8	1	0	0	2,5-Pyrrolidinedione, 1,3-dimethyl-		14.1, 17.4
8543.	33425-47-7	1	0	0	2,5-Pyrrolidinedione, 3,4-dimethyl-		14.1, 17.4
8544.	58467-27-9	1	0	0	2,5-Pyrrolidinedione, 3-ethyl-		14.1, 17.4
8545.		1	0	0	2,5-Pyrrolidinedione, ethylmethyl-		14.1, 17.4
8546.	15542-97-9	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-1-methyl-		14.1, 17.4
8547.	77-67-8	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-3-methyl-		14.1, 17.4
8548.	58501-92-1	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-		14.1, 17.4
8549.	16824-61-6	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*Z*)-		14.1, 17.4
8550.	15510-11-9	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*E*)-		14.1, 17.4
8551.		1	0	0	2,5-Pyrrolidinedione, 3-ethylene-4-methyl-		14.1, 17.4
8552.	14156-12-8	1	0	0	2,5-Pyrrolidinedione, 3-ethylidene-		14.1, 17.4
8553.	61892-74-8	1	0	0	2,5-Pyrrolidinedione, 3-ethylidene-1-methyl-		14.1, 17.4
8554.	16395-79-2	1	1	1	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-		14.1, 17.4
8555.	28098-82-0	0	1	0	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-, (*E*)-		14.1, 17.4
8556.	18366-19-3	1	0	0	2,5-Pyrrolidinedione, 3-hydroxy- (S)		2.5, 14.1, 17.4
8557.	1121-07-9	1	1	1	2,5-Pyrrolidinedione, 1-methyl-		14.1, 17.4
8558.	5615-90-7	1	1	1	2,5-Pyrrolidinedione, 3-methyl-		14.1, 17.4
8559.	72693-03-9	1	0	0	2,5-Pyrrolidinedione, 3-(1-methylethyl)-		14.1, 17.4
8560.	15542-99-1	1	0	0	2,5-Pyrrolidinedione, 1-methyl-3-(1-methylethyl)-		14.1, 17.4
8561.	71099-03-1	1	1	1	2,5-Pyrrolidinedione, 1,3,4-trimethyl-		14.1, 17.4
8562.	61892-97-5	1	0	0	2-Pyrrolidinemethanol, 5-methyl-		2.5, 17.4
8563.	25110-79-6	1	0	0	2-Pyrrolidinol, 1-methyl-5-(3-pyridinyl)-		17.9
8564.	28261-54-3	1	0	0	Pyrrolidinone		17.4
8565.	616-45-5	1	1	1	2-Pyrrolidinone {γ-butyrolactam}		17.4, 17.13
8566.	932-17-2	1	0	0	2-Pyrrolidinone, 1-acetyl-		17.4, 17.13
8567.		1	0	0	2-Pyrrolidinone, 1,?-dimethyl-		17.4, 17.13
8568.	5075-92-3	1	0	0	2-Pyrrolidinone, 1,5-dimethyl-		17.4, 17.13
8569.	88-12-0	1	0	0	2-Pyrrolidinone, 1-ethenyl-		17.4, 17.13
8570.	2687-91-4	1	0	0	2-Pyrrolidinone, 1-ethyl-		17.4, 17.13
8571.	872-50-4	1	1	1	2-Pyrrolidinone, 1-methyl-		17.4, 17.13
8572.	2555-05-7	1	0	0	2-Pyrrolidinone, 3-methyl-		17.4, 17.13
8573.	2996-58-9	1	1	1	2-Pyrrolidinone, 4-methyl-		17.4, 17.13
8574.	108-27-0	1	0	0	2-Pyrrolidinone, 5-methyl-		17.4, 17.13
8575.	75202-09-4	1	1	1	2-Pyrrolidinone,1-methyl-5-(3-pyridinyl)-		17.9, 17.13

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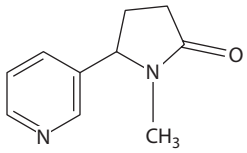
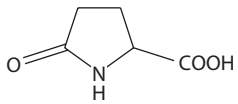
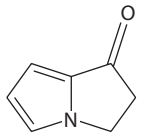
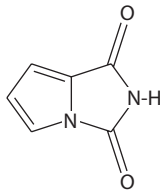
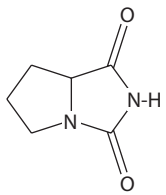
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
8576.	486-56-6	1	1	1	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, (S)- {cotinine}		17.9, 17.13, 26.9
8577.	15569-85-4 36508-80-2	1	0	0	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, 1-oxide {cotinine 1-oxide}		17.9, 17.13
8578.	61892-90-8	1	0	0	2-Pyrrolidinone, 1-(2-oxopropyl)-		17.4, 17.13
8579.	5980-06-3	1	1	1	2-Pyrrolidinone, 5-(3-pyridinyl)-, (S)- {norcotinine}		17.9, 17.13
8580.	98-79-3	0	1	0	5-Pyrrolidinone-2-carboxylic acid {5-oxoproline}		4.3, 17.4, 17.13
8581.	61892-89-5	1	0	0	3-Pyrrolidinone, 1-methyl-5-(2-oxopropyl)-		17.4
8582.	18028-53-0	1	0	0	2*H*-Pyrrolium, 3,4-dihydro-1-methyl-, chloride		17.4, 18.4
8583.	17266-64-7	1	0	0	1*H*-Pyrrolizin-1-one, 2,3-dihydro-		3.13
8584.	13939-91-8	1	0	0	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione		14.1, 17.23
8585.	5768-79-6	1	0	0	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione, tetrahydro-		14.1, 17.23
8586.	54036-77-0	1	0	0	2*H*-Pyrrol-2-one		17.4, 17.13
8587.	61892-80-6	1	0	0	2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-3-ethyl-4-methyl-		13.1, 14.1, 17.4, 17.13
8588.		1	0	0	2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-4-ethyl-3-methyl-		13.1, 14.1, 17.4, 17.13
8589.	62003-47-8	1	0	0	2*H*-Pyrrol-2-one, 1,3-dihydro-5-(3-pyridinyl)-		17.9, 17.13
8590.	4031-15-6	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-		17.4, 17.13
8591.	13950-21-5	0	1	0	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-		17.4, 17.13
8592.	78210-72-7	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-5-(1-methylethylidene)-		17.4, 17.13
8593.	4030-23-3	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4,5-trimethyl-		17.4, 17.13
8594.	4030-22-2	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4-dimethyl-		17.4, 17.13

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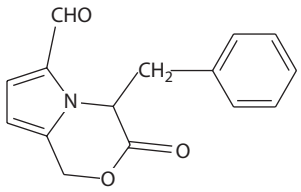
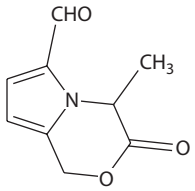
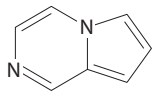
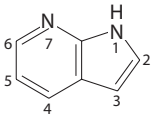
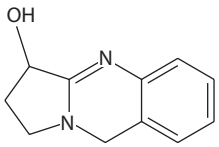
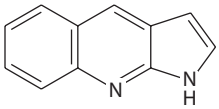
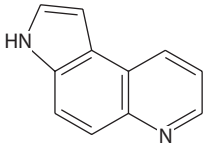
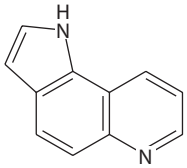
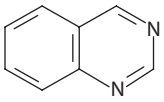
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8595.	51088-90-5	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-		17.4, 17.13
8596.	4030-24-4	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-4-ethyl-		17.4, 17.13
8597.		1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-4,5-dimethyl-3-ethyl-		17.4, 17.13
8598.	27406-77-5	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3-methyl-		17.4, 17.13
8599.	766-36-9	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3-ethyl-4-methyl-		17.4, 17.13
8600.	78210-71-6	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3-ethyl-5-methylene-		17.4, 17.13
8601.	115600-67-4	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-4-ethyl-		17.4, 17.13
8602.	53598-99-5	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-4-methyl-		17.4, 17.13
8603.	766-45-0	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-4-ethyl-3-methyl-		17.4, 17.13
8604.	60026-28-0	0	1	0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-3-oxo-4-(phenylmethyl)-		3.12, 6.3, 17.15
8605.	35674-33-0	0	1	0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-4-methyl-3-oxo-		3.12, 6.3, 17.15
8606.	274-45-3	1	0	0	Pyrrolo[1,2-*a*]pyrazine		17.21
8607.		1	0	0	Pyrrolo[1.2-*a*]pyrazine, 3,6-dimethyl-		17.21
8608.	19179-12-5	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-		17.13, 17.23
8609.	19943-28-3 36357-32-1	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-methyl-, (3R-*trans*)-		17.13, 17.23
8610.	5654-86-4	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-		17.13, 17.23
8611.	61949-29-9	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-propyl-		17.13, 17.23
8612.	26626-89-1	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-propyl-, (3S-*trans*)-		17.13, 17.23
8613.		1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, 3-(1-methylethyl)-		17.13, 17.23
8614.	61891-74-5	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, tetrahydro-		17.13, 17.23
8615.	274-40-8	1	0	0	Pyrrolo[1,2-*a*]pyridine		17.21

(*continued*)

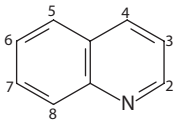
(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8616.	271-63-6	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine {7-azaindole}		17.21
8617.		1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, C_3-alkyl-		17.21
8618.		1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, diethyl-		17.21
8619.	78249-85-1	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, ethyl-		17.21
8620.	72692-80-9	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, methyl- {at least 4 methyl isomers other than the 1- and 2-methyl- compounds}		17.21
8621.	27257-15-4	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, 1-methyl-		17.21
8622.	23612-48-8	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, 2-methyl-		17.21
8623.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, diethyl-		17.21
8624.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, dimethyl-		17.21
8625.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, ethylmethyl-		17.21
8626.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, (1-methylethyl)-		17.21
8627.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, methyl- (1-methylethyl)-		17.21
8628.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, pentamethyl-		17.21
8629.		1	0	0	1*H*-Pyrrolo[2,3-*g*]pyridine, trimethyl-		17.21
8630.	6159-55-3	0	1	0	Pyrrolo[2,1-*b*]quinazolin-3-ol, 1,2,3,9-tetrahydro- {*l*-peganin, *l*-vasicin}		2.5, 17.23
8631.		1	0	0	Pyrroloquinoline		17.21
8632.		1	0	0	Pyrroloquinoline, dimethyl-		17.21
8633.		1	0	0	Pyrroloquinoline, methyl-		17.21
8634.		1	0	0	Pyrroloquinoline, trimethyl-		17.21
8635.	268-91-7	1	0	0	1*H*-Pyrrolo[2,3-*b*]quinoline		17.21
8636.	233-36-3	1	0	0	1*H*-Pyrrolo[2,3-*f*]quinoline		17.21
8637.	232-85-9	1	0	0	3*H*-Pyrrolo[3,2-*f*]quinoline		17.21
8638.	29036-02-0	1	0	0	Quaterphenyl		1.13
8639.	253-82-7	1	0	0	Quinazoline {1,3-benzodiazine}		17.21
8640.	64811-59-2	1	0	0	Quinazoline, dihydro-		17.21
8641.	64828-47-3	1	0	0	Quinazoline, ethyl-		17.21
8642.	64828-48-4	1	0	0	Quinazoline, methyl-		17.21

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8643.	700-79-8	1	0	0	Quinazoline, 2-methyl-		17.21
8644.	700-46-9	1	0	0	Quinazoline, 4-methyl-		17.21
8645.	31135-62-3	1	0	0	Quinolinamine		12.2
8646.	580-22-3	1	0	0	2-Quinolinamine		12.2
8647.	91-22-5	1	1	1	Quinoline {1-azanaphthalene}		0.4, 17.21, 23.5
8648.		1	0	0	Quinoline, C_3-alkyl-		17.21
8649.		1	0	0	Quinoline, alkyl-2-methyl-		17.21
8650.		1	0	0	Quinoline, alkyl-3-methyl-		17.21
8651.		1	1	1	Quinoline, alkyl-4-methyl-		17.21
8652.	611-34-7	1	0	0	Quinoline, 5-amino-		12.2
8653.		0	1	0	Quinoline, 5-amino-6,8-dimethoxy-		10.2, 12.2
8654.		0	1	0	Quinoline, 5-amino-2-hydroxymethyl-6-methoxy-		2.5, 10.2, 12.2
8655.	53452-65-6	1	0	0	Quinoline, butyl-		17.21
8656.	7634-74-4	1	0	0	Quinoline, 6-butyl-		17.21
8657.		1	0	0	Quinoline, 7-butyl-		17.21
8658.	2051-28-7	1	0	0	Quinoline, decahydro-		17.21
8659.	29968-14-7	1	0	0	Quinoline, dihydro-		17.21
8660.	65312-76-7	1	0	0	Quinoline, dihydroethyl-		17.21
8661.	65312-78-9	1	0	0	Quinoline, dihydromethyl-		17.21
8662.	28351-04-4	1	0	0	Quinoline, dimethyl-		17.21
8663.	1198-37-4	1	0	0	Quinoline, 2,4-dimethyl-		17.21
8664.	26190-82-9	1	0	0	Quinoline, 2,5-dimethyl-		17.21
8665.	877-43-0	1	1	1	Quinoline, 2,6-dimethyl-		17.21
8666.	1463-17-8	1	0	0	Quinoline, 2,8-dimethyl-		17.21
8667.		1	0	0	Quinoline, 3.6-dimethyl-		17.21
8668.	2623-50-9	1	0	0	Quinoline, 5,8-dimethyl-		17.21
8669.	53123-73-2	1	0	0	Quinoline, ethyl-		17.21
8670.	1613-34-9	1	0	0	Quinoline, 2-ethyl-		17.21
8671.	56717-33-0	1	0	0	Quinoline, 2-ethyl-5,6,7,8-tetrahydro-		17.21
8672.	1873-54-7	1	0	0	Quinoline, 3-ethyl-		17.21
8673.	19020-26-9	1	0	0	Quinoline, 4-ethyl-		17.21
8674.	65745-66-6	1	0	0	Quinoline, 5-ethyl-		17.21
8675.	7661-47-4	1	0	0	Quinoline, 7-ethyl-		17.21
8676.	78249-84-0	1	0	0	Quinoline, 7-ethyl-5,6,7,8-tetrahydro-		17.21
8677.	19655-56-2	1	0	0	Quinoline, 8-ethyl-		17.21
8678.	6931-16-4	1	0	0	Quinoline, 2-methoxy-		10.2
8679.	6931-17-5	1	0	0	Quinoline, 3-methoxy-		10.2
8680.	5263-87-6	1	0	0	Quinoline, 6-methoxy-		10.2
8681.	4964-76-5	1	0	0	Quinoline, 7-methoxy-		10.2
8682.	938-33-0	1	0	0	Quinoline, 8-methoxy-		10.2
8683.	27601-00-9	1	0	0	Quinoline, methyl-		17.21
8684.	65312-74-5	1	0	0	Quinoline, methyltetrahydro-		17.21
8685.	78249-82-8	1	0	0	Quinoline, methyl-1,2,3,4-tetrahydro- {several isomers present in MSS}		17.21
8686.	91-63-4	1	0	0	Quinoline, 2-methyl-		17.21
8687.	2617-98-3	1	0	0	Quinoline, 2-methyl-5,6,7,8-tetrahydro-		17.21
8688.	612-58-8	1	0	0	Quinoline, 3-methyl-		17.21
8689.	28712-62-1	1	0	0	Quinoline, 3-methyl-5,6,7,8-tetrahydro-		17.21

(*continued*)

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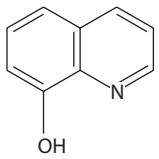
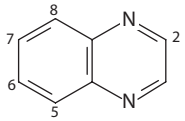
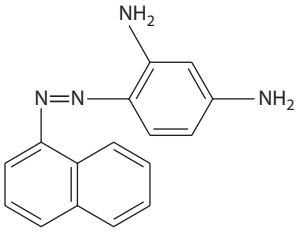
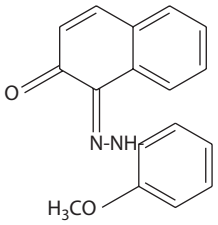
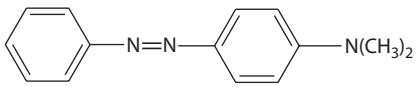
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8690.	491-35-0	1	1	1	Quinoline, 4-methyl-		17.21
8691.	7661-55-4	1	0	0	Quinoline, 5-methyl-		17.21
8692.	91-62-3	1	0	0	Quinoline, 6-methyl-		17.21
8693.	612-60-2	1	0	0	Quinoline, 7-methyl-		17.21
8694.	78249-83-9	1	0	0	Quinoline, 7-methyl-5,6,7,8-tetrahydro-		17.21
8695.	611-32-5	1	0	0	Quinoline, 8-methyl-		17.21
8696.	1333-53-5	1	0	0	Quinoline, (1-methylethyl)-		17.21
8697.	17507-24-3	1	0	0	Quinoline, 2-(1-methylethyl)-		17.21
8698.	17507-25-4	1	0	0	Quinoline, 4-(1-methylethyl)-		17.21
8699.	64828-52-0	1	0	0	Quinoline, propyl-		17.21
8700.	7661-53-2	1	0	0	Quinoline, 8-propyl-		17.21
8701.	6294-65-1	1	0	0	Quinoline, 2-(3-pyridyl)-		17.7, 17.21
8702.		1	0	0	Quinoline, tetrahydro-		17.21
8703.	635-46-1	1	0	0	Quinoline, 1,2,3,4-tetrahydro-		17.21
8704.	10500-57-9	1	0	0	Quinoline, 5,6,7,8-tetrahydro-		17.21
8705.	76602-27-2	1	0	0	Quinoline, tetramethyl-		17.21
8706.	51366-52-0	1	0	0	Quinoline, trimethyl-		17.21
8707.	4945-28-2	1	0	0	Quinoline, 2,3,8-trimethyl-		17.21
8708.	64850-00-6	1	0	0	Quinolinecarbonitrile		11.2
8709.	59551-02-9	1	0	0	5-Quinolinecarbonitrile		11.2
8710.	23395-72-4	1	0	0	6-Quinolinecarbonitrile		11.2
8711.	67360-38-7	1	0	0	7-Quinolinecarbonitrile		11.2
8712.	2739-16-4	0	1	0	1(2*H*)-Quinolinecarboxaldehyde, 3,4-dihydro-		3.12
8713.	4363-93-3	0	1	0	4-Quinolinecarboxaldehyde		3.12
8714.	3778-29-8	0	1	0	2-Quinolinecarboxylicacid,4,6-dihydroxy- {6-hydroxykynurenic acid}		4.3, 9.22
8715.	492-27-3	1	0	0	2-Quinolinecarboxylic acid, 4-hydroxy-		4.3, 9.22
8716.	643-38-9	0	1	0	2,3-Quinolinedicarboxylic acid		4.3
8717.	148-24-3	1	1	1	8-Quinolinol		9.22
8718.	13207-66-4	0	1	0	8-Quinolinol, 5-amino-		9.22, 12.2
8719.	5541-68-4	1	0	0	8-Quinolinol, 7-methyl-		9.22
8720.	91-19-0	1	0	0	Quinoxaline {1,4-benzodiazine}		17.21
8721.	64811-58-1	1	0	0	Quinoxaline, dihydro-		17.21
8722.	72692-77-4	1	0	0	Quinoxaline, dimethyl-		17.21
8723.	2379-55-7	1	0	0	Quinoxaline, 2,3-dimethyl-		17.21
8724.	64828-46-2	1	0	0	Quinoxaline, ethyl-		17.21
8725.		1	0	0	Quinoxaline, 2-ethyl-		17.21
8726.	37920-99-3	1	0	0	Quinoxaline, 2-ethyl-3-methyl-		17.21
8727.	7251-61-8	1	0	0	Quinoxaline, 2-methyl-		17.21
8728.	38917-65-6	1	0	0	Quinoxaline, 2-methyl-5,6,7,8-tetrahydro-		17.21
8729.	13708-12-8	0	1	0	Quinoxaline, 5-methyl-		17.21
8730.	64828-56-4	1	0	0	Quinoxaline, 7-methyl-		17.21
8731.	34413-35-9	1	1	1	Quinoxaline, 5,6,7,8-tetrahydro-		17.21
8732.	72692-78-5	1	0	0	Quinoxaline, trimethyl-		17.21
8733.		1	0	0	Radicals, free {general discussion}		27.1

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8734.	7440-14-4 13982-63-3	1	1	1	Radium, isotope of mass 226	^{226}Ra	0.4, 20.5
8735.	15262-20-1	0	1	0	Radium, isotope of mass 228	^{228}Ra	20.5
8736.	10043-92-2	1	0	0	Radon	Rn	0.4, 19.5, 20.5
8737.	14859-67-7	1	1	1	Radon, isotope of mass 222	^{226}Rn	19.5, 20.5
8738.	9037-80-3	0	1	0	Reductase		0.4, 22.2
8739.	9028-31-3	0	1	0	Reductase, aldose		22.2
8740.	9023-03-4	0	1	0	Reductase, cytochrome c (reduced nicotinamide adenine dinucleotide phosphate)		22.2
8741.	37256-44-3	0	1	0	Reductase, ferredoxin–nitrite		22.2
8742.	9001-48-3	0	1	0	Reductase, glutathione		22.2
8743.	9028-32-4	0	1	0	Reductase, glyoxylate		22.2
8744.	9032-06-8	0	1	0	Reductase, hydroxylamine		22.2
8745.	9028-35-7	0	1	0	Reductase, hydroxymethylglutaryl coenzyme A (reduced nicotinamide adenine dinucleotide phosphate)		22.2
8746.	9013-03-0	0	1	0	Reductase, nitrate		22.2
8747.	9029-27-0	0	1	0	Reductase, nitrate (reduced nicotinamide adenine dinucleotide (phosphate))		22.2
8748.	9080-03-9	0	1	0	Reductase, nitrite		22.2
8749.	9029-29-2	0	1	0	Reductase, nitrite (reduced nicotinamide adenine dinucleotide (phosphate))		22.2
8750.	9029-17-8	0	1	0	Reductase, pyrroline-5-carboxylate		22.2
8751.	6416-57-5	0	1	0	Resinol, brown		12.2
	69772-40-3				Resinol, red		3.13, 10.2, 12.2
	60-11-7				Resinol, yellow		12.2
8752.	51848-43-2	0	1	0	Retine		22.2
8753.	5328-43-8	0	1	0	Rhamnitol	$H_3C\text{-}(CHOH)_4\text{-}CH_2OH$	2.5, 8.3
8754.		0	1	0	Rhamnitol, 2,4-di-*O*-methyl-		2.5, 8.3, 10.2
8755.		0	1	0	Rhamnitol, 3,4-di-*O*-methyl-		2.5, 8.3, 10.2
8756.		0	1	0	Rhamnitol, 3-*O*-methyl-		2.5, 8.3, 10.2
8757.		0	1	0	Rhamnitol, 2,3,4-tri-*O*-methyl-		2.5, 8.3, 10.2

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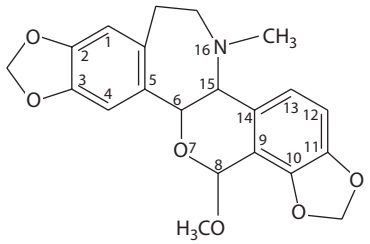
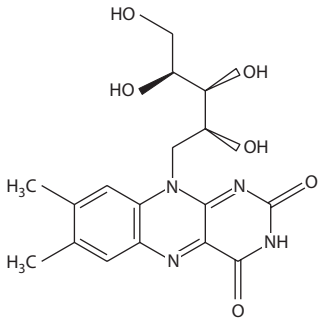
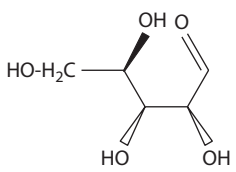
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8758.	39280-21-2	0	1	0	(1→2)-*L*-Rhamno-(1→4)-α-*D*-galacturonan		2.5, 8.3, 10.2
8759.	2718-25-4	0	1	0	Rheadan, 8-β-methoxy-6-methyl-2,3,10,11-[methylenebis(oxy)]-{rhoeadin}		10.2
8760.	7440-15-5	1	1	1	Rhenium	Re	20.5
8761.	7440-16-6	1	1	1	Rhodium	Rh	20.5
8762.	488-81-3	1	0	0	Ribitol [pentahydroxypentane]		2.5
8763.	83-88-5	0	1	0	Riboflavin		0.4, 2.5, 14.1, 17.13
8764.	146-17-8	0	1	0	Riboflavin 5′-(dihydrogen phosphate)		2.5, 14.1, 17.13
8765.	106777-19-9	0	1	0	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-		4.3, 2.5
8766.	27442-42-8	0	1	0	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-, 5-(dihydrogen phosphate)		4.3, 2.5
8767.	9001-99-4	0	1	0	Ribonuclease		22.2
8768.	63231-63-0	0	1	0	Ribonucleic acid		5.3, 22.2
8769.	9067-16-7	0	1	0	Ribonucleic acid (*Bombyx mori* fibroin-specifying messenger)		22.2
8770.	139872-63-2	0	1	0	Ribonucleic acid (tobacco clone lambda 5A gene RB7 protein-specifying 1524-nucleotide messenger)		22.2
8771.	139872-64-3	0	1	0	Ribonucleic acid (tobacco clone lambda 5A gene RB7 protein-specifying 1549-nucleotide messenger)		22.2
8772.	128285-01-8	0	1	0	Ribonucleic acid (tobacco clone lambda CHN17 chitinase basic isoenzyme-specifying messenger)		22.2
8773.	9014-25-9	0	1	0	Ribonucleic acids, transfer		22.2
8774.	3615-55-2	0	1	0	Ribose, 5-(dihydrogen phosphate)		2.5, 3.12, 5.3, 8.3
8775.	50-69-1	1	1	1	*D*-Ribose		2.5, 3.12
8776.	24259-59-4	0	1	0	*L*-Ribose		2.5, 3.12

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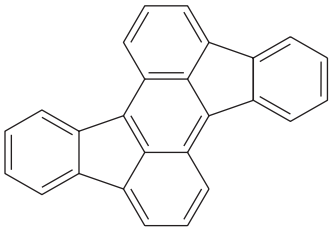
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8777.	9027-23-0	0	1	0	Ribulose-1,5-bisphosphate carboxylase {Rubisco, Fraction 1 protein (F-1 protein), also known as carboxylase, ribulose diphosphate}		22.2
8778.	197-61-5	1	0	0	Rubicene		1.20
8779.	7440-17-7	1	1	1	Rubidium	Rb	0.4, 20.5
8780.	22537-38-8	0	1	0	Rubidium, ion	Rb^{+1}	20.5
8781.	7440-18-8	1	1	1	Ruthenium	Ru	20.5
8782.	7440-19-9	1	1	1	Samarium	Sa	20.5
8783.	10361-82-7	0	1	0	Samarium chloride		18.4, 20.6
8784.	129990-04-1	0	1	0	Saponin B, from tobacco		0.4, 2.5
8785.	7440-20-2	1	1	1	Scandium	Sc	20.5
8786.	13967-63-0	1	1	1	Scandium, isotope of mass 46	^{46}Sc	20.5
8787.	14391-97-0	0	1	0	Scandium, isotope of mass 49	^{49}Sc	20.5
8788.	7782-49-2	1	1	1	Selenium	Se	0.4, 20.5, 23.5, 26.9
8789.	14265-71-5	1	1	1	Selenium, isotope of mass 75	^{75}Se	20.5
8790.	6898-95-9	1	1	1	Serine	$HO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	0.4, 2.5, 4.3, 4.10, 12.2, 25.29
8791.	35688-48-3	0	1	0	*D*-Serine, *N*-(carboxyacetyl)-		2.5, 4.3, 4.10, 12.2
8792.	56-45-1	0	1	0	*L*-Serine		2.5, 4.3, 4.10, 12.2
8793.	5147-00-2	0	1	0	*L*-Serine, acetate (ester)	$H_3C\text{-}COO\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$	4.3, 4.10, 5.3, 12.2
8794.	5692-15-9	0	1	0	*L*-Serine, labeled with ^{14}C		2.5, 4.3, 4.10, 12.2
8795.	142785-07-7	0	1	0	*L*-Serine, *L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-		2.5, 4.3, 4.10, 13.1
8796.	146440-48-4	0	1	0	*L*-Serine, *L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-		2.5, 4.3, 4.10, 13.1
8797.	7631-86-9	1	1	1	Silica	SiO_2	0.4, 20.6
8798.	60676-86-0	0	1	0	Silica, vitreous		20.6
8799.	19088-13-2	0	1	0	Silicic acid, aluminum salt	$Al_2(SiO_3)_3$	20.6
8800.	7440-21-3	1	1	1	Silicon	Si	0.4, 20.5
8801.	12141-45-6	1	0	0	Sillimanite	$Al_2O(SiO_4)$	20.6
8802.	7440-22-4	1	1	1	Silver	Ag	0.4, 20.5
8803.	14391-76-5	1	1	1	Silver, isotope of mass 110	^{110}Ag	20.5

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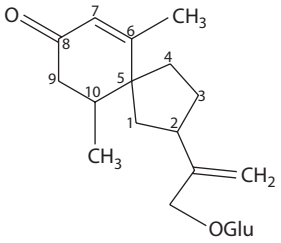
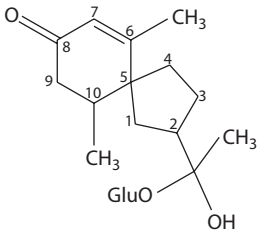
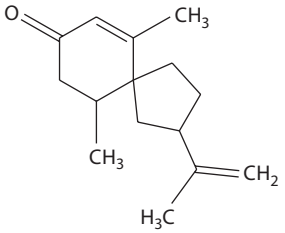
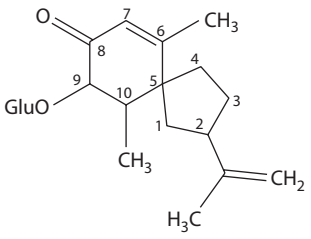
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8804.	7440-23-5	1	1	1	Sodium	Na	0.4, 20.5
8805.	7647-14-5	0	1	0	Sodium chloride	NaCl	20.6
8806.	1310-73-2	0	1	0	Sodium hydroxide	NaOH	20.6
8807.	1313-59-3	0	1	0	Sodium oxide	Na_2O	20.6
8808.	17341-25-2	0	1	0	Sodium, ion	Na^{+1}	20.5
8809.	16759-28-7	0	1	0	Sodium, isotope of mass 24	^{24}Na	20.5
8810.	62574-27-0	0	1	0	Spiro[4.5]dec-6-en-8-one, 2-[1-[(β-*D*-glucopyranosyloxy)methyl] ethenyl]-6,10-dimethyl-		2.5, 3.13
8811.	62574-29-2	0	1	0	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6, 10-dimethyl-		2.5, 3.13
8812.	62623-87-4	0	1	0	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-		2.5, 3.13
8813.	54878-25-0	0	1	0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-2-(1-methylethenyl)-, [2R-[2α,5α(R*)]]-		3.13
8814.		0	1	0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethenyl)- {isomer}		2.5, 3.13
8815.		0	1	0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethyl)-		2.5, 3.13
8816.	18444-79-6	0	1	0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethylidene)-, (5R-*cis*)-		2.5, 3.13
8817.	62574-25-8	0	1	0	Spiro[4.5]dec-6-en-8-one, 9-(β-*D*-glucopyranosyloxy)-6, 10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]-		2.5, 3.13
8818.	117407-01-9	0	1	0	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6, 10-dimethyl-2-(1-methylethenyl)- {spirovetivan A}		2.5, 3.13

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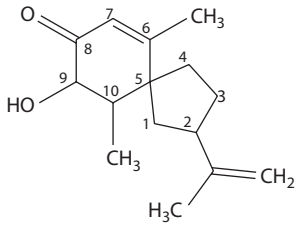
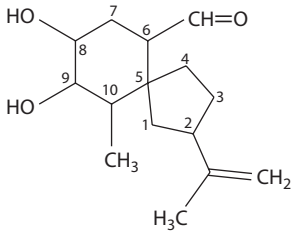
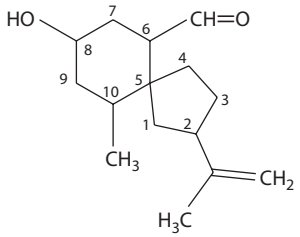
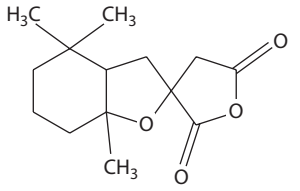
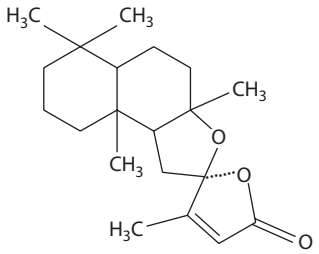
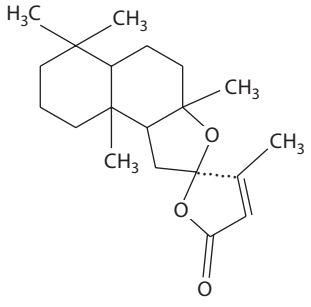
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8819.	117332-54-4	0	1	0	Spiro[4.5]dec-6-en-8-one,2-[1-(hydroxymethyl)ethenyl]-6-methyl- {spirovetivan B}		2.5, 3.13
8820.	62623-88-5	0	1	0	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]-		2.5, 3.13
8821.	55784-90-2	0	1	0	Spiro[4.5]decane-6-carboxaldehyde, 8, 9-dihydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,9α,10β]]-		2.5, 3.12
8822.	35951-50-9	0	1	0	Spiro[4.5]decane-6-carboxaldehyde, 8-hydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,10β]]-		2.5, 3.12
8823.	162188-94-5	0	1	0	Spiro[benzofuran-6(2*H*),2′-[1,3] dioxolan]-2-one, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-, (±)-		7.1, 10.2
8824.	5989-24-2 30987-48-5	1	1	1	Spiro[furan-2(3*H*),2′(1′*H*)-naphtho [2,1-*b*]furan]-5(4*H*)-one, decahydro-3, 3′a,6′,6′,9′a-pentamethyl- {α-levantenolide}		6.3, 10.2
8825.	1235-78-5	1	1	1	Spiro[furan-2(5*H*),2′(1′*H*)-naphtho [2,1-*b*]furan]-5-one, 3′a,4′,5′, 5′a,6′,7′,8′,9′,9′a,9′b-decahydro-3,3′a,6′,6′, 9′a-pentamethyl-, [2′S-(2′α,3′aα,5′aβ,9′aα,9′bβ)]- {β-levantenolide}		6.3, 10.2

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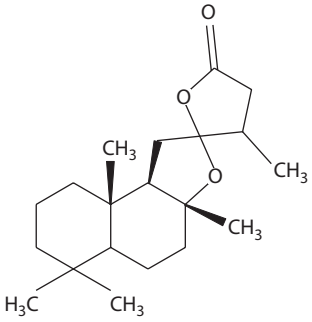
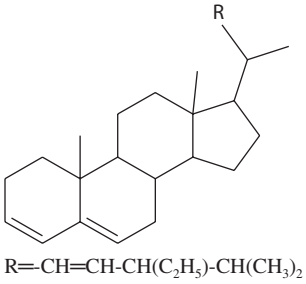
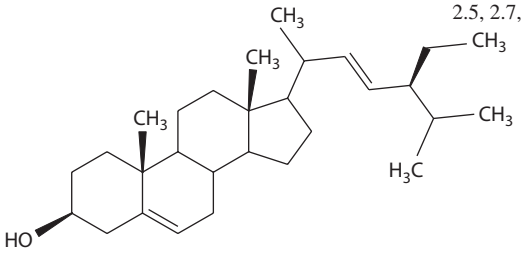
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8826.		0	1	0	Spiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one, dodecahydro-3,3′a,6′,9′a-pentamethyl-{α_2-levantanolide}		2.5, 3.12
8827.	9005-25-8	1	1	1	Starch		0.4, 2.5, 8.3, 25.29
8828.	39341-47-4	0	1	0	Starch, labeled with ^{13}C, labeled with ^{13}C {starch-^{13}C}		2.5, 8.3
8829.	70226-57-2	0	1	0	Starch, labeled with ^{14}C {starch-^{14}C}		2.5, 8.3, 25.29
8830.		0	1	0	*Staphylococcus saprophyticus*		22.2
8831.		0	1	0	*Staphylococcus epidermidis*		22.2
8832.		0	1	0	*Staphylococcus cohnii*		22.2
8833.		0	1	0	*Staphylococcus sciuri*		22.2
8834.		0	1	0	*Stenotrophomonas maltophilia*		22.2
8835.	79897-80-6	1	1	1	Stigmasta-3,5-diene, (24ξ)-		2.7, 1.12
8836.	83-48-7	1	1	1	Stigmasta-5,22-dien-3-ol, (3β,22E)-{stigmasterol}		2.5, 2.7, 25.29
8837.	71607-87-9	1	1	1	Stigmasta-5,22-dien-3-ol, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]-{stigmasteryl linolenate}		2.7, 5.3
8838.	71278-15-4	1	1	1	Stigmasta-5,22-dien-3-ol, 9,12-octadecadienoate, [3β(9*Z*,12*Z*),22*E*]-{stigmasteryl linoleate}		2.7, 5.3
8839.	31615-93-7	1	1	1	Stigmasta-5,22-dien-3-ol, 9-octadecenoate, [3β(*Z*),22*E*]- {stigmasteryl oleate}		2.7, 5.3
8840.	20242-97-1	1	1	1	Stigmasta-5,22-dien-3-ol, dodecanoate, (3β,22*E*)- {stigmasteryl laurate}		2.7, 5.3
8841.	2308-84-1	1	1	1	Stigmasta-5,22-dien-3-ol, hexadecanoate, (3β,22*E*)-{stigmasteryl palmitate}		2.7, 5.3

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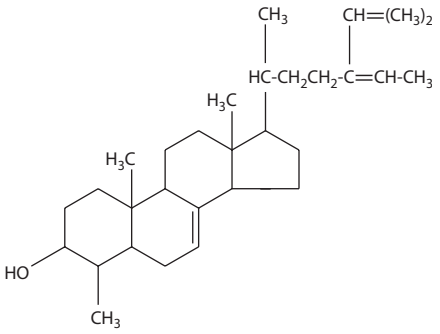
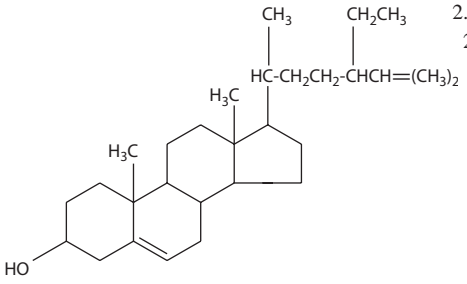
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8842.	23838-16-6	1	1	1	Stigmasta-5,22-dien-3-ol, octadecanoate, (3β,22*E*)- {stigmasteryl stearate}		2.7, 5.3
8843.	20242-98-2	1	1	1	Stigmasta-5,22-dien-3-ol, tetradecanoate, (3β,22*E*)- {stigmasteryl myristate}		2.7, 5.3
8844.	28949-66-8	0	1	0	Stigmasta-5,24-dien-3-ol, (β)-		2.5, 2.7
8845.	18472-36-1	1	1	1	Stigmasta-5,24(28)-dien-3-ol, (3β)-		2.5, 2.7
8846.	17605-67-3	1	1	1	Stigmasta-5,24(28)-dien-3-ol, (3β,24*E*)-		2.5, 2.7
8847.	481-14-1	0	1	0	Stigmasta-5,24(28)-dien-3-ol, (3β,24*Z*)-		2.5, 2.7
8848.	2364-23-0	0	1	0	Stigmasta-5,25-dien-3-ol, (3β,24S)-		2.5, 2.7
8849.	7212-91-1	0	1	0	Stigmasta-7,24(28)-dien-3-ol, (3β,5α)-		2.5, 2.7
8850.	23290-26-8	0	1	0	Stigmasta-7,24(28)-dien-3-ol,(3β,5α,24*Z*)-		2.5, 2.7
8851.	12002-39-0	0	1	0	Stigmasta-7,24(28)-dien-3-ol, 4-methyl- {sitosterols}		2.5, 2.7
8852.	39006-52-5	0	1	0	Stigmasta-7,24(28)-diene-3-ol, 4-methyl- (3β,4α,5α,24*E*)		2.5, 2.7
8853.	474-40-8	1	1	1	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α,24*Z*)- {α-sitosterol}		2.5, 2.7
8854.	120056-15-7	1	0	0	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,5α)-		2.5, 2.7
8855.	11040-28-1	1	1	1	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,5α)-		2.5, 2.7
8856.	34347-65-4	0	1	0	Stigmasta-8,14-dien-3-ol, (3β,5α)-		2.5, 2.7
8857.	159169-57-0	0	1	0	Stigmasta-8,24(28)-dien-3-ol, 4, 14-dimethyl-, (3β,4α,5α)-		2.5, 2.7
8858.	102491-96-3	1	1	1	Stigmasta-3,5,22-triene, (22*E*)-		2.7, 1.12
8859.	81531-12-6	1	1	1	Stigmasta-3,5,22-triene, (22*E*,24ξ)-		2.7, 1.12
8860.	86709-50-4	1	1	1	Stigmasta-3,5,24(28)-triene		2.7, 1.12
8861.	34350-85-1	0	1	0	Stigmasta-8,14,24(28)-trien-3-ol,(3β,5α)-		2.5, 2.7
8862.	159169-58-1	0	1	0	Stigmasta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-		2.5, 2.7
8863.	83-46-5	1	1	1	Stigmast-5-en-3-ol, (3β)- {β-sitosterol}		2.5, 2.7, 25.29, 26.9

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
8864.	83-47-6	1	1	1	Stigmast-5-en-3-ol, (3β, 24*S*)- {γ-sitosterol}		2.5, 2.7
8865.	3177-92-2	1	1	1	Stigmast-5-en-3-ol, 9,12,15-octadecatrienoate, [3β(9*Z*,12*Z*,15*Z*)]- {β-sitosteryl linolenate}		2.7, 5.3
8866.	3577-13-7	1	1	1	Stigmast-5-en-3-ol, 9,12-octadecadienoate, [3β(*Z*,*Z*)]- {β-sitosteryl linoleate}		2.7, 5.3
8867.	3712-16-1	1	1	1	Stigmast-5-en-3-ol, 9-octadecenoate, [3β(*Z*)]- {β-sitosteryl oleate}		2.7, 5.3
8868.	41005-65-6	1	1	1	Stigmast-5-en-3-ol, dodecanoate, (3β)- {β-sitosteryl laurate}		2.7, 5.3
8869.	2308-85-2	1	1	1	Stigmast-5-en-3-ol, hexadecanoate, (3β)- {β-sitosteryl palmitate}		2.7, 5.3
8870.	34137-25-2	1	1	1	Stigmast-5-en-3-ol, octadecanoate, (3β)- {β-sitosteryl stearate}		2.7, 5.3
8871.	10473-40-2	1	1	1	Stigmast-5-en-3-ol, tetradecanoate, (3β)- {β-sitosteryl myristate}		2.7, 5.3
8872.	6869-99-4	0	1	0	Stigmast-7-en-3-ol, (3β)-		2.5, 2.7
8873.	521-03-9	0	1	0	Stigmast-7-en-3-ol, (3β,5α)-		2.5, 2.7
8874.	4736-56-5	0	1	0	Stigmast-22-en-3-ol (3β,5α,22Z,24S)		2.5, 2.7
8875.	57-92-1	0	1	0	Streptomycin		21.3
8876.	7440-24-6	1	1	1	Strontium	Sr	0.4, 20.5
8877.	14158-27-1	0	1	0	Strontium, isotope of mass 89	^{89}Sr	20.5
8878.	10098-97-2	0	1	0	Strontium, isotope of mass 90	^{90}Sr	20.5
8879.	14808-79-8	1	1	1	Sulfate	SO_4^{-2}	0.4, 18.1, 20.5
8880.	18496-25-8	1	1	1	Sulfide	S^{-2}	18.1, 20.5
8881.	14265-45-3	1	1	1	Sulfite	SO_3^{-2}	18.1, 20.5
8882.		0	1	0	Sulfonium		18.1, 20.6
8883.	7704-34-9	1	1	1	Sulfur	S	0.4, 18.1, 20.5, 21.3
8884.	7446-09-5	1	0	0	Sulfur dioxide	SO_2	18.1
8885.	2551-62-4	0	1	0	Sulfur hexafluoride	SF_6	18.1, 18.4
8886.	7446-11-9	1	0	0	Sulfur trioxide	$S0_3$	18.1
8887.	7664-93-9	0	1	0	Sulfuric acid	H_2SO_4	0.4, 18.1, 20.6, 21.3
8888.	7783-20-2	0	1	0	Sulfuric acid, ammonium salt		18.1, 20.6
8889.	7778-18-9	0	1	0	Sulfuric acid, calcium salt	$CaSO_4$	18.1, 20.6
8890.	7758-98-7	0	1	0	Sulfuric acid, copper salt	$CuSO_4$	20.6, 21.3
8891.	10377-48-7	0	1	0	Sulfuric acid, dilithium salt	Li_2SO_4	18.1, 20.6
8892.	7778-80-5	0	1	0	Sulfuric acid, dipotassium salt	K_2SO_4	18.1, 20.6
8893.	7757-82-6	0	1	0	Sulfuric acid, disodium salt	Na_2SO_4	18.1, 20.6
8894.	7757-83-7	0	1	0	Sulfurous acid, disodium salt	Na_2SO_3	18.1, 20.6
8895.	7487-88-9	0	1	0	Sulfuric acid, magnesium salt	$MgSO_4$	18.1, 20.6
8896.	7488-54-2	0	1	0	Sulfuric acid, rubidium salt		18.1, 20.6
8897.	7733-02-0	0	1	0	Sulfuric acid, zinc salt		18.1, 20.6
8898.	7773-03-7	0	1	0	Sulfurous acid, monopotassium salt	$KHSO_3$	18.1, 20.6
8899.	11062-77-4	1	0	0	Superoxide (anion radical)		27.1
8900.	72506-68-4	0	1	0	Synthase, 1-aminocyclopropanecarboxylate		22.2
8901.	37211-77-1	0	1	0	Synthase, 5-dehydroquinate		22.2
8902.	9068-73-9	0	1	0	Synthase, 5-enolpyruvoylshikimate 3-phosphate		22.2

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8903.	144324-42-5	0	1	0	Synthase, 5-enolpyruvoylshikimate 3-phosphate (petunia clone pMON9531/pMON9556 reduced) 101-*L*-alanine-		22.2
8904.	144324-43-6	0	1	0	Synthase, 5-enolpyruvoylshikimate 3-phosphate (petunia clone pMON9531/pMON9556 reduced) 101-*L*-alanine-192-*L*-threonine-		22.2
8905.	9027-45-6	0	1	0	Synthase, acetolactate		22.2
8906.	9031-59-8	0	1	0	Synthase, anthranilate		22.2
8907.	37290-89-4	0	1	0	Synthase, cysteine {acetylserine sulfhydrylase}		22.2
8908.	9055-59-8	0	1	0	Synthase, dihydrodipicolinate		22.2
8909.	56803-04-4	0	1	0	Synthase, flavanone		22.2
8910.	9013-48-3	0	1	0	Synthase, malate		22.2
8911.	108281-08-9	0	1	0	Synthase, mannopine		22.2
8912.	131754-88-6	0	1	0	Synthase, nicotine		22.2
8913.	9036-37-7	0	1	0	Synthase, porphobilinogen		22.2
8914.	9023-35-2	0	1	0	Synthase, pseudouridylate		22.2
8915.	9077-14-9	0	1	0	Synthase, squalene		22.2
8916.	9014-52-2	0	1	0	Synthase, tryptophan		22.2
8917.	9031-56-5	0	1	0	Synthetase		22.2
8918.	37205-63-3	0	1	0	Synthetase, adenosine triphosphate		22.2
8919.	9028-02-8	0	1	0	Synthetase, aminoacyl-transfer ribonucleate		22.2
8920.	9037-14-3	0	1	0	Synthetase, aminolevulinate {synthase, aminolevulinate}		22.2
8921.	37205-35-9	0	1	0	Synthetase, arginyl-transfer ribonucleate		22.2
8922.	37332-51-7	0	1	0	Synthetase, *p*-coumaroyl coenzyme A		22.2
8923.	37211-77-1	0	1	0	Synthetase, 5-dehydroquinate		22.2
8924.	9023-70-5	0	1	0	Synthetase, glutamine		22.2
8925.	147626-93-5	0	1	0	Synthetase, glutamine (tobacco clone pcGS2-17 isoenzyme 2 subunit precursor reduced)		22.2
8926.	9068-76-2	0	1	0	Synthetase, glutamyl-transfer ribonucleate		22.2
8927.	39341-90-7	0	1	0	Synthetase, indoleacetate		22.2
8928.	9031-15-6	0	1	0	Synthetase, leucyl-transfer ribonucleate		22.2
8929.	37318-64-2	0	1	0	Synthetase, methenyltetrahydrofolate		22.2
8930.	9014-36-2	0	1	0	Synthetase, succinyl coenzyme A (guanosine diphosphate-forming)		22.2
8931.	9023-47-6	0	1	0	Synthetase, valyl-transfer ribonucleate		22.2
8932.	71010-48-5	0	1	0	α-Tabacenic acid		0.4, 4.3
8933.	71010-46-3	0	1	0	β-Tabacenic acid		0.4, 4.3
8934.	71010-47-4	0	1	0	γ-Tabacenic acid		0.4, 4.3
8935.	1401-55-4	0	1	0	Tannins {tannic acid}		0.4, 2.5, 4.3, 5.3, 24.3
8936.	7440-25-7	1	1	1	Tantalum	Ta	20.5
8937.	13494-80-9	1	1	1	Tellurium	Te	20.5
8938.	7440-27-9	0	1	0	Terbium	Tb	20.5
8939.		1	0	0	Tergitol ether I[d]: R = CH_3, x = 1		10.2
8940.		1	0	0	Tergitol ether II[d]: R = CH_3, x = 2		10.2

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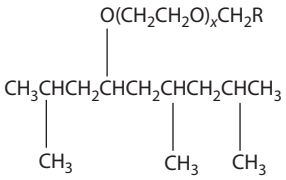
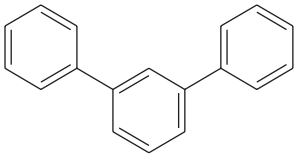
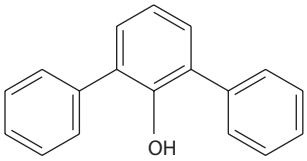
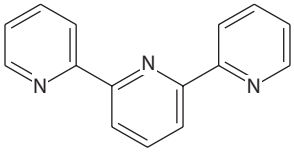
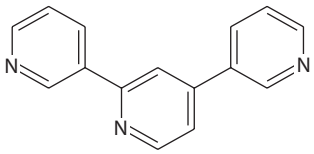
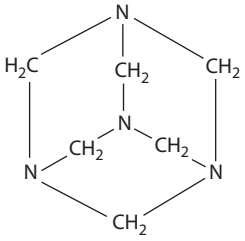
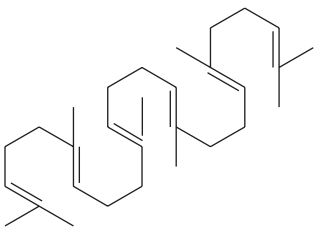
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8941.		1	0	0	Tergitol ether III[d]: R = CH_3, x = 3		10.2
8942.		1	0	0	Tergitol ether IV[d]: R = H, x = 1[d]. The Tergitol ethers possessed the structures indicated		10.2
8943.	92-06-8 26140-60-3	1	0	0	1,1′:3′,1″-Terphenyl {*m*-terphenyl}		1.13
8944.	2432-11-3	1	0	0	1,1′,3′-Terphenyl-2′-ol		9.22
8945.	92-94-4	1	0	0	1,1′:4′,1″-Terphenyl		1.13
8946.	1148-79-4	1	1	1	2,2′:6′,2″-Terpyridine		17.11
8947.	494-04-2	1	1	1	3,2′:4′,3″-Terpyridine {nicotelline}		0.4, 17.11
8948.	100-97-0	1	0	0	1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}] decane {hexamethylenetetramine}		12.2
8949.	4181-95-7	1	0	0	Tetracontane	H_3C-$(CH_2)_{38}$-CH_3	1.10
8950.	11030-10-7	1	0	0	1,6,10,14,18,23-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- {isosqualene}		1.11
8951.	7683-64-9	1	1	1	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-		1.11
8952.	111-02-4	1	1	1	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-*E*)- {squalene}		1.11, 25.29

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8953.		0	1	0	2,6,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-pentamethyl-		1.11
8954.	646-31-1	1	1	1	Tetracosane	H_3C-$(CH_2)_{22}$-CH_3	1.10, 25.29
8955.	28503-88-0	1	1	1	Tetracosane, methyl-		1.10
8956.	1560-78-7	1	0	0	Tetracosane, 2-methyl-		1.10
8957.		1	1	1	Tetracosane, 3-methyl-		1.10
8958.	557-59-5	1	1	1	Tetracosanoic acid {lignoceric acid}	H_3C-$(CH_2)_{22}$-COOH	4.3
8959.	42233-59-0	1	1	1	Tetracosanoic acid, docosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{21}$-CH_3	5.3
8960.	42233-49-8	1	1	1	Tetracosanoic acid, dodecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{11}$-CH_3	5.3
8961.	42233-57-8	1	1	1	Tetracosanoic acid, eicosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{19}$-CH_3	5.3
8962.		1	1	1	Tetracosanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl tetracosanoate}		2.7, 5.3
8963.	42233-58-9	1	1	1	Tetracosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{20}$-CH_3	5.3
8964.		1	1	1	Tetracosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{26}$-CH_3	5.3
8965.	42233-54-5	1	1	1	Tetracosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{16}$-CH_3	5.3
8966.	121878-03-3	1	1	1	Tetracosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{25}$-CH_3	5.3
8967.	42233-53-4	1	1	1	Tetracosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{15}$-CH_3	5.3
8968.	42233-56-7	1	1	1	Tetracosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{18}$-CH_3	5.3
8969.	24897-95-8	1	1	1	Tetracosanoic acid, octacosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{27}$-CH_3	5.3
8970.	42233-55-6	1	1	1	Tetracosanoic acid, octadecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{17}$-CH_3	5.3
8971.		1	1	1	Tetracosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{24}$-CH_3	5.3
8972.	42233-52-3	1	1	1	Tetracosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{14}$-CH_3	5.3
8973.	1001-43-0	1	1	1	Tetracosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{23}$-CH_3	5.3
8974.	42233-51-2	1	1	1	Tetracosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{13}$-CH_3	5.3
8975.	42233-60-3	1	1	1	Tetracosanoic acid, tricosyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{22}$-CH_3	5.3
8976.	42233-50-1	1	1	1	Tetracosanoic acid, tridecyl ester	H_3C-$(CH_2)_{22}$-COO-$(CH_2)_{12}$-CH_3	5.3
8977.	36378-43-5	0	1	0	Tetracosanoic acid, 22-methyl-		4.3
8978.	121877-84-7	1	1	1	Tetracosanoic acid, 22-methyl-, docosyl ester		5.3
8979.	121877-77-8	1	1	1	Tetracosanoic acid, 22-methyl-, eicosyl ester		5.3
8980.		0	1	0	Tetracosanoic acid, 23-methyl-		4.3
8981.	71608-05-4	1	0	0	Tetracosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-		5.3
8982.	506-51-4	1	1	1	1-Tetracosanol	H_3C-$(CH_2)_{22}$-CH_2OH	2.5
8983.	63785-29-5	0	1	0	1-Tetracosanol, 22-methyl-		2.5
8984.		0	1	0	1-Tetracosanol, 23-methyl-		2.5
8985.	10192-32-2	1	0	0	1-Tetracosene	H_2C=CH-$(CH_2)_{21}$-CH_3	1.11
8986.		1	0	0	1-Tetracosene, 2-methyl-	H_2C=C(CH_3)-$(CH_2)_{21}$-CH_3	1.11
8987.		1	0	0	2-Tetracosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{20}$-CH_3	1.11
8988.		1	0	0	2-Tetracosene, (*E*)-		1.11
8989.		1	0	0	2-Tetracosene, 2-methyl-	H_3C-C(CH_3)=CH-$(CH_2)_{20}$-CH_3	1.11
8990.		1	0	0	2-Tetracosene, 22-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{18}$-CH(CH_3)-CH_2-CH_3	1.11
8991.		1	0	0	2-Tetracosene, 22-methyl-, (*E*)-		1.11
8992.		1	0	0	2-Tetracosene, 23-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{19}$-CH$(CH_3)_2$	1.11
8993.		1	0	0	2-Tetracosene, 23-methyl-, (*E*)-		1.11
8994.	14490-79-0	1	0	0	15-Tetracosenoic acid {nervonic acid}		4.3
8995.	506-37-6	1	0	0	15-Tetracosenoic acid, (*Z*)-		4.3
8996.	69521-46-6	0	1	0	Tetracosen-1-ol		2.5
8997.	58879-40-6	0	1	0	1,13-Tetradecadien-3-one		3.13
8998.	124-25-4	1	1	1	Tetradecanal {myristaldehyde}	H_3C-$(CH_2)_{12}$-CH=O	3.12, 24.3

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	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
8999.	629-59-4	1	1	1	Tetradecane	H_3C-$(CH_2)_{12}$-CH_3	1.10
9000.	1560-95-8	0	1	0	Tetradecane, 2-methyl-	H_3C-$(CH_2)_{11}$-CH═$(CH_3)_2$	1.10
9001.	18435-22-8	0	1	0	Tetradecane, 3-methyl-	H_3C-$(CH_2)_{10}$-$CH(CH_3)$-CH_2-CH_3	1.10
9002.	14905-56-7	0	1	0	Tetradecane, 2,6,10-trimethyl-		1.10
9003.	821-38-5	1	0	0	Tetradecanedioic acid	HOOC-$(CH_2)_{12}$-COOH	4.3
9004.	544-63-8	1	1	1	Tetradecanoic acid {myristic acid}	H_3C-$(CH_2)_{12}$-COOH	0.4, 4.3, 24.3
9005.	110-36-1	1	0	0	Tetradecanoic acid, butyl ester		5.3
9006.	42232-05-3	1	1	1	Tetradecanoic acid, docosyl ester	H_3C-$(CH_2)_{12}$-$COO(CH_2)_{21}$-CH_3	5.3
9007.	2040-64-4	1	1	1	Tetradecanoic acid, dodecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{11}$-CH_3	5.3
9008.	22413-00-9	1	1	1	Tetradecanoic acid, eicosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{19}$-CH_3	5.3
9009.	124-06-1	0	1	0	Tetradecanoic acid, ethyl ester {ethyl myristate}	H_3C-$(CH_2)_{12}$-COO-C_2H_5	5.3, 24.3, 25.29
9010.	42218-21-3	1	1	1	Tetradecanoic acid, heneicosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{20}$-CH_3	5.3
9011.		1	1	1	Tetradecanoic acid, heptacosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{26}$-CH_3	5.3
9012.	18299-78-0	1	1	1	Tetradecanoic acid, heptadecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{16}$-CH_3	5.3
9013.	80252-34-2	1	1	1	Tetradecanoic acid, hexacosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{25}$-CH_3	5.3
9014.	2599-01-1	1	1	1	Tetradecanoic acid, hexadecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{15}$-CH_3	5.3
9015.	124-10-7	1	1	1	Tetradecanoic acid, methyl ester	H_3C-$(CH_2)_{12}$-COO-CH_3	5.3
9016.	110-27-0	0	1	0	Tetradecanoic acid, 1-methylethyl ester	H_3C-$(CH_2)_{12}$-COO-CH═$(CH_3)_2$	5.3
9017.	36617-28-4	1	1	1	Tetradecanoic acid, nonadecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{18}$-CH_3	5.3
9018.	3234-81-9	1	1	1	Tetradecanoic acid, octadecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{17}$-CH_3	5.3
9019.	121877-45-0	1	1	1	Tetradecanoic acid, pentacosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{24}$-CH_3	5.3
9020.	18299-74-6	1	1	1	Tetradecanoic acid, pentadecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{14}$-CH_3	5.3
9021.	18653-39-9	1	1	1	Tetradecanoic acid, tetracosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{23}$-CH_3	5.3
9022.	3234-85-3	1	1	1	Tetradecanoic acid, tetradecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{13}$-CH_3	5.3
9023.	42232-06-4	1	1	1	Tetradecanoic acid, tricosyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{22}$-CH_3	5.3
9024.	36617-27-3	1	1	1	Tetradecanoic acid, tridecyl ester	H_3C-$(CH_2)_{12}$-COO-$(CH_2)_{12}$-CH_3	5.3
9025.	1961-72-4	1	1	1	Tetradecanoic acid, 3-hydroxy-	H_3C-$(CH_2)_{10}$-$CHOH$-CH_2-COOH	2.5, 4.3
9026.	5502-94-3 5746-58-7	1	1	1	Tetradecanoic acid, 12-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COOH	4.3
9027.	121877-30-3	1	1	1	Tetradecanoic acid, 12-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{21}$-CH_3	5.3
9028.	121877-23-4	1	1	1	Tetradecanoic acid, 12-methyl-, eicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{19}$-CH_3	5.3
9029.	121877-28-9	1	1	1	Tetradecanoic acid, 12-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{20}$-CH_3	5.3
9030.	121877-56-3	1	1	1	Tetradecanoic acid, 12-methyl-, hexacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{25}$-CH_3	5.3
9031.	121877-08-5	1	1	1	Tetradecanoic acid, 12-methyl-, hexadecyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{15}$-CH_3	5.3
9032.	121877-17-6	1	1	1	Tetradecanoic acid, 12-methyl-, octadecyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{17}$-CH_3	5.3
9033.	121877-48-3	1	1	1	Tetradecanoic acid, 12-methyl-, pentacosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{24}$-CH_3	5.3
9034.	121877-40-5	1	1	1	Tetradecanoic acid, 12-methyl-, tetracosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{23}$-CH_3	5.3
9035.	121877-34-7	1	1	1	Tetradecanoic acid, 12-methyl-, tricosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{10}$-COO-$(CH_2)_{22}$-CH_3	5.3
9036.	2485-71-4	0	1	0	Tetradecanoic acid, 13-methyl-	$(H_3C)_2$═CH-$(CH_2)_{11}$-COOH	4.3
9037.	121877-29-0	1	1	1	Tetradecanoic acid, 13-methyl-, docosyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{21}$-CH_3	5.3
9038.	121877-21-2	1	1	1	Tetradecanoic acid, 13-methyl-, eicosyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{19}$-CH_3	5.3

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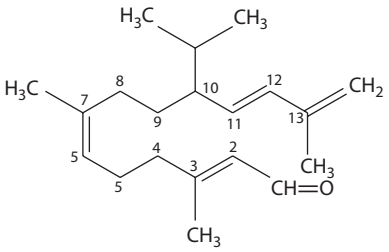
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
9039.	121877-26-7	1	1	1	Tetradecanoic acid, 13-methyl-, heneicosyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{20}$-CH_3	5.3
9040.	121877-49-4	1	1	1	Tetradecanoic acid, 13-methyl-, hexacosyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{25}$-CH_3	5.3
9041.	71801-84-8	1	1	1	Tetradecanoic acid, 13-methyl-, hexadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{15}$-CH_3	5.3
9042.	121877-12-1	1	1	1	Tetradecanoic acid, 13-methyl-, octadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{17}$-CH_3	5.3
9043.	121877-35-8	1	1	1	Tetradecanoic acid, 13-methyl-, tetracosyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{23}$-CH_3	5.3
9044.	121877-32-5	1	1	1	Tetradecanoic acid, 13-methyl-, tricosyl ester	$(H_3C)_2$═CH-$(CH_2)_{11}$-COO-$(CH_2)_{22}$-CH_3	5.3
9045.	71607-88-0 110053-62-8	1	1	1	Tetradecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl tetradecanoate}		5.3
9046.	62172-52-5	1	0	0	Tetradecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
9047.	112-72-1	1	1	1	1-Tetradecanol	H_3C-$(CH_2)_{12}$-CH_2OH	2.5
9048.	50313-71-8	0	1	0	1-Tetradecanol, 12-methyl-		2.5
9049.	15371-32-1	0	1	0	2,6,11,13-Tetradecatetraenal, 3,7,13-trimethyl-10-(1-methylethyl)-, [S-(*E,E,E*)]-		3.12
9050.	125572-76-1	1	1	1	2,6,11,13-Tetradecatetraenal, 3,7,13-trimethyl-10-(1-methylethyl)-		3.12
9051.	150405-77-9	0	1	0	2,6,11,13-Tetradecatetraen-1-ol, 3,7,13-trimethyl-10-(1-methylethyl)-		2.5
9052.	30790-23-9	0	1	0	Tetradecatrienoic acid		4.3
9053.	1120-36-1	1	1	1	1-Tetradecene	H_2C═CH-$(CH_2)_{11}$-CH_3	1.11
9054.	52254-38-3	1	0	0	1-Tetradecene, 2-methyl-	H_2C═$C(CH_3)$-$(CH_2)_{11}$-CH_3	1.11
9055.	1652-97-7	1	0	0	2-Tetradecene		1.11
9056.	35953-53-8	1	0	0	2-Tetradecene, (*Z*)-	H_3C-CH═CH-$(CH_2)_{10}$-CH_3	1.11
9057.	35953-54-9	1	0	0	2-Tetradecene, (*E*)-		1.11
9058.	52254-38-3	1	0	0	2-Tetradecene, 2-methyl-	H_3C-$C(CH_3)$═CH-$(CH_2)_{10}$-CH_3	1.11
9059.		1	0	0	2-Tetradecene, 12-methyl-,(*Z*)-	H_3C-CH═CH-$(CH_2)_8$-$CH(CH_3)$-CH_2-CH_3	1.11
9060.		1	0	0	2-Tetradecene, 12-methyl-, (*E*)-		1.11
9061.		1	0	0	2-Tetradecene, 13-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_9$-$CH(CH_3)_2$	1.11
9062.		1	0	0	2-Tetradecene, 13-methyl-, (*E*)-		1.11
9063.	26444-03-1	1	1	1	Tetradecenoic acid		4.3
9064.	56219-06-8	0	1	0	9-Tetradecenoic acid, methyl ester, (*Z*)-		5.3
9065.	14167-59-0	1	1	1	Tetratriacontane	H_3C-$(CH_2)_{32}$-CH_3	1.10
9066.	14167-65-8	1	1	1	Tetratriacontane, 2-methyl-	H_3C-$CH(CH_3)$-$(CH_2)_{31}$-CH_3	1.10
9067.	66309-88-4	1	1	1	Tetratriacontane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{30}$-CH_3	1.10
9068.	38232-04-1	1	0	0	Tetratriacontanoic acid	H_3C-$(CH_2)_{32}$-COOH	4.3
9069.	7440-28-0	1	1	1	Thallium	Tl	0.4, 20.5
9070.	420-12-2	0	1	0	Thiacyclopropane {ethylene sulfide}		18.1

(*continued*)

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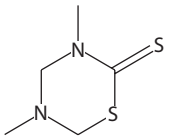
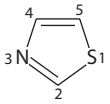
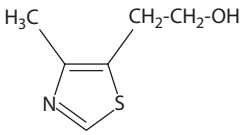
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9071.	533-74-4	0	1	0	1,3,5-Thiadiazine, 2-thio-3,5-dimethyl-tetrahydro- {Dazomet®, Mylone®}		18.1, 21.3
9072.	288-47-1	1	1	1	Thiazole		18.1, 24.3
9073.		1	0	0	Thiazole, methyl-5-propyl-		18.1
9074.	37645-61-7	1	0	0	Thiazole, 2-butyl-		18.1
9075.	15679-09-1	1	0	0	Thiazole, 2-ethyl-		18.1
9076.	19961-53-6	1	0	0	Thiazole, 2-ethyl-5-methyl-		18.1
9077.	3581-87-1	1	0	0	Thiazole, 2-methyl-		18.1
9078.	15679-11-5	1	0	0	Thiazole, 2-methyl-4-(1,1-dimethylethyl)-		18.1
9079.	17626-75-4	1	0	0	Thiazole, 2-propyl-		18.1
9080.		1	0	0	Thiazole, 2-(3-methylbutyl)-		18.1
9081.	15679-10-4	1	0	0	Thiazole, 2-(1-methylethyl)-		18.1
9082.	18277-27-5	1	0	0	Thiazole, 2-(1-methylpropyl)-		18.1
9083.	18640-74-9	1	0	0	Thiazole, 2-(2-methylpropyl)-		18.1
9084.	32272-49-4	1	0	0	Thiazole, 2,4-diethyl-		18.1
9085.	52414-89-8	1	0	0	Thiazole, 2,4-diethyl-5-methyl-		18.1
9086.	541-58-2	1	0	0	Thiazole, 2,4-dimethyl-		18.1
9087.	13623-11-5	1	0	0	Thiazole, 2,4,5-trimethyl-		18.1
9088.	41981-71-9	1	0	0	Thiazole, 2,5-diethyl-4-methyl-		18.1
9089.	4175-66-0	1	0	0	Thiazole, 2,5-dimethyl-		18.1
9090.	15679-12-6	1	0	0	Thiazole, 2-ethyl-4-methyl-		18.1
9091.	32272-48-3	1	0	0	Thiazole, 4-ethyl-2-methyl-		18.1
9092.	52414-91-2	1	0	0	Thiazole, 4-ethyl-5-methyl-		18.1
9093.	87116-68-5	1	0	0	Thiazole, 4-ethyl-5-methyl-2-(1-methylethyl)-		18.1
9094.	693-95-8	1	0	0	Thiazole, 4-methyl-		18.1
9095.	656-53-1	1	0	0	Thiazole, 4-methyl-5-(2-acetoxyethyl)-		5.3, 18.1
9096.	137-00-8	0	1	0	Thiazole, 4-methyl-5-(2′-hydroxyethyl)-		18.1
9097.	15679-13-7	1	0	0	Thiazole, 4-methyl-2-(1-methylethyl)-		18.1
9098.		1	0	0	Thiazole, 4-(2-methylpropyl)-		18.1
9099.	41981-60-6	1	0	0	Thiazole, 4-propyl-		18.1
9100.	2346-00-1	1	0	0	Thiazole, 4,5-dihydro-2-methyl-		18.1
9101.	3581-91-7	1	0	0	Thiazole, 4,5-dimethyl-		18.1
9102.	873-64-3	1	0	0	Thiazole, 4,5-dimethyl-2-ethyl-		18.1
9103.	53498-30-9	1	0	0	Thiazole, 4,5-dimethyl-2-(1-methylethyl)-		18.1
9104.	53498-32-1	1	0	0	Thiazole, 4,5-dimethyl-2-(2-methylpropyl)-		18.1
9105.	1759-28-0	1	0	0	Thiazole, 5-ethenyl-4-methyl-		18.1
9106.	17626-73-2	1	0	0	Thiazole, 5-ethyl-		18.1
9107.	38205-61-7	1	0	0	Thiazole, 5-ethyl-2,4-dimethyl-		18.1
9108.	19961-52-5	1	0	0	Thiazole, 5-ethyl-2-methyl-		18.1
9109.	31883-01-9	1	0	0	Thiazole, 5-ethyl-4-methyl-		18.1

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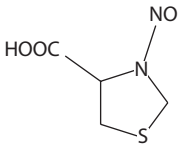
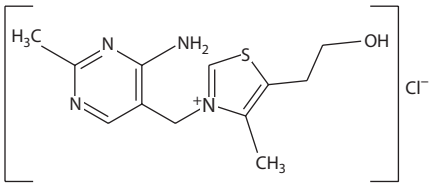
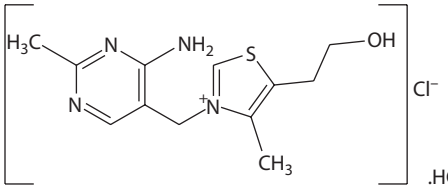
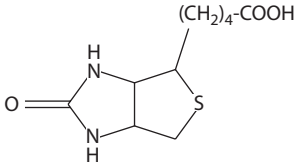
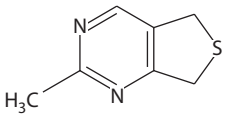
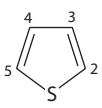
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9110.	3581-89-3	1	0	0	Thiazole, 5-methyl-		18.1
9111.	72611-71-3	1	0	0	Thiazole, 5-methyl-2-(2-methylpropyl)-		18.1
9112.	88381-44-6	0	1	0	4-Thiazolidinecarboxylic acid, 3-nitroso- {*N*-nitrosothioproline}		4.3, XV-9, 18.1
9113.	154-87-0	0	1	0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, *P*,*P*′-dioxide		5.3, 12.2, 17.7, 18.1, 18.4
9114.	59-43-8	0	1	0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride {thiamine}		0.4, 2.5, 12.2, 17.7, 18.1, 18.4
9115.	67-03-8	0	1	0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride, monohydrochloride {thiamine hydrochloride}		2.5, 12.2, 17.7, 18.1, 18.4
9116.	58-85-5	0	1	0	1*H*-Thieno[3,4-*d*]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3aS-(3aα,4β,6aα)]-		4.3, 17.4, 17.23, 18.1
9117.	36267-71-7	0	1	0	Thieno(3,4-*d*)pyrimidine, 5,7-dihydro-2-methyl-		17.7, 17.23, 18.1
9118.	302-04-5	1	0	0	Thiocyanate		18.1
9119.	463-56-9	1	1	1	Thiocyanic acid	HSCN	0.4, 11.2, 18.1
9120.	556-64-9	1	0	0	Thiocyanic acid, methyl ester	H_3C-SCN	5.3, 11.2, 18.1
9121.	505-14-6 15941-77-2	1	0	0	Thiocyanogen	$(SCN)_2$	0.4, 11.2, 18.1
9122.	137-26-8	0	1	0	Thioformamide, 1,1′-dithiobis (*N*,*N*-dimethyl- {Thiram®}		18.1, 21.3
9123.	22223-61-6	1	0	0	Thionitrous acid (HNOS), S-methyl ester		5.3, 18.1
9124.	110-02-1	1	1	1	Thiophene		18.1, 25.29
9125.	638-00-6	1	0	0	Thiophene, 2,4-dimethyl-		18.1
9126.	872-55-9	1	0	0	Thiophene, 2-ethyl-		18.1
9127.	25154-40-9	1	1	1	Thiophene, methyl-		18.1

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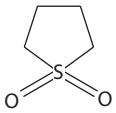
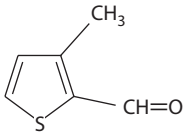
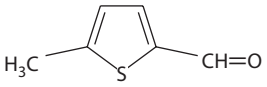
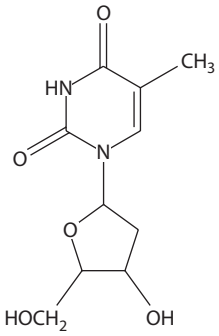
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9128.	554-14-3	1	0	0	Thiophene, 2-methyl-		18.1, 25.29
9129.	616-44-4	1	0	0	Thiophene, 3-methyl-		18.1
9130.	126-33-0	1	0	0	Thiophene, tetrahydro-, 1, 1-dioxide {Sulfolan®}		18.1, 21.3
9131.	98-03-3	1	1	1	2-Thiophenecarboxaldehyde		3.12, 18.1
9132.	5834-16-2	1	1	1	2-Thiophenecarboxaldehyde, 3-methyl-		3.12, 18.1
9133.	13679-70-4	1	1	1	2-Thiophenecarboxaldehyde, 5-methyl-		3.12, 18.1, 24.3
9134.	149956-84-3	0	1	0	Thioredoxin h2 (tobacco)		22.2
9135.	7772-98-7	0	1	0	Thiosulfuric acid, disodium salt		18.1, 20.6
9136.	14274-82-9	1	1	1	Thorium, isotope of mass 228	^{228}Th	20.5
9137.	14269-63-7	1	1	1	Thorium, isotope of mass 230	^{230}Th	20.5
9138.	7440-29-1	1	1	1	Thorium, isotope of mass 232	^{232}Th	20.5
9139.	72-19-5	1	1	1	*L*-Threonine	H_3C-CHOH-CH(NH_2)-COOH	0.4, 2.5, 4.3, 4.10, 12.2, 24.3, 25.29
9140.	32190-57-1	0	1	0	*L*-Threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]-		2.5, 4.3, 4.10, 17.1
9141.		0	1	0	*L*-Threonine, *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 10.2
9142.	7440-30-4	1	1	1	Thulium	Tm	20.5
9143.	50-89-5	0	1	0	Thymidine		2.5, 10.2
9144.	7440-31-5 7740-31-5	1	1	1	Tin	Sn	0.4, 20.5
9145.	1344-13-4	0	1	0	Tin chloride (stannic chloride)	$SnCl_4$	18.4, 20.6
9146.	7440-32-6	1	1	1	Titanium	Ti	0.4, 20.5
9147.	13463-67-7	0	1	0	Titanium oxide	TiO_2	20.6
9148.		0	1	0	Transaminase		22.2
9149.	50812-37-8	0	1	0	Transferase, glutathione S-		22.2
9150.	9014-48-6	0	1	0	Transketolase		22.2
9151.	99-20-7	0	1	0	Trehalose		2.5, 8.3
9152.	638-68-6	1	1	1	Triacontane	H_3C-(CH_2)$_{28}$-CH_3	0.4, 1.10
9153.	1560-72-1	1	1	1	Triacontane, 2-methyl-	H_3C-CH(CH_3)-(CH_2)$_{27}$-CH_3	1.10

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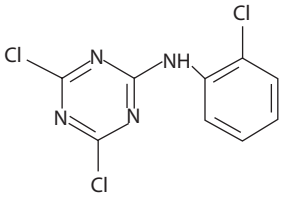
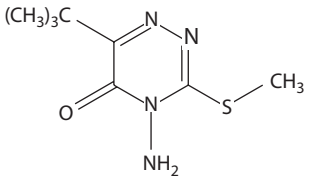
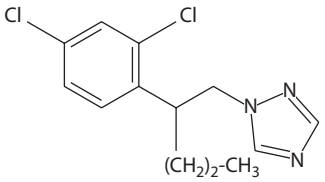
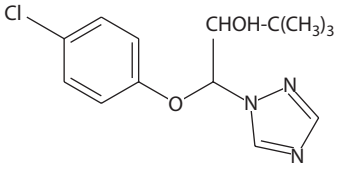
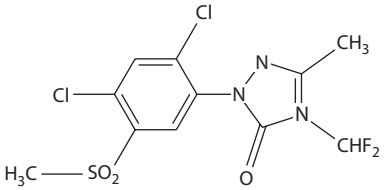
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9154.	72227-01-1	1	1	1	Triacontane, 3-methyl-	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{26}\text{-}CH_3$	1.10
9155.	506-50-3	1	0	0	Triacontanoic acid	$H_3C\text{-}(CH_2)_{28}\text{-}COOH$	4.3
9156.	121878-07-7	1	1	1	Triacontanoic acid, docosyl ester	$H_3C\text{-}(CH_2)_{28}\text{-}COO\text{-}(CH_2)_{21}\text{-}CH_3$	5.3
9157.		1	1	1	Triacontanoic acid, ester with olean-12-en-3-ol, (3β)- {β-amyrenyl triacontanoate}		2.7, 5.3
9158.	104932-26-5	1	1	1	Triacontanoic acid, eicosyl ester	$H_3C\text{-}(CH_2)_{28}\text{-}COO\text{-}(CH_2)_{19}\text{-}CH_3$	5.3
9159.	593-50-0	1	1	1	1-Triacontanol	$H_3C\text{-}(CH_2)_{28}\text{-}CH_2OH$	2.5
9160.	18435-53-5	1	0	0	1-Triacontene	$H_2C{=}CH\text{-}(CH_2)_{27}\text{-}CH_3$	1.11
9161.		1	0	0	1-Triacontene, 2-methyl-	$H_2C{=}C(CH_3)\text{-}(CH_2)_{27}\text{-}CH_3$	1.11
9162.		1	0	0	2-Triacontene, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{26}\text{-}CH_3$	1.11
9163.		1	0	0	2-Triacontene, (*E*)-		1.11
9164.		1	0	0	2-Triacontene, 2-methyl-	$H_3C\text{-}C(CH_3){=}CH\text{-}(CH_2)_{26}\text{-}CH_3$	1.11
9165.		1	0	0	2-Triacontene, 28-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{24}\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$	1.11
9166.		1	0	0	2-Triacontene, 28-methyl-, (*E*)-		1.11
9167.		1	0	0	2-Triacontene, 29-methyl-, (*Z*)-	$H_3C\text{-}CH{=}CH\text{-}(CH_2)_{25}\text{-}CH(CH_3)_2$	1.11
9168.		1	0	0	2-Triacontene, 29-methyl-, (*E*)-		1.11
9169.	101-05-3	0	1	0	1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-(2-chlorophenyl)- {Anilazine®, Dyrene®}		17.7, 18.4, 21.3
9170.		1	0	0	1,3,5-Triazine,1.4-dihydro-1,2-dimethyl-		17.7
9171.	21087-64-9	0	1	0	1,2,4-Triazin-5(4*H*)-one, 4-amino-6-*tert*-butyl-3-(methylthio)- {Metribuzin®}		17.7, 12.2, 18.1, 21.3
9172.	66246-88-6	0	1	0	1,2,4-Triazole, 1-(2-(2,4-dichlorophenyl) pentyl)- {Penconazole®}		17.4, 18.4, 21.3
9173.	55219-65-3	0	1	0	1*H*-1,2,4-Triazol-1-ethanol, 8-(4-chlorophenoxy)-α-(1,1-dimethylethyl)- {Triadimenol®}		10.2, 17.4, 18.4, 21.3
9174.	122836-35-5	0	1	0	1*H*-1,2,4-Triazol-1-yl)phenyl)methanesulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, N-(2,4-dichloro-5(4-difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl)phenyl)-; Sulfentrazone®}		17.4, 18.1, 18.4, 21.3

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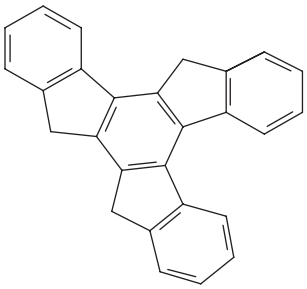
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9175.	27096-03-3 548-35-6	1	0	0	5*H*-Tribenzo[*a,f,l*]trindene,10,15-dihydro-{5*H*-diindeno[1,2-*a*:1′,2′-*c*] fluorene, truxene}		1.20
9176.	638-67-5	1	1	1	Tricosane	H_3C-$(CH_2)_{21}$-CH_3	1.10
9177.	1928-30-9	1	1	1	Tricosane, 2-methyl-	H_3C-$CH(CH_3)$-$(CH_2)_{20}$-CH_3	1.10
9178.	13410-45-2	0	1	0	Tricosane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-CH_3	1.10
9179.	2433-96-7	1	1	1	Tricosanoic acid	H_3C-$(CH_2)_{21}$-$COOH$	4.3
9180.	42233-37-4	1	1	1	Tricosanoic acid, docosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{21}$-CH_3	5.3
9181.	42233-27-2	1	1	1	Tricosanoic acid, dodecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{11}$-CH_3	5.3
9182.	42233-35-2	1	1	1	Tricosanoic acid, eicosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{19}$-CH_3	5.3
9183.	42233-36-3	1	1	1	Tricosanoic acid, heneicosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{20}$-CH_3	5.3
9184.		1	1	1	Tricosanoic acid, heptacosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{26}$-CH_3	5.3
9185.	42233-32-9	1	1	1	Tricosanoic acid, heptadecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{16}$-CH_3	5.3
9186.	121877-98-3	1	1	1	Tricosanoic acid, hexacosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{25}$-CH_3	5.3
9187.	42233-31-8	1	1	1	Tricosanoic acid, hexadecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{15}$-CH_3	5.3
9188.	2433-97-8	0	1	0	Tricosanoic acid, methyl ester	H_3C-$(CH_2)_{21}$-COO-CH_3	5.3
9189.	42233-34-1	1	1	1	Tricosanoic acid, nonadecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{18}$-CH_3	5.3
9190.	42233-33-0	1	1	1	Tricosanoic acid, octadecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{17}$-CH_3	5.3
9191.		1	1	1	Tricosanoic acid, pentacosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{24}$-CH_3	5.3
9192.	42233-30-7	1	1	1	Tricosanoic acid, pentadecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{14}$-CH_3	5.3
9193.	42233-39-6	1	1	1	Tricosanoic acid, tetracosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{23}$-CH_3	5.3
9194.	42233-29-4	1	1	1	Tricosanoic acid, tetradecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{13}$-CH_3	5.3
9195.	42233-38-5	1	1	1	Tricosanoic acid, tricosyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{22}$-CH_3	5.3
9196.	42233-28-3	1	1	1	Tricosanoic acid, tridecyl ester	H_3C-$(CH_2)_{21}$-COO-$(CH_2)_{12}$-CH_3	5.3
9197.	36332-96-4	1	1	1	Tricosanoic acid, 21-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-$COOH$	4.3
9198.	121877-82-5	1	1	1	Tricosanoic acid, 21-methyl-, docosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{21}$-CH_3	5.3
9199.	121877-72-3	1	1	1	Tricosanoic acid, 21-methyl-, eicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{19}$-CH_3	5.3
9200.	121877-73-4	1	1	1	Tricosanoic acid, 21-methyl-, heneicosyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{20}$-CH_3	5.3
9201.	121877-63-2	1	1	1	Tricosanoic acid, 21-methyl-, nonadecyl ester	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_{19}$-COO-$(CH_2)_{18}$-CH_3	5.3
9202.	4730-63-6	1	1	1	Tricosanoic acid, 22-methyl-	$(H_3C)_2$=CH-$(CH_2)_{20}$-$COOH$	4.3
9203.	71608-06-5	1	0	0	Tricosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
9204.	3133-01-5	1	1	1	1-Tricosanol	H_3C-$(CH_2)_{21}$-CH_2OH	2.5
9205.	63907-54-0	0	1	0	1-Tricosanol, 22-methyl-	$(H_3C)_2$=CH-$(CH_2)_{20}$-CH_2OH	2.5
9206.	540-09-0	1	1	1	12-Tricosanone	$[H_3C$-$(CH_2)_{10}]_2$=C=O	3.13
9207.	66309-85-1	1	1	1	5,9,13,17,21-Tricosapentaen-2-one, 6,10,14,18,22-pentamethyl-		3.13
9208.	18835-32-0	1	1	1	1-Tricosene	H_3C-$(CH_2)_{20}$-CH=CH_2	1.11
9209.		1	0	0	1-Tricosene, 2-methyl-	H_2C=$C(CH_3)$-$(CH_2)_{20}$-CH_3	1.11
9210.		1	0	0	2-Tricosene, (*Z*)-	H_3C-CH=CH-$(CH_2)_{19}$-CH_3	1.11
9211.		1	0	0	2-Tricosene, (*E*)-		1.11
9212.		1	0	0	2-Tricosene, 2-methyl-	H_3C-$C(CH_3)$=CH-$(CH_2)_{19}$-CH_3	1.11
9213.		1	0	0	2-Tricosene, 21-methyl-, (*Z*)-	H_3C-CH=CH-$(CH_2)_{17}$-$CH(CH_3)$-CH_2-CH_3	1.11

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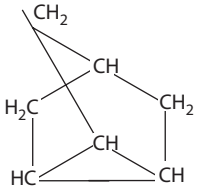
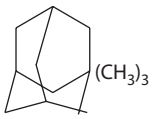
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9214.		1	0	0	2-Tricosene, 21-methyl-, (*E*)-		1.11
9215.		1	0	0	2-Tricosene, 22-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_{18}$-CH$(CH_3)_2$	1.11
9216.		1	0	0	2-Tricosene, 22-methyl-, (*E*)-		1.11
9217.	27519-02-4	0	1	0	9-Tricosene		1.11
9218.	30326-99-9	1	0	0	Tricosenoic acid		4.3
9219.	279-19-6	1	0	0	Tricyclo[2.2.1.02,6]heptane		1.12
9220.	707-35-7	0	1	0	Tricyclo[3.3.1.1]decane, 1,3,5-trimethyl-		1.12
9221.	472-97-9	0	1	0	Tricyclo[6.3.1.02,5]dodecan-1-ol, 4,4,8-trimethyl-, [1R-(1α,2α,5β,8β)]-		2.5
9222.	195-84-6	1	0	0	Tricycloquinazoline		17.21
9223.	28522-57-8	1	0	0	Tricycloquinazoline, 3-methyl-		17.21
9224.	129777-24-8	0	1	0	3,7-Tridecadiene-2,12-dione, 6-hydroxy-6-methyl-9-(1-methylethyl)-		2.5, 3.13
9225.	60593-18-2	0	1	0	3,8-Tridecadiene-2,12-dione, 8-methyl-5-(1-methylethyl)-, [S-(*E,E*)]-		3.13
9226.	10486-19-8	0	1	0	Tridecanal	H_3C-$(CH_2)_{11}$-CH═O	3.12
9227.	629-50-5	1	1	1	Tridecane	H_3C-$(CH_2)_{11}$-CH_3	1.10
9228.	1590-96-9	0	1	0	Tridecane, 2-methyl-	H_3C-$(CH_2)_{10}$-CH═$(CH_3)_2$	1.10
9229.	6418-41-3	0	1	0	Tridecane, 3-methyl-	H_3C-$(CH_2)_9$-CH(CH_3)-CH_2-CH_3	1.10
9230.	19780-80-4	0	1	0	Tridecane, 7-methylene-	$[H_3C$-$(CH_2)_5]_2$═C═CH_2	1.11
9231.	505-52-2	1	0	0	Tridecanedioic acid	HOOC-$(CH_2)_{11}$-COOH	4.3
9232.	638-53-9	1	1	1	Tridecanoic acid	H_3C-$(CH_2)_{11}$-COOH	4.3
9233.	36617-26-2	1	1	1	Tridecanoic acid, eicosyl ester	H_3C-$(CH_2)_{11}$-COO-$(CH_2)_{19}$-CH_3	5.3
9234.	1731-88-0	0	1	0	Tridecanoic acid, methyl ester	H_3C-$(CH_2)_{11}$-COO-CH_3	5.3
9235.	121877-24-5	1	1	1	Tridecanoic acid, 11-methyl-, heneicosyl ester	H_3C-CH_2-CH(CH_3)-$(CH_2)_9$-COO-$(CH_2)_{20}$-CH_3	5.3
9236.	121877-57-4	1	1	1	Tridecanoic acid, 11-methyl-, heptacosyl ester	H_3C-CH_2-CH(CH_3)-$(CH_2)_9$-COO-$(CH_2)_{26}$-CH_3	5.3
9237.	121877-07-4	1	1	1	Tridecanoic acid, 11-methyl-, heptadecyl ester	H_3C-CH_2-CH(CH_3)-$(CH_2)_9$-COO-$(CH_2)_{16}$-CH_3	5.3
9238.	121877-16-5	1	1	1	Tridecanoic acid, 11-methyl-, nonadecyl ester	H_3C-CH_2-CH(CH_3)-$(CH_2)_9$-COO-$(CH_2)_{18}$-CH_3	5.3
9239.	2724-57-4	1	1	1	Tridecanoic acid, 12-methyl-	$(H_3C)_2$═CH-$(CH_2)_{10}$-COOH	4.3
9240.	121877-25-6	1	1	1	Tridecanoic acid, 12-methyl-, docosyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-$(CH_2)_{21}$-CH_3	5.3
9241.	121877-19-8	1	1	1	Tridecanoic acid, 12-methyl-, eicosyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-$(CH_2)_{19}$-CH_3	5.3
9242.	121877-22-3	1	1	1	Tridecanoic acid, 12-methyl-, heneicosyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-$(CH_2)_{20}$-CH_3	5.3
9243.	121877-14-3	1	1	1	Tridecanoic acid, 12-methyl-, heptadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-$(CH_2)_{16}$-CH_3	5.3
9244.	5129-58-8	0	1	0	Tridecanoic acid, 12-methyl-, methyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-CH_3	5.3

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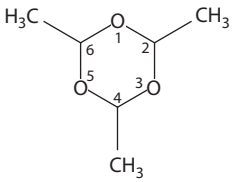
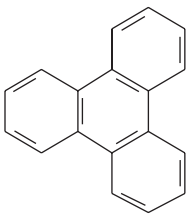
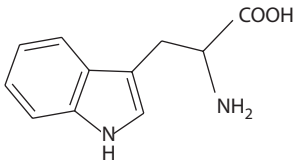
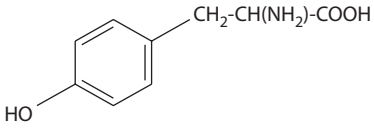
	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9245.	121877-11-0	1	1	1	Tridecanoic acid, 12-methyl-, nonadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-$(CH_2)_{18}$-CH_3	5.3
9246.	121877-09-6	1	1	1	Tridecanoic acid, 12-methyl-, octadecyl ester	$(H_3C)_2$═CH-$(CH_2)_{10}$-COO-$(CH_2)_{17}$-CH_3	5.3
9247.	71608-07-6	1	0	0	Tridecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
9248.	112-70-9	1	1	1	1-Tridecanol	H_3C-$(CH_2)_{11}$-CH_2OH	2.5
9249.	21987-21-3	0	1	0	1-Tridecanol, 12-methyl-	$(H_3C)_2$═CH-$(CH_2)_{10}$-CH_2OH	2.5
9250.	593-08-8	0	1	0	2-Tridecanone	H_3C-$(CH_2)_{10}$-CO-CH_3	3.13, 24.3
9251.	117210-51-2	0	1	0	2-Tridecanone, 4,8,12-trimethyl-		3.13
9252.	41678-34-6	0	1	0	Tridecatrienoic acid		4.3
9253.	122855-83-8	0	1	0	5,10,12-Tridecatrien-2-one, 6,12-dimethyl-9-(1-methylethyl)-		3.13
9254.	59573-83-0	0	1	0	5,10,12-Tridecatrien-2-one, 6,12-dimethyl-9-(1-methylethyl)-, [S-(*E,E*)]-		3.13
9255.	7774-82-5	0	1	0	2-Tridecenal	H_3C-$(CH_2)_9$-CH═CH-CH═O	3.12
9256.		1	1	1	Tridecene	H-$(CH_2)_n$-CH═CH-$(CH_2)_{(11-n)}$-H	1.11
9257.	2437-56-1	1	1	1	1-Tridecene	H_3C-$(CH_2)_{10}$-CH═CH_2	1.11
9258.	18094-01-4	1	0	0	1-Tridecene, 2-methyl-	H_2C═$C(CH_3)$-$(CH_2)_{10}$-CH_3	1.11
9259.	19150-20-0	1	0	0	2-Tridecene, (*Z*)-	H_3C-CH═CH-$(CH_2)_9$-CH_3	1.11
9260.	25377-82-6	1	0	0	2-Tridecene, (*E*)-		1.11
9261.	62060-10-0	1	0	0	2-Tridecene, 2-methyl-	H_3C-$C(CH_3)$═CH-$(CH_2)_9$-CH_3	1.11
9262.		1	0	0	2-Tridecene, 11-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_7$-$CH(CH_3)$-CH_2-CH_3	1.11
9263.		1	0	0	2-Tridecene, 11-methyl-, (*E*)-		1.11
9264.		1	0	0	2-Tridecene, 12-methyl-, (*Z*)-	H_3C-CH═CH-$(CH_2)_8$-$CH(CH_3)_2$	1.11
9265.		1	0	0	2-Tridecene, 12-methyl-, (*E*)-		1.11
9266.	60026-14-4	0	1	0	3-Tridecene-2,8-diol, 4,8,12-trimethyl-		2.5
9267.		1	0	0	Tridecenoic acid		4.3
9268.	123-63-7	1	0	0	1,3,5-Trioxane, 2,4,6-trimethyl- {paraldehyde, acetaldehyde trimer}		3.12, 10.2
9269.	81901-03-3	0	1	0	3,5,9-Trioxa-4-phosphaheptacosadien-1-aminium, 4-hydroxy-*N*,*N*,*N*-trimethyl-10-oxo-7-[(1-oxooctadecadienyl) oxy]-, hydroxide, inner salt, 4-oxide		12.2
9270.	70106-56-8	0	1	0	3,5,9-Trioxa-4-phosphaheptacosan-1-aminium, 4-hydroxy-*N*,*N*,*N*-trimethyl-10-oxo-7-[(1-oxooctadecatrienyl)oxy]-, hydroxide, inner salt, 4-oxide, hexadehydro derivative, (R)-		12.2
9271.	217-59-4	1	0	0	Triphenylene {9,10-benzophenanthrene}		1.20
9272.	60826-76-8	1	0	0	Triphenylene, dimethyl-		1.20

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9273.	41637-89-2	1	0	0	Triphenylene, methyl-		1.20
9274.	60826-79-1	1	0	0	Triphenylene, trimethyl-		1.20
9275.	76-87-9	0	1	0	Triphenylstannium hydroxide {Fentin hydroxide®}	$(C_6H_5)_3{\equiv}Sn\text{-}OH$	20.6, 21.3
9276.	3658-80-8	1	0	0	Trisulfide, dimethyl-		18.1
9277.	630-05-7	1	1	1	Tritriacontane	$H_3C\text{-}(CH_2)_{31}\text{-}CH_3$	1.10
9278.	*66214*-27-5	1	1	1	Tritriacontane, 2-methyl-	$(H_3C)_2{=}CH\text{-}(CH_2)_{30}\text{-}CH_3$	1.10
9279.	14167-69-2	1	1	1	Tritriacontane, 3-methyl-	$H_3C\text{-}CH_2\text{-}CH(CH_3)\text{-}(CH_2)_{29}\text{-}CH_3$	1.10
9280.	38232-03-0	1	0	0	Tritriacontanoic acid	$H_3C\text{-}(CH_2)_{31}\text{-}COOH$	4.3
9281.	22986-69-2	1	0	0	17-Tritriacontanone		3.13
9282.	9035-81-8	0	1	0	Trypsin inhibitor		22.2
9283.	150498-11-6	0	1	0	Trypsin inhibitor, TTI (tobacco isoform 1 reduced)		22.2
9284.	6912-86-3	0	1	0	Tryptophan		4.3, 4.10
9285.	73-22-3	0	1	0	*L*-Tryptophan		0.4, 4.3, 4.10, 12.2, 25.29
9286.	60738-11-6	0	1	0	*L*-Tryptophan, labeled with ^{14}C		4.3, 4.10
9287.	7440-33-7	1	1	1	Tungsten	W	20.5
9288.	55520-40-6	0	1	0	Tyrosine		4.3, 4.10
9289.	587-45-1	0	1	0	Tyrosine, 3-hydroxy-		4.3, 4.10
9290.	60-18-4	0	1	0	*L*-Tyrosine		0.4, 4.3, 4.10, 12.2, 25.29
9291.	34393-22-1	0	1	0	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 10.2
9292.	120904-94-1	0	1	0	Ubiquitin, poly-		22.2
9293.	129970-88-3	0	1	0	5,9-Undecadienal, 6,10-dimethyl-2-methylene-		3.12
9294.	55976-13-1	0	1	0	1,4-Undecadiene, (*E*)-	$H_3C\text{-}(CH_2)_5\text{-}CH{=}CH\text{-}CH_2\text{-}CH{=}CH_2$	1.11
9295.	53837-34-6	1	1	1	5,9-Undecadien-2-ol, 6,10-dimethyl-		2.5
9296.		0	1	0	5,8-Undecadien-2-one, 6,10-dimethyl-		3.13
9297.	65017-84-7 133561-45-2	0	1	0	5,8-Undecadien-2-one, 6,10-dimethyl-10-hydroxy- (*E,E*)-		2.5, 3.13
9298.	689-67-8	0	1	0	5,9-Undecadien-2-one, 6,10-dimethyl-		3.13
9299.	3796-70-1	1	1	1	5,9-Undecadien-2-one, 6,10-dimethyl-, (*E*)- {geranylacetone}	$H(CH_2\text{-}C(CH_3){=}CH\text{-}CH_2)_2\text{-}CH_2\text{-}CO\text{-}CH_3$	3.13, 24.3, 25.29
9300.	3879-26-3	1	1	1	5,9-Undecadien-2-one, 6,10-dimethyl-, (*Z*)- {nerylacetone}		3.13
9301.	74233-43-5	0	1	0	5,10-Undecadien-2-one, 6,10-dimethyl-9-hydroxy-		2.5, 3.13
9302.	152209-56-8	0	1	0	6,10-Undecadien-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-2-methyl-2-furanyl)-		2.5, 3.13, 10.2
9303.	51297-36-0	0	1	0	8,10-Undecadien-4-one, 2,10-dimethyl-7-(1-methylethyl)-, (*E*)-(±)-		3.13
9304.	112-44-7	1	1	1	Undecanal	$H_3C\text{-}(CH_2)_9\text{-}CH{=}O$	3.12

(*continued*)

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Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9305.	1120-21-4	1	1	1	Undecane	H_3C-$(CH_2)_9$-CH_3	1.10
9306.		1	0	0	Undecane, dimethyl-		1.10
9307.	17301-23-4	0	1	0	Undecane, 2,6-dimethyl-		1.10
9308.	7045-71-8	1	1	1	Undecane, 2-methyl-	$(H_3C)_2$═CH-$(CH_2)_8$-CH_3	1.10
9309.	1002-43-3	1	1	1	Undecane, 3-methyl-	H_3C-CH_2-$CH(CH_3)$-$(CH_2)_7$-CH_3	1.10
9310.	1852-04-6	1	1	1	Undecanedioic acid	HOOC-$(CH_2)_9$-COOH	4.3
9311.	112-37-8	1	1	1	Undecanoic acid	H_3C-$(CH_2)_9$-COOH	0.4, 4.3
9312.	10580-24-2	0	1	0	Undecanoic acid, butyl ester		5.3
9313.	1731-86-8	0	1	0	Undecanoic acid, methyl ester	H_3C-$(CH_2)_9$-$COOCH_3$	5.3
9314.	71608-08-7	1	0	0	Undecanoicacid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-		5.3
9315.	112-42-5	1	1	1	1-Undecanol	H_3C-$(CH_2)_9$-CH_2OH	2.5
9316.	1731-81-3	0	1	0	1-Undecanol, acetate	H_3C-$(CH_2)_9$-CH_2-OOC-CH_3	5.3
9317.	38713-13-2	0	1	0	2-Undecanol, 6,10-dimethyl-	H-$[CH_2$-$CH(CH_3)$-$(CH_2)_2]_2$-CH_2-CHOH-CH_3	2.5
9318.	112-12-9	1	1	1	2-Undecanone {methyl nonyl ketone}	H_3C-$(CH_2)_8$-CO-CH_3	3.13, 24.3, 25.29
9319.	1604-34-8	1	1	1	2-Undecanone, 6,10-dimethyl- {tetrahydrogeranylacetone}		3.13
9320.	927-49-1	0	1	0	6-Undecanone	H_3C-$(CH_2)_4$-CO-$(CH_2)_4$-CH_3	3.13
9321.	16356-11-9	1	0	0	1,3,5-Undecatriene		1.11
9322.	141-10-6	1	1	1	3,5,9-Undecatrien-2-one, 6,10-dimethyl- {pseudoionone}		3.13
9323.	3548-78-5	0	1	0	3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (*E,E*)- {pseudoionone}		3.13
9324.	13927-47-4	0	1	0	3,5,9-Undecatrien-2-one, 6, 10-dimethyl-, (*E,Z*)- {pseudoionone}		3.13
9325.	112-45-8	0	1	0	10-Undecenal		3.12
9326.	28761-27-5	1	0	0	Undecene		1.11
9327.	821-95-4	1	0	0	1-Undecene	H_3C-$(CH_2)_8$-CH═CH_2	1.11
9328.	2244-02-2	1	0	0	2-Undecene		1.11
9329.	31613-73-7	0	1	0	5-Undecene, 5-methyl-	H_3C-$(CH_2)_4$-CH═$C(CH_3)$-$(CH_2)_3$-CH_3	1.11
9330.	133561-48-5	0	1	0	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-		2.5, 3.13
9331.	129777-22-6	0	1	0	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-, (*E*)-		2.5, 3.13
9332.	112-38-9	0	1	0	10-Undecenoic acid		4.3
9333.	109-42-2	0	1	0	10-Undecenoic acid, butyl ester		5.3
9334.	692-86-4	0	1	0	10-Undecenoic acid, ethyl ester		5.3
9335.	29093-90-1	0	1	0	5-Undecen-2-one, 10-hydroxy-6, 10-dimethyl-		2.5, 3.13
9336.	160115-56-0	0	1	0	6-Undecen-2-one, 10-(acetyloxy)-8,11-dihydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-5-hydroxy-2-methyl-2-furanyl)-		2.5, 3.13, 5.3, 10.2
9337.	13966-29-5	0	1	0	Uranium, isotope of mass 234	^{234}U	20.5
9338.	15117-96-1	0	1	0	Uranium, isotope of mass 235	^{235}U	20.5
9339.	7440-61-1	1	1	1	Uranium, isotope of mass 238	^{238}U	0.4, 20.5
9340.	57-13-6	1	1	1	Urea	H_2N-CO-NH_2	13.1, 24.3, 25.29

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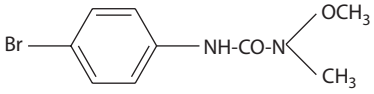
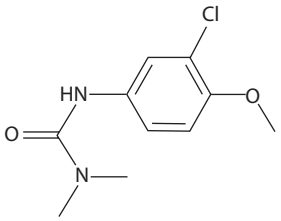
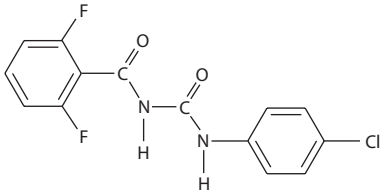
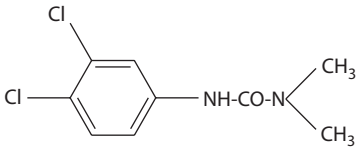
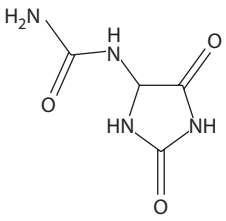
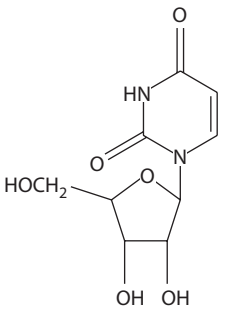
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
9341.	3060-89-7	1	1	1	Urea, *N′*-(4-bromophenyl)-*N′*-methoxy-*N′*-methyl- {Metobromuron®, Patoran®}		18.4, 21.3
9342.	19937-59-8	0	1	0	Urea, *N′*-(3-chloro-4-methoxyphenyl)-*N,N*-dimethyl- {Metoxuron®}		21.3
9343.	1746-81-2	1	1	1	Urea, *N′*-(4-chlorophenyl)-*N*-methoxy-*N*-methyl- {Linuron®, 30% of Molipan®}		18.4, 21.3
9344.	35367-38-5	1	1	1	Urea, 1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)- {Diflubenzuron®}		21.3
9345.	330-55-2	1	1	1	Urea, *N′*-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methyl- {Monolinuron®, 20% of Molipan®}		18.4, 21.3
9346.	150-68-5	0	1	0	Urea, 1,1-dimethyl-3-(4-chlorophenyl) {Monuron®}		18.4, 21.3
9347.	330-54-1	0	1	0	Urea, 1,1-dimethyl-3-(3,4-dichlorophenyl) {Diuron®}		18.4, 21.3
9348.	97-59-6	0	1	0	Urea, (2,5-dioxo-4-imidazolidinyl)- {allantoin}		0.4, 13.1, 17.4
9349.	9002-13-5	0	1	0	Urease		0.4, 22.2
9350.	58-96-8	0	1	0	Uridine		2.5, 10.2
9351.	133-89-1	0	1	0	Uridine 5′-(trihydrogen diphosphate), *P′*-α-*D*-glucopyranosyl ester		2.5, 5.3, 10.2

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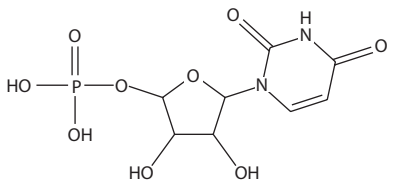
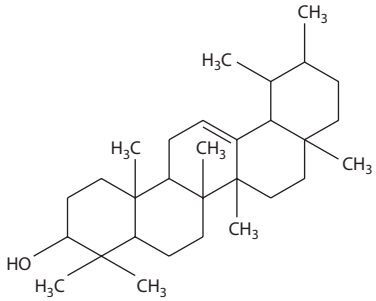
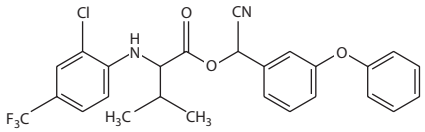
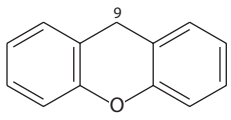
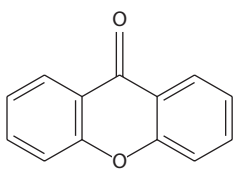
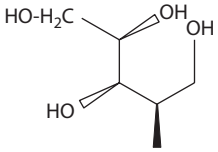
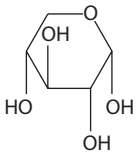
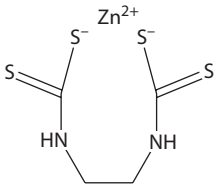
Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	S T	Name (per CA Collective Index)	Selected Structures	Chapter Table
9352.	3616-06-6	0	1	0	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester		2.5, 5.3, 10.2
9353.	19253-25-9	0	1	0	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester		2.5, 5.3, 10.2
9354.	58-97-9	0	1	0	5′-Uridylic acid		2.5, 5.3, 10.2
9355.	9026-22-6	0	1	0	Uridylyltransferase, glucose 1-phosphate		22.2
9356.	94414-19-4	0	1	0	Urs-12-en-28-oic acid, 3,23-dihydroxy-, (3β,4α)-		2.5, 2.7, 4.3
9357.	77-52-1	0	1	0	Urs-12-en-28-oic acid, 3-hydroxy-, (3β)-		2.5, 2.7, 4.3
9358.	638-95-9	1	1	1	Urs-12-en-3-ol, (3β)- {α-amyrin}		2.5, 2.7
9359.	7004-03-7	1	1	1	Valine	$(H_3C)_2$═CH-CH(NH_2)-COOH	0.4, 4.3, 4.10, 24.3, 25.29
9360.	72-18-4	1	1	1	*L*-Valine		4.3, 4.10, 12.2
9361.		0	1	0	*L*-Valine, *N*-(1-deoxy-*D*-fructos-1-yl)-		2.5, 4.3, 4.10, 10.2
9362.	102851-06-9	0	1	0	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl) methyl ester {Fluvalinate®}		5.3, 10.2, 11.2, 18.4, 21.3, 25.29
9363.	7440-62-2	1	1	1	Vanadium	V	0.4, 20.5
9364.	11105-12-7	0	1	0	Vanadium chloride		18.4, 20.6
9365.	1314-62-1	0	1	0	Vanadium pentoxide	V_2O_5	20.6
9366.	12001-76-2	0	1	0	Vitamin B		2.5
9367.	7732-18-5	1	1	1	Water	H_2O	0.4, 19.5, 24.3, 25.29
9368.	92-83-1	1	1	1	9*H*-Xanthene {dibenzopyran}		10.2
9369.	6279-07-8	1	1	1	9*H*-Xanthene, 2-methyl-		10.2
9370.	90-47-1	0	1	0	9*H*-Xanthen-9-one {xanthone}		3.13
9371.	9014-63-5	0	1	0	Xylan		2.5, 8.3
9372.		0	1	0	Xylan, 4′-(*O*-methylglucuronyloxy)-		2.5, 8.3
9373.	9025-57-4	0	1	0	Xylanase, endo-1,4-β-		22.2

(continued)

Alphabetical Index to Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

	CAS No.	S	T	ST	Name (per CA Collective Index)	Selected Structures	Chapter Table
9374.	87-99-0	1	1	1	Xylitol		2.5
9375.	82796-87-0	1	0	0	*D*-Xylonic acid, δ-lactone		2.5, 6.3
9376.	58-86-6	1	1	1	Xylose		2.5, 10.2
9377.	25990-60-7	1	1	1	*DL*-Xylose		1.5, 10.2, 25.29
9378.	31178-70-8	0	1	0	α-*D*-Xylose		2.5, 10.2
9379.	31178-71-9	0	1	0	β-*D*-Xylose		2.5, 10.2
9380.	9025-53-0	0	1	0	β-Xylosidase		22.2
9381.	7440-64-4	1	1	1	Ytterbium	Yb	20.5
9382.	7440-65-5	1	1	1	Yttrium	Y	20.5
9383.	10098-91-6	0	1	0	Yttrium, isotope of mass 90	^{90}Y	20.5
9384.	7440-66-6	1	1	1	Zinc	Zn	0.4, 20.5
9385.	12122-67-7	0	1	0	Zinc, [[1,2-ethanediylbis [carbamodithioato]](2-)]- {Zineb®}		18.1, 20.5, 21.3
9386.	18920-65-5	0	1	0	Zinc, bis(thiocarbamato)-		18.1, 20.6
9387.	23713-49-7	0	1	0	Zinc, ion	Zn^{+2}	20.5
9388.	13982-39-3	1	1	1	Zinc, isotope of mass 65	^{65}Zn	20.5
9389.	7440-67-7	1	1	1	Zirconium	Zr	20.5
9390.	11126-30-0	0	1	0	Zirconium chloride		18.4, 20.6
	Totals	**6**	**5**	**–**	**9390**		
		0	**5**	**2**			
		1	**9**	**2**			
		0	**5**	**1**			
				5			

There were 292 partially identified isomers listed in the preceding index. Thus, the number of identified/partially identified components in tobacco and tobacco smoke totals **9582 (9390 + 292 – 100)**.

At the end of our Index on the last page of our published book, the totals and assessment were as follows:

Totals	**5**	**4**	**–**	**8430**
	3	**9**	**1**	
	1	**9**	**8**	
	5	**4**	**7**	
			9	

There were 292 partially identified isomers listed in the index for the First Edition. Thus, the number of identified/partially identified components in tobacco and tobacco smoke totaled **8622 (8430 + 292 – 100).**

Note: S, tobacco smoke component; T, tobacco component; ST, component of both S and T.

Sequence of CAS Registry Numbers for Components Identified in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

After the publication of our initial catalog and the Alphabetical Index of the chemical components of tobacco and tobacco smoke, several items were noted in the scientific literature. Whenever there was a substantial list of chemical compounds with specific properties, a list other than an alphabetical one was also generated, namely, a listing of the chemical compounds in the sequence of their CAS Registry Numbers. A classical example, of course, is the Merck Index which in one catalog lists the chemical compounds alphabetically, each with its CAS No., and in a second catalog lists the chemical compounds in the sequence of their CAS Nos. Another such list was by Acree and Arn (5095a), a listing of 738 chemical components noted for their flavor. Comparison of the Acree–Arn list with our CAS No. sequence of tobacco and/or tobacco smoke components indicates that many of the compounds classified as flavors by Acree and Arn are components of tobacco and/or its smoke.

Another example of the sequential listing of chemical compounds by CAS Nos. beginning with 1, 2, 3, or 4, etc., may be found at:

http://msds.chem.ox.ac.uk/cas1.html
http://msds.chem.ox.ac.uk/cas2.html
http://msds.chem.ox.ac.uk/cas3.html

These lists are linked to safety/hazard data for the listed compounds. Because of the magnitude of our Alphabetical Index on tobacco and tobacco smoke components and the considerable interest in those components categorized as tobacco additives or flavor formulation ingredients, a second tabulation, based on the sequence of CAS Nos., has been prepared. The sequential tabulation, which follows the Alphabetical Index, is divided into three parts: The first and lengthy one, comprising over 8350 entries, is the listing of the chemical components of tobacco and tobacco smoke arranged in their CAS No. sequence. Components with more than one CAS No. appear in the list for each of their assigned CAS Nos. In this list, as in the Alphabetical Index, each component is designated as a tobacco component or a tobacco smoke component or both.

The authors hope that this CAS Registry Number sequence together with the format of the Alphabetical Index will not only help the reader in his/her search for a particular component but also provide a better understanding of the components of tobacco and tobacco smoke.

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
50-00-0	1	1	1	Formaldehyde
50-06-6	0	1	0	2,4,6(1*H*,3*H*, 5*H*)-Pyrimidinetrione, 5-ethyl-5-phenyl- {phenobarbital}
50-21-5	1	1	1	Propanoic acid, 2-hydroxy- [2 CAS Nos.] {lactic acid}
598-82-3				
50-29-3	1	1	1	Benzene, 1,1′-(2,2,2-trichloroethylidene)bis[4-chloro- {*p,p′*-DDT}
50-32-8	1	1	1	Benzo[*a*]pyrene {B[*a*]P}
50-67-9	1	1	1	1*H*-Indol-5-ol, 3-(2-aminoethyl)-
50-69-1	0	1	0	*D*-Ribose
50-70-4	1	1	1	Hexane, hexahydroxy- {sorbitol, glucitol}
50-76-0	0	1	0	Actinomycin D
50-78-2	0	1	0	Benzoic acid, 2-acetoxy-
50-81-7	1	1	1	*L*-Ascorbic acid {*L*-gulofuranolactone, 3-oxo-}
50-85-1	1	0	0	Benzoic acid, 2-hydroxy-4-methyl-
50-89-5	0	1	0	Thymidine
50-99-7	1	1	1	α-*D*-Glucose
26655-34-5				
51-03-6	0	1	0	1,3-Benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl- {piperonyl butoxide}
51-17-2	1	0	0	1*H*-Benzimidazole
51-35-4	0	1	0	*L*-Proline, 4-hydroxy-, *trans*-
51-45-6	0	1	0	1*H*-Imidazole-4-ethanamine {histamine}
51-55-8	0	1	0	Benzeneacetic acid, α-(hydroxymethyl)-(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester {atropine}
51-67-2	1	1	1	Phenol, 4-(2-aminoethyl)- {tyramine}
51-75-2	1	0	0	Ethanamine, 2-chloro-*N*-(2-chloroethyl)-*N*-methyl-
51-79-6	1	1	1	Carbamic acid, ethyl ester {urethane}
51-90-1	1	0	0	Carbon-^{14}C dioxide
52-68-6	1	1	1	Phosphonic acid, 2,2,2-trichloromethyl-1-hydroxyethyl-, dimethyl ester {Trichlorphon®, Dylox®, Dipterex®}
52-90-4	1	1	1	*L*-Cysteine {propanoic acid, 2-amino-3-mercapto- (R)}
53-19-0	1	1	1	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDD, *o.p′*-TDE}
53-57-6	0	1	0	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P′*→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide
53-59-8	0	1	0	Adenosine 5′-(trihydrogen diphosphate), 2′-(dihydrogen phosphate), *P′*→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt
53-69-0	1	0	0	Benz[*a*]acridine, 8,10-dimethyl-
53-70-3	1	1	1	Dibenz[*a,h*]anthracene {DB[*a,h*]A}
53-84-9	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *P′*→5′-ester with 3-(aminocarbonyl)-1-β-*D*-ribofuranosylpyridinium hydroxide, inner salt
54-11-5	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {*l*-nicotine}
55-18-5	1	1	1	Ethanamine, *N*-ethyl-*N*-nitroso- {NDEA}
55-21-0	1	1	1	Benzamide
55-38-9	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-methylthio)-3-methylphenyl ester {Fenthion®}
56-12-2	1	1	1	Butanoic acid, 4-amino-
56-18-8	1	0	0	1,3-Propanediamine, *N*-(3-aminopropyl)- {norspermidine}
56-23-5	1	1	1	Carbon tetrachloride
56-25-7	0	1	0	1,3-Isobenzofurandione, 3a,7a-dimethyl-4,7-epoxy-hexahydro- {cantharidin}
56-38-2	1	1	1	Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester {Parathion®}
56-40-6	1	1	1	Glycine
56-41-7	1	1	1	*L*-α-Alanine
56-45-1	0	1	0	*L*-Serine
56-49-5	1	0	0	Benz[*j*]aceanthrylene, 1,2-dihydro-3-methyl- {3-methylcholanthrene}
56-55-3	1	1	1	Benz[*a*]anthracene {B*a*A or B[*a*]A}
56-65-5	0	1	0	Adenosine 5′-(tetrahydrogen triphosphate)
56-81-5	1	1	1	1,2,3-Propanetriol {glycerol}
56-84-8	1	1	1	*L*-Aspartic acid
56-85-9	1	1	1	*L*-Glutamine
56-86-0	1	1	1	*L*-Glutamic acid
56-87-1	0	1	0	*L*-Lysine

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
56-89-3	0	1	0	*L*-Cystine
13028-62-1				
57-03-4	0	1	0	1,2,3-Propanetriol, 1-(dihydrogen phosphate)
57-04-5	0	1	0	2-Propanone, 1-hydroxy-3-(phosphonooxy)-
57-10-3	1	1	1	Hexadecanoic acid {palmitic acid}
57-11-4	1	1	1	Octadecanoic acid {stearic acid}
57-12-5	1	0	0	Cyanide ion
57-13-6	1	1	1	Urea
57-14-7	1	1	1	Hydrazine, 1,1-dimethyl-
57-48-7	1	1	1	*D*-Fructose {levulose}
57-50-1	1	1	1	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl- {sucrose}
57-55-6	1	1	1	1,2-Propanediol {propylene glycol}
57-74-9	0	1	0	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro {chlordane}
12789-03-6				
57-83-0	0	1	0	Pregn-4-ene-3,20-dione
57-87-4	1	1	1	Ergosta-5,7,22-trien-3-ol, (3β,22*E*)- {ergosterol}
57-88-5	1	1	1	Cholest-5-en-3-ol (3β)- {cholesterol}
57-92-1	0	1	0	Streptomycin
57-97-6	1	0	0	Benz[*a*]anthracene, 7,12-dimethyl- {DMBA}
58-05-9	0	1	0	*L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-
58-08-2	1	1	1	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- {caffeine}
58-27-5	1	0	0	1,4-Naphthalenedione, 2-methyl-
58-55-9	0	1	0	1*H*-Purine-2,6-dione, 3,7-dihydro-1,7-dimethyl-
58-56-0	0	1	0	3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride
58-61-7	0	1	0	Adenosine
58-64-0	0	1	0	Adenosine 5′-(trihydrogen diphosphate)
58-68-4	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *P*′→5′-ester with 1,4-dihydro-1-β-*D*-ribofuranosyl-3-pyridinecarboxamide
58-85-5	0	1	0	1*H*-Thieno[3,4-*d*]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3aS-(3aα,4β,6aα)]-
58-86-6	1	1	1	Xylose
58-89-9	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1α,2α,3β,4α,5α,6β)- {gamma-HCH, HCH-gamma, γ-Lindane®}
58-96-8	0	1	0	Uridine
58-97-9	0	1	0	5′-Uridylic acid
59-02-9	1	1	1	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- {α-tocopherol}
59-23-4	1	1	1	*D*-Galactose
59-43-8	0	1	0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride {thiamine}
59-48-3	1	0	0	2*H*-Indol-2-one, 1,3-dihydro- {phthalimidine, oxindole}
59-56-3	0	1	0	α-*D*-Glucopyranose, 1-(dihydrogen phosphate)
59-67-6	1	1	1	3-Pyridinecarboxylic acid {nicotinic acid}
59-89-2	1	1	1	Morpholine, 4-nitroso- {NMOR}
60-11-7	0	1	0	Resinol: resinol, yellow
60-12-8	1	1	1	Benzeneethanol {phenethyl alcohol} Occasionally listed as 1321-27-3 Ethanol, phenyl-
60-18-4	0	1	0	*L*-Tyrosine
60-27-5	0	1	0	4*H*-Imidazol-4-one, 2-amino-1,5-dihydro-1-methyl- {creatinine}
60-29-7	1	1	1	Ethane, 1,1′-oxybis- {ethyl ether}
60-33-3	1	1	1	9,12-Octadecadienoic acid, (*Z,Z*)- {linoleic acid}
60-34-4	1	0	0	Hydrazine, methyl-
60-35-5	1	0	0	Acetamide
60-51-5	1	1	1	Phosphorodithioic acid, *O*,*O*-dimethyl-S-[2-(methylamino)-2-oxoethyl] ester {Dimethoate®}
60-57-1	1	1	1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aα,3β,6β,6aα,7β,7aα)- {Dieldrin®}
60-92-4	0	1	0	Adenosine, cyclic 3′,5′-(hydrogen phosphate)

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
61-19-8	0	1	0	5′-Adenylic acid
61-54-1	0	1	0	1*H*-Indole-3-ethanamine
61-90-5	1	1	1	*L*-Leucine
62-49-7	0	1	0	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl- [2 CAS Nos.] {choline}
123-41-1				
62-53-3	1	1	1	Benzenamine {aniline}
62-57-7	0	1	0	Alanine, 2-methyl-
62-73-7	0	1	0	Phosphoric acid, 2,2,-dichloroethenyl-, dimethyl ester {DDVP, Dichlorvos®}
62-75-9	1	1	1	Methanamine, *N*-methyl-*N*-nitroso- {NDMA}
63-25-2	1	1	1	1-Naphthalenol, methylcarbamate {Sevin®, Carbaryl®}
63-37-6	0	1	0	5′-Cytidylic acid
63-42-3	0	1	0	Lactose
63-68-3	0	1	0	*L*-Methionine
63-91-2	1	1	1	*L*-Phenylalanine
64-04-0	1	1	1	Benzeneethanamine
64-17-5	1	1	1	Ethanol {ethyl alcohol}
64-18-6	1	1	1	Formic acid
64-19-7	1	1	1	Acetic acid
65-30-5	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate (2:1)
65-46-3	0	1	0	Cytidine {2(1*H*)-pyrimidinone, 4-amino-1-β-*D*-ribofuranosyl-}
65-47-4	0	1	0	Cytidine 5′-(tetrahydrogen triphosphate)
65-71-4	1	1	1	2,4(1*H*,3*H*)-Pyrimidinedione, 5-methyl- {thymine}
65-85-0	1	1	1	Benzoic acid {benzenecarboxylic acid}
66-22-8	0	1	0	2,4(1*H*,3*H*)-Pyrimidinedione {uracil}
66-25-1	1	1	1	Hexanal {caproic aldehyde}
66-76-2	1	0	0	2*H*-1-Benzopyran-2-one, 3,3′-methylenebis[4-hydroxy]- {dicumarol}
67-03-8	0	1	0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- chloride, monohydrochloride {thiamine hydrochloride}
67-47-0	1	1	1	2-Furancarboxaldehyde, 5-(hydroxymethyl)-
67-51-6	1	0	0	1*H*-Pyrazole, 3,5-dimethyl-
67-56-1	1	1	1	Methanol
67-63-0	1	1	1	2-Propanol
67-64-1	1	1	1	2-Propanone {acetone}
67-66-3	1	1	1	Methane, trichloro- {chloroform}
67-68-5	0	1	0	Methane, sulfinylbis-
67-72-1	1	0	0	Ethane, hexachloro-
68-04-2	1	1	1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, sodium salt
68-12-2	1	1	1	Formamide, *N*,*N*-dimethyl-
68-26-8	0	1	0	2,4,6,8-Nonatetraen-1-ol, 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (all-*E*)- {retinol}
68-94-0	0	1	0	6*H*-Purin-6-one, 1,7-dihydro- {hypoxanthine}
69-65-8	1	1	1	*D*-Mannitol {cordycepic acid}
69-72-7	1	1	1	Benzoic acid, 2-hydroxy- {salicylic acid}
69-79-4	0	1	0	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin, α-maltose}
69-89-6	0	1	0	1*H*-Purine-2,6-dione, 3,7-dihydro- {xanthine}
69-93-2	1	0	0	1*H*-Purine-2,6,8-trione, 7,9-dihydro- {uric acid}
70-18-8	0	1	0	Glycine, *N*-(*N*-*L*-γ-glutamyl-*L*-cysteinyl)- {glutathione}
70-26-8	1	1	1	*L*-Ornithine
70-30-4	1	0	0	Phenol, 2,2′-methylenebis[3,4,6-trichloro-
70-47-3	0	1	0	*L*-Asparagine
71-00-1	0	1	0	*L*-Histidine
71-23-8	1	1	1	1-Propanol
71-30-7	1	1	1	2(1*H*)-Pyrimidinone, 4-amino- {cytosine}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
71-36-3	1	1	1	1-Butanol {*n*-butyl alcohol}
71-41-0	1	1	1	1-Pentanol {amyl alcohol}
71-43-2	1	1	1	Benzene
71-44-3	0	1	0	1,4-Butanediamine, *N*,*N*′-bis(3-aminopropyl)- {spermine}
71-47-6	1	1	1	Formate
71-50-1	1	1	1	Acetate
71-55-6	1	0	0	Ethane, 1,1,1-trichloro-
72-17-3	0	1	0	Propanoic acid, 2-hydroxy-, sodium salt {sodium lactate}
16595-31-6				
72-18-4	0	1	0	*L*-Valine
72-19-5	1	1	1	*L*-Threonine
72-20-8	1	1	1	2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aβ,3α,6α,6aβ,7β,7aα)- {Endrin®}
72-43-5	0	1	0	Ethane, 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)- {Methoxychlor®}
72-54-8	1	1	1	Benzene, 1,1′-(2,2-dichloroethylidene)bis[4-chloro- {*p*,*p*′-DDD, *p*,*p*′-TDE}
72-55-9	1	1	1	Benzene, 1,1′-(dichloroethenylidene)bis[4-chloro- {*p*,*p*′-DDE}
73-22-3	0	1	0	*L*-Tryptophan
73-24-5	0	1	0	1*H*-Purin-6-amine {adenine}
73-32-5	0	1	0	*L*-Isoleucine
73-40-5	1	1	1	6*H*-Purin-6-one, 2-amino-1,7-dihydro- {guanine}
74-79-3	0	1	0	*L*-Arginine
74-82-8	1	0	0	Methane
74-83-9	1	1	1	Methane, bromo- {Brom-o-Gas®, Meth-o-Gas®, ProFum®, Terr-o-Gas®, Zytox®}
74-84-0	1	0	0	Ethane
74-85-1	1	1	1	Ethene {ethylene}
74-86-2	1	0	0	Ethyne {acetylene}
74-87-3	1	1	1	Methane, chloro-
74-88-4	1	1	1	Methane, iodo-
74-89-5	1	1	1	Methanamine {methylamine}
74-90-8	1	1	1	Hydrocyanic acid {hydrogen cyanide}
74-93-1	1	1	1	Methanethiol {methyl mercaptan}
74-98-6	1	0	0	Propane
74-99-7	1	0	0	1-Propyne
75-00-3	1	0	0	Ethane, chloro-
75-01-4	0	1	0	Ethene, chloro- {vinyl chloride}
75-04-7	1	1	1	Ethanamine {ethylamine}
75-05-8	1	1	1	Acetonitrile
75-07-0	1	1	1	Acetaldehyde
75-08-1	1	0	0	Ethanethiol {ethyl mercaptan}
75-09-2	1	1	1	Methane, dichloro-
75-12-7	1	0	0	Formamide
75-13-8	0	1	0	Isocyanic acid
75-15-0	1	1	1	Carbon disulfide
75-18-3	1	1	1	Methane, thiobis- {methyl sulfide}
75-21-8	1	0	0	Oxirane {ethylene oxide}
75-28-5	1	0	0	Propane, 2-methyl- {isobutane}
75-31-0	1	1	1	2-Propanamine
75-33-2	1	0	0	2-Propanethiol {isopropyl mercaptan}
75-44-5	0	1	0	Carbon oxychloride {phosgene}
75-50-3	1	1	1	Methanamine, *N*,*N*-dimethyl- {trimethylamine}
75-52-5	1	0	0	Methane, nitro-
75-56-9	1	0	0	Oxirane, methyl- {propylene oxide}
75-64-9	1	1	1	2-Propanamine, 2-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
75-65-0	1	1	1	2-Propanol, 2-methyl- {*tert*-butanol}
75-69-4	1	1	1	Methane, trichlorofluoro-
75-71-8	1	0	0	Methane, dichlorodifluoro-
75-83-2	1	0	0	Butane, 2,2-dimethyl-
75-85-4	1	0	0	2-Butanol, 2-methyl-
75-86-5	1	0	0	Propanenitrile, 2-hydroxy-2-methyl- {acetone cyanohydrin}
75-88-7	1	1	1	Ethane, 1-chloro-2,2,2-trifluoro- {Freon® 133a}
75-97-8	1	0	0	2-Butanone, 3,3-dimethyl-
75-98-9	0	1	0	Propanoic acid, 2,2-dimethyl- {pivalic acid}
76-06-2	0	1	0	Methane, nitrotrichloro- {Chloropicrin®}
76-19-7	0	1	0	Propane, octafluoro- {Freon® 218, Perfluoropropane}
76-22-2	0	1	0	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- {camphor}
76-44-8	1	1	1	4,7-Methano-1*H*-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- {Heptachlor®}
76-49-3	0	1	0	Acetic acid, *endo*-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl ester {bornyl acetate}
76-50-6	0	1	0	Butanoic acid, 3-methyl-, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, endo- {bornyl isovalerate}
76-87-9	0	1	0	Triphenylstannium hydroxide {Fentin hydroxide®}
77-06-5	0	1	0	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)- {gibberellic acid}
77-10-1	1	0	0	Piperidine, 1-(1-phenylcyclohexyl)-
77-52-1	0	1	0	Urs-12-en-28-oic acid, 3-hydroxy-, (3β)-
77-53-2	0	1	0	1*H*-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,6α,7β,8aα)]-
77-67-8	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-3-methyl-
77-73-6	1	0	0	Dicyclopentadiene
77-74-7	1	0	0	3-Pentanol, 3-methyl-
77-76-9	1	0	0	Propane, 2,2-dimethoxy-
77-83-8	0	1	0	Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester {ethyl methylphenylglycidate}
77-92-9	1	1	1	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid}
77-93-0	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester {triethyl citrate}
77-95-2	1	1	1	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy- [2 CAS Nos.] {quinic acid}
562-73-2				
78-35-3	0	1	0	Butanoic acid, 3-methyl-, 3,7-dimethyl-1,6-octadien-6-yl ester {linalyl isobutyrate}
78-51-3	1	0	0	Ethanol, 2-butoxy-, phosphate (3:1)
78-59-1	1	1	1	2-Cyclohexen-1-one, 3,5,5-trimethyl- {isophorone}
78-67-1	0	1	0	Propanenitrile, 2-methyl-, 2,2′-azobis- {Porofor-57®}
78-69-3	0	1	0	3-Octanol, 3,7-dimethyl- {tetrahydrolinalool}
78-70-6	1	1	1	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool}
78-78-4	1	1	1	Butane, 2-methyl- {methylbutane}
102056-77-9				
78-79-5	1	1	1	1,3-Butadiene, 2-methyl- {isoprene}
78-81-9	1	1	1	1-Propanamine, 2-methyl-
78-82-0	1	1	1	Propanenitrile, 2-methyl- {isobutyronitrile}
78-83-1	1	1	1	1-Propanol, 2-methyl- {isobutyl alcohol}
78-84-2	1	1	1	Propanal, 2-methyl- {isobutyraldehyde}
78-85-3	1	1	1	2-Propenal, 2-methyl- {methacrolein}
78-87-5	0	1	0	Propane, 1,2-dichloro-
78-92-2	1	1	1	2-Butanol {*sec*-butyl alcohol}
15892-23-6				
78-93-3	1	1	1	2-Butanone {methyl ethyl ketone}
78-94-4	1	1	1	3-Buten-2-one {methyl vinyl ketone}
78-95-5	1	0	0	2-Propanone, 1-chloro-
78-97-7	1	0	0	Propanenitrile, 2-hydroxy-
78-98-8	1	1	1	Propanal, 2-oxo- {pyruvaldehyde, methylglyoxal}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
79-01-6	1	0	0	Ethene, trichloro-
79-05-0	1	0	0	Propanamide
79-06-1	1	1	1	2-Propenamide {acrylamide}
79-09-4	1	1	1	Propanoic acid {propionic acid}
79-10-7	1	1	1	2-Propenoic acid {acrylic acid}
79-14-1	1	1	1	Acetic acid, hydroxy- {glycolic acid}
79-16-3	1	0	0	Acetamide, *N*-methyl-
79-20-9	1	1	1	Acetic acid, methyl ester
79-24-3	1	0	0	Ethane, nitro-
79-31-2	1	1	1	Propanoic acid, 2-methyl- {isobutyric acid}
79-35-6	1	1	1	Ethene, 1,1-dichloro-2,2-difluoro- {Freon® 1112a}
79-38-9	1	1	1	Ethene, chlorotrifluoro- {Freon® 1113}
79-39-0	1	0	0	2-Propenamide, 2-methyl- {methacrylamide}
79-41-4	1	0	0	2-Propenoic acid, 2-methyl- {methacrylic acid}
79-43-6	0	1	0	Acetic acid, dichloro-
79-46-9	1	0	0	Propane, 2-nitro-
79-62-9	0	1	0	Lanost-8-en-3-ol, (3β)-
79-63-0	0	1	0	Lanosta-8,24-dien-3-ol, (3β)- {lanosterol}
79-69-6	0	1	0	3-Buten-2-one, 4-(2,5,6,6-tetramethyl-2-cyclohexen-1-yl)- {α-irone}
79-77-6	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)-
79-78-7	0	1	0	1,6-Heptadien-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {allylionone}
79-83-4	0	1	0	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- [2 CAS Nos.] {pantothenic acid}
137-08-8				
79-92-5	1	1	1	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- {camphene}
80-26-2	1	1	1	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate {α-terpinyl acetate}
80-53-5	1	0	0	Cyclohexanemethanol, 4-hydroxy-α,α,4-trimethyl- {*p*-menthane-1,8-diol}
80-56-8	1	1	1	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- [2 CAS Nos.] {α-pinene}
7785-26-4				
80-59-1	1	1	1	2-Butenoic acid, 2-methyl-, (*E*)- {tiglic acid}
80-60-4	1	1	1	Butanoic acid, 2-amino-
80-62-6	0	1	0	2-Propenoic acid, 2-methyl-, methyl ester
80-69-3	1	1	1	Propanedioic acid, hydroxy-
80-71-7	1	1	1	2-Cyclopenten-1-one, 2-hydroxy-3-methyl- {methylcyclopentenolone}
80-72-8	1	0	0	2-Cyclopenten-1-one, 2,3-dihydroxy- {reductic acid}
80-97-7	0	1	0	Cholestan-3-ol (3β) {dihydrocholesterol}
81-15-2	0	1	0	Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro- {musk xylene}
82-68-8	0	1	0	Benzene, nitropentachloro- {Quintocen®}
83-32-9	1	1	1	Acenaphthylene, 1,2-dihydro- {acenaphthene}
83-33-0	1	0	0	1*H*-Inden-1-one, 2,3-dihydro- {1-indanone}
83-34-1	1	1	1	1*H*-Indole, 3-methyl- {skatole}
83-46-5	1	1	1	Stigmast-5-en-3-ol, (3β)- {β-sitosterol}
83-47-6	1	1	1	Stigmast-5-en-3-ol, (3β, 24*S*)- {γ-sitosterol}
83-48-7	1	1	1	Stigmasta-5,22-dien-3-ol, (3β,22*E*)- {stigmasterol}
83-66-9	0	1	0	Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro- {musk ambrette}
83-67-0	1	1	1	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- {theobromine}
83-79-4	0	1	0	Benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6a*H*)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, [2R-(2α,6aα,12aα)]- {Rotenone®}
83-88-5	0	1	0	Riboflavin
84-11-7	1	0	0	9,10-Phenanthrenedione {phenanthrenequinone, phenanthraquinone}
84-21-9	0	1	0	3′-Adenylic acid
84-54-8	1	1	1	9,10-Anthracenedione, 2-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
84-65-1	1	1	1	9,10-Anthracenedione {9,10-anthraquinone}
84-66-2	1	1	1	1,2-Benzenedicarboxylic acid, diethyl ester {diethyl phthalate}
84-69-5	0	1	0	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
84-74-2	1	1	1	1,2-Benzenedicarboxylic acid, dibutyl ester {dibutyl phthalate}
84-75-3	0	1	0	1,2-Benzenedicarboxylic acid, dihexyl ester
84-80-0	0	1	0	1,4-Naphthalenedione, 2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [R-[R*,R*-(*E*)]]- {vitamin K1}
85-01-8	1	0	0	Phenanthrene
85-02-9	1	0	0	Benzo[*f*]quinoline {1-azaphenanthrene}
85-41-6	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione {phthalimide}
85-44-9	1	1	1	1,3-Isobenzofurandione {phthalic anhydride}
85-61-0	0	1	0	Coenzyme A
85-68-7	0	1	0	1,2-Benzenedicarboxylic acid, butyl, phenylmethyl ester
85-69-8	1	1	1	1,2-Benzenedicarboxylic acid, butyl, 2-ethylhexyl ester
85-91-6	0	1	0	Benzoic acid, 2-(methylamino)-, methyl ester
86-01-1	0	1	0	Guanosine 5′-(tetrahydrogen triphosphate)
86-28-2	1	0	0	9*H*-Carbazole, 9-ethyl-
86-30-6	1	0	0	Benzenamine, *N*-nitroso-*N*-phenyl-
86-50-0	1	1	1	Phosphorodithioic acid, *O,O*-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Guthion®, Azinphos-Methyl®}
86-51-1	1	1	1	Benzaldehyde, 2,3-dimethoxy-
86-53-3	1	0	0	1-Naphthalenecarbonitrile
86-57-7	1	1	1	Naphthalene, 1-nitro-
86-73-7	1	1	1	9*H*-Fluorene
86-74-8	1	0	0	9*H*-Carbazole {dibenzo[*b,d*]pyrrole}
86-87-3	0	1	0	1-Naphthaleneacetic acid
87-19-4	0	1	0	Benzoic acid, 2-hydroxy-, 2-methylpropyl ester {isobutyl salicylate}
87-20-7	0	1	0	Benzoic acid, 2-hydroxy-, 3-methylbutyl ester {isoamyl salicylate}
87-22-9	0	1	0	Benzoic acid, 2-hydroxy-, 2-phenylethyl ester {phenethyl salicylate}
87-25-2	0	1	0	Benzoic acid, 2-amino-, ethyl ester
87-40-1	0	1	0	Benzene, 1,3,5-trichloro-2-methoxy-
87-41-2	0	1	0	1(3*H*)-Isobenzofuranone {phthalide}
87-44-5	0	1	0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4*E*,9S*)]- {β-caryophyllene}
87-51-4	1	1	1	1*H*-Indole-3-acetic acid
87-59-2	1	1	1	Benzenamine, 2,3-dimethyl- {2,3-xylidine}
87-62-7	1	1	1	Benzenamine, 2,6-dimethyl- {2,6-xylidine}
87-66-1	1	1	1	1,2,3-Benzenetriol {pyrogallol}
87-69-4	0	1	0	Butanedioic acid, 2,3-dihydroxy- {*l*-tartaric acid}
87-72-9	1	1	1	*L*-Arabinose
5328-37-0				
87-89-8	1	1	1	myo-Inositol
87-99-0	1	1	1	Xylitol
88-05-1	1	1	1	Benzenamine, 2,4,6-trimethyl- {mesitylamine}
88-09-5	1	1	1	Butanoic acid, 2-ethyl- {diethylacetic acid}
88-12-0	1	0	0	2-Pyrrolidinone, 1-ethenyl-
88-14-2	1	1	1	2-Furancarboxylic acid {furoic acid}
88-15-3	0	1	0	Ethanone, 1-(2-thienyl)- {2-acetylthiophene}
88-18-6	1	1	1	Phenol, 2-(1,1-dimethylethyl)-
88-32-4	1	0	0	Phenol, 3-(1,1-dimethylethyl)-4-methoxy-
88-69-7	1	1	1	Phenol, 2-(1-methylethyl)- {2-isopropylphenol}
88-72-2	1	0	0	Benzene, 1-methyl-2-nitro-
88-75-5	1	0	0	Phenol, 2-nitro-
88-99-3	1	1	0	1,2-Benzenedicarboxylic acid {phthalic acid}
89-00-9	0	1	0	2,3-Pyridinedicarboxylic acid {quinolinic acid}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
89-48-5	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate [2 CAS Nos.] {menthyl acetate}
16409-45-3				
89-58-7	1	0	0	Benzene, 1,4-dimethyl-2-nitro- {2,5-dimethyl-1-nitrobenzene}
89-72-5	1	1	1	Phenol, 2-(1-methylpropyl)-
89-74-7	0	1	0	Ethanone, 1-(2,4-dimethylphenyl)-
89-78-1	1	1	1	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {menthol}
89-79-2	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, [1R-(1α,2β,5α)]-
89-80-5	1	1	1	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}
10458-16-7				
14073-97-3				
89-81-6	1	1	1	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- {*D*-piperitone}
89-82-7	0	1	0	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)- {pulegone}
89-83-8	1	0	0	Phenol, 5-methyl-2-(1-methylethyl)- {thymol}
89-86-1	1	0	0	Benzoic acid, 2,4-dihydroxy- {β-resorcylic acid}
89-87-2	1	0	0	Benzene, 2,4-dimethyl-1-nitro-
89-95-2	1	1	1	Benzenemethanol, 2-methyl-
90-00-6	1	0	0	Phenol, 2-ethyl-
90-02-8	1	1	1	Benzaldehyde, 2-hydroxy- {salicylaldehyde}
90-04-0	1	1	1	Benzenamine, 2-methoxy- {*o*-anisidine}
90-05-1	1	1	1	Phenol, 2-methoxy- {guaiacol}
90-12-0	1	1	1	Naphthalene, 1-methyl-
90-15-3	1	0	0	1-Naphthalenol {1-naphthol = α-naphthol}
90-33-5	0	1	0	2*H*-1-Benzopyran-2-one, 7-hydroxy-4-methyl-
90-41-5	1	0	0	[1,1′-Biphenyl]-2-amine
90-43-7	1	1	1	[1,1′-Biphenyl]-2-ol
90-44-8	1	0	0	9(10*H*)-Anthracenone {anthrone}
90-47-1	0	1	0	9*H*-Xanthen-9-one {xanthone}
90-50-6	0	1	0	2-Propenoic acid, 3-(3,4,5-trimethoxyphenyl)-
90-64-2	0	1	0	Benzeneacetic acid, α-hydroxy- {mandelic acid}
90-65-3	1	1	1	2,5-Hexadienoic acid, 3-methoxy-5-methyl-4-oxo-
90-74-4	0	1	0	*D*-Glucose, 6-*O*-(6-deoxy-α-*L*-mannopyranosyl)- {rutinose}
90-80-2	1	0	0	2*H*-Pyran-2-one, tetrahydro-6-hydroxymethyl, 3,4,5-trihydroxy- {gluconic acid, δ-lactone}
90-98-2	1	0	0	Methanone, bis(4-chlorophenyl)-
91-10-1	1	1	1	Phenol, 2,6-dimethoxy- {syringol}
91-15-6	1	0	0	1,2-Benzenedicarbonitrile
91-16-7	1	1	1	Benzene, 1,2-dimethoxy- {veratrole}
91-17-8	1	0	0	Naphthalene, decahydro-
91-19-0	1	0	0	Quinoxaline {1,4-benzodiazine}
91-20-3	1	1	1	Naphthalene
91-21-4	1	0	0	Isoquinoline, 1,2,3,4- tetrahydro-
91-22-5	1	1	1	Quinoline {1-azanaphthalene}
91-55-4	1	0	0	1*H*-Indole, 2,3-dimethyl-
91-57-6	1	1	1	Naphthalene, 2-methyl-
91-59-8	1	0	0	2-Naphthalenamine {naphthalene, 2-amino-, β-naphthylamine}
91-62-3	1	0	0	Quinoline, 6-methyl-
91-63-4	1	0	0	Quinoline, 2-methyl-
91-64-5	1	1	1	2*H*-1-Benzopyran-2-one {coumarin}
92-06-8	1	0	0	1,1′:3′,1″-Terphenyl [2 CAS Nos.] {*m*-terphenyl}
26140-60-3				
92-07-9	1	0	0	Pyridine, 3,5-diphenyl-
92-24-0	1	0	0	Naphthacene

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
92-44-4	1	0	0	2,3-Naphthalenediol
92-48-8	1	0	0	2*H*-1-Benzopyran-2-one, 6-methyl- {6-methylcoumarin}
92-51-3	1	1	1	1,1′-Bicyclohexyl {cyclohexylcyclohexane}
92-52-4	1	1	1	1,1′-Biphenyl {diphenyl}
92-61-5	1	1	1	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- {scopoletin}
92-67-1	1	0	0	[1,1′-Biphenyl]-4-amine {4-aminobiphenyl}
92-69-3	1	0	0	[1,1′-Biphenyl]-4-ol
92-81-9	1	0	0	Acridine, 9,10-dihydro- {acridan}
92-83-1	1	1	1	9*H*-Xanthene {dibenzopyran}
92-87-5	1	0	0	1,1′-Biphenyl, 4,4′-diamino-
92-93-3	1	0	0	1,1′-Biphenyl, 4-nitro-
92-94-4	1	0	0	1,1′:4′,1″-Terphenyl
93-02-7	1	1	1	Benzaldehyde, 2,5-dimethoxy-
93-03-8	0	1	0	Benzenemethanol, 3,4-dimethoxy-{benzyl alcohol, 3,4-dimethoxy-}
93-04-9	1	1	1	Naphthalene, 2-methoxy-
93-07-2	0	1	0	Benzoic acid, 3,4-dimethoxy-
93-08-3	1	1	1	Ethanone, 1-(2-naphthalenyl)- {methyl naphthyl ketone}
1333-52-4				
93-15-2	1	1	1	Phenol, 2-methoxy-methyl-4-(2-propenyl)- {eugenol, methyl-}
93-16-3	1	1	1	Benzene, 1,2-dimethoxy-4-(1-propenyl)-
93-18-5	1	1	1	Naphthalene, 2-ethoxy- {β-naphthyl ethyl ether}
93-35-6	0	1	0	2*H*-1-Benzopyran-2-one, 7-hydroxy-
93-51-6	1	1	1	Phenol, 2-methoxy-4-methyl- {4-methylguaiacol}
93-54-9	0	1	0	Benzenemethanol, α-ethyl- {1-phenyl-1-propanol}
93-55-0	1	1	1	1-Propanone, 1-phenyl- {propiophenone}
93-58-3	1	1	1	Benzoic acid, methyl ester {methyl benzoate}
93-60-7	1	1	1	3-Pyridinecarboxylic acid, methyl ester {methyl nicotinate}
93-76-5	0	1	0	Acetic acid, 2,4,5-trichlorophenoxy- {2,4,5-T®}
93-89-0	1	0	0	Benzoic acid, ethyl ester {ethyl benzoate}
93-92-5	0	1	0	Benzenemethanol, α-methyl-, acetate
93-99-2	0	1	0	Benzoic acid, phenyl ester
94-13-3	1	0	0	Benzoic acid, 4-hydroxy-, propyl ester
94-26-8	0	1	0	Benzoic acid, 4-hydroxy-, butyl ester
1322-01-6				
94-41-7	1	0	0	2-Propen-1-one, 1,3-diphenyl- {chalcone}
94-46-2	1	1	1	1-Butanol, 3-methyl-, benzoate {isoamyl benzoate}
94-47-3	0	1	0	Benzoic acid, 2-phenylethyl ester {2-phenylethyl benzoate}
94-59-7	0	1	0	1,3-Benzodioxole, 5-(2-propenyl)- {safrole}
94-68-8	1	0	0	Benzenamine, *N*-ethyl-2-methyl-
94-75-7	0	1	0	Acetic acid, 2,4-dichlorophenoxy- {2,4-D}
94-86-0	0	1	0	Phenol, 2-ethoxy-5-propenyl- {5-propenylguaethol}
95-01-2	1	0	0	Benzaldehyde, 2,4-dihydroxy-
95-13-6	1	0	0	1*H*-Indene
95-14-7	1	0	0	1*H*-Benzotriazole {1,2,3-triaza-1*H*-indene}
95-15-8	1	0	0	Benzo[*b*]thiophene
95-16-9	1	1	1	Benzothiazole {benzosulfonazole}
95-20-5	1	1	1	1*H*-Indole, 2-methyl-
95-21-6	1	0	0	Benzoxazole, 2-methyl-
95-47-6	1	1	1	Benzene, 1,2-dimethyl- {*o*-xylene}
95-48-7	1	1	1	Phenol, 2-methyl- {*o*-cresol}
95-50-1	1	1	1	Benzene, 1,2-dichloro-
95-51-2	1	1	1	Benzenamine, 2-chloro- {2-chloroaniline}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
95-53-4	1	1	1	Benzenamine, 2-methyl- {*o*-toluidine, 2-toluidine}
95-54-5	1	0	0	1,2-Benzenediamine {*o*-phenylenediamine}
95-57-8	1	0	0	Phenol, 2-chloro-
95-63-6	1	1	1	Benzene, 1,2,4-trimethyl- {pseudocumene}
95-64-7	1	1	1	Benzenamine, 3,4-dimethyl- {3,4-xylidine}
95-65-8	1	1	1	Phenol, 3,4-dimethyl- {3,4-xylenol}
95-68-1	1	1	1	Benzenamine, 2,4-dimethyl- {2,4-xylidine}
95-71-6	1	1	1	1,4-Benzenediol, 2-methyl- = 1,4-benzenediol, methyl-
95-76-1	0	1	0	Benzenamine, 3,4-dichloro-
95-78-3	1	1	1	Benzenamine, 2,5-dimethyl- {2,5-xylidine}
95-80-7	1	0	0	1,3-Benzenediamine, 4-methyl-
95-87-4	1	1	1	Phenol, 2,5-dimethyl- {2,5-xylenol}
95-92-1	0	1	0	Ethanedioic acid, diethyl ester
95-93-2	1	1	1	Benzene, 1,2,4,5-tetramethyl-
96-04-8	1	0	0	2,3-Heptanedione
96-09-3	1	1	1	Oxirane, phenyl- {phenylethylene oxide}
96-12-8	0	1	0	Propane, 1,2-dibromo-3-chloro- {DBCP®}
96-14-0	1	1	1	Pentane, 3-methyl-
96-15-1	1	1	1	1-Butanamine, 2-methyl-
96-17-3	1	1	1	Butanal, 2-methyl- {2-methylbutyraldehyde}
96-22-0	1	1	1	3-Pentanone
96-24-2	1	0	0	1,2-Propanediol, 3-chloro-
96-26-4	1	0	0	2-Propanone, 1,3-dihydroxy-
96-33-3	1	1	1	2-Propenoic acid, methyl ester
96-35-5	1	0	0	Acetic acid, hydroxy-, methyl ester
96-37-7	1	0	0	Cyclopentane, methyl-
96-38-8	1	0	0	1,3-Cyclopentadiene, 5-methyl-
96-39-9	1	0	0	1,3-Cyclopentadiene, 1-methyl-
96-45-7	1	0	0	2-Imidazolidinethione {ethylenethiourea}
96-47-9	1	0	0	Furan, 2-methyltetrahydro-
96-48-0	1	0	0	2(3*H*)-Furanone, dihydro- {butyrolactone}
96-49-1	1	0	0	1,3-Dioxalan-2-one {ethylene glycol carbonate}
96-54-8	1	1	1	1*H*-Pyrrole, 1-methyl-
97-41-6	1	1	1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ethyl ester
97-53-0	1	1	1	Phenol, 2-methoxy-4-(2-propenyl)- {eugenol}
97-54-1	1	1	1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}
97-59-6	0	1	0	Urea, (2,5-dioxo-4-imidazolidinyl)- {allantoin}
97-61-0	1	1	1	Pentanoic acid, 2-methyl- {2-methylvaleric acid}
97-62-1	0	1	0	Propanoic acid, 2-methyl-, ethyl ester
97-64-3	1	1	1	Propanoic acid, 2-hydroxy-, ethyl ester {ethyl lactate}
97-65-4	1	1	1	Butanedioic acid, methylene- {itaconic acid}
97-73-4	0	1	0	Propanoic acid, 2-hydroxy-, anhydride
97-87-0	0	1	0	Propanoic acid, 2-methylbutyl ester
97-89-2	0	1	0	Propanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester
97-95-0	1	1	1	1-Butanol, 2-ethyl-
97-96-1	1	1	1	Butanal, 2-ethyl- {diethylacetaldehyde}
97-99-4	1	1	1	2-Furanmethanol, tetrahydro-
98-00-0	1	1	1	2-Furanmethanol {furfuryl alcohol}
98-01-1	1	1	1	2-Furancarboxaldehyde {furfural, 2-furaldehyde}
98-02-2	0	1	0	2-Furanmethanethiol
98-03-3	1	1	1	2-Thiophenecarboxaldehyde

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
98-06-6	1	1	1	Benzene, (1,1-dimethylethyl)-
98-29-3	1	0	0	1,2-Benzenediol, 4-(1,1-dimethylethyl)-
98-54-4	1	1	1	Phenol, 4-(1,1-dimethylethyl)-
98-55-5	1	1	1	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {α-terpineol}
98-79-3	0	1	0	5-Pyrrolidinone-2-carboxylic acid {5-oxoproline}
98-82-8	1	1	1	Benzene, (1-methylethyl)- {cumene}
98-83-9	1	0	0	Benzene, (1-methylethenyl)- {α-methylstyrene}
98-85-1	1	1	1	Benzenemethanol, α-methyl-
98-86-2	1	1	1	Ethanone, 1-phenyl- {acetophenone}
98-92-0	1	1	1	3-Pyridinecarboxamide {nicotinamide}
98-95-3	1	0	0	Benzene, nitro-
99-04-7	1	1	1	Benzoic acid, 3-methyl- {*m*-toluic acid}
99-06-9	1	1	1	Benzoic acid, 3-hydroxy-
99-08-1	1	0	0	Benzene, 1-methyl-3-nitro-
99-10-5	1	0	0	Benzoic acid, 3,5-dihydroxy-
99-14-3	0	1	0	1,2,3-Propanetricarboxylic acid
99-20-7	0	1	0	Trehalose
99-30-9	0	1	0	Benzenamine, 2,6-dichloro-4-nitro- {Dicloran®}
99-49-0	1	1	1	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*l*-carvone}
6485-40-1				
99-50-3	1	1	1	Benzoic acid, 3,4-dihydroxy- {protocatechuic acid}
99-51-4	1	0	0	Benzene, 1,2-dimethyl-4-nitro-
99-53-6	1	0	0	Phenol, 2-methyl-4-nitro-
99-62-1	1	0	0	Cyclohexane, 1-methyl-4-(1-methylethyl)- {*p*-menthane}
99-71-8	1	1	1	Phenol, 4-(1-methylpropyl)-
99-76-3	1	0	0	Benzoic acid, 4-hydroxy-, methyl ester
99-83-2	1	1	1	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- {α-phellandrene}
1329-99-3				
99-85-4	0	1	0	1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
99-86-5	1	1	1	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- {α-terpinene}
99-87-6	1	1	1	Benzene, 1-methyl-4-(1-methylethyl)- {*p*-cymene}
99-89-8	1	1	1	Phenol, 4-(1-methylethyl)-
99-93-4	1	1	1	Ethanone, 1-(4-hydroxyphenyl)-
99-94-5	0	1	0	Benzoic acid, 4-methyl- {*p*-toluic acid}
99-96-7	1	1	1	Benzoic acid, 4-hydroxy- {*p*-salicylic acid}
99-99-0	1	0	0	Benzene, 1-methyl-4-nitro-
100-02-7	1	0	0	Phenol, 4-nitro-
100-06-1	1	1	1	Ethanone, 1-(4-methoxyphenyl)- {acetanisole}
100-10-7	1	0	0	Benzaldehyde, 4-(dimethylamino)-
100-18-5	1	1	1	Benzene, 1,4-bis(1-methylethyl)-
100-21-0	1	1	1	1,4-Benzenedicarboxylic acid {terephthalic acid}
100-40-3	1	0	0	Cyclohexene, 4-ethenyl-
100-41-4	1	1	1	Benzene, ethyl-
100-42-5	1	1	1	Benzene, ethenyl- {styrene}
100-43-6	1	1	1	Pyridine, 4-ethenyl-
100-46-9	1	1	1	Benzenemethanamine {benzylamine}
100-47-0	1	1	1	Benzonitrile {phenyl cyanide}
100-48-1	1	0	0	4-Pyridinecarbonitrile
100-51-6	1	1	1	Benzenemethanol {benzyl alcohol}
100-52-7	1	1	1	Benzaldehyde
100-54-9	1	1	1	3-Pyridinecarbonitrile {nicotinonitrile}
100-55-0	0	1	0	3-Pyridinemethanol

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
100-61-8	1	1	1	Benzenamine, *N*-methyl- {*N*-methylaniline}
100-66-3	1	1	1	Benzene, methoxy- {anisole}
100-69-6	1	1	1	Pyridine, 2-ethenyl-
100-70-9	1	0	0	2-Pyridinecarbonitrile
100-71-0	1	1	1	Pyridine, 2-ethyl-
100-73-2	1	1	1	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro- {acrolein dimer}
100-75-4	1	1	1	Piperidine, 1-nitroso- {NPIP}
100-79-8	1	0	0	1,3-Dioxalane-4-methanol, 2,2-dimethyl-
100-80-1	1	0	0	Benzene, 1-ethenyl-3-methyl-
100-83-4	0	1	0	Benzaldehyde, 3-hydroxy-
100-84-5	1	0	0	Benzene, 1-methoxy-3-methyl- {*m*-methylanisole}
100-97-0	1	0	0	1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane {hexamethylenetetramine}
101-05-3	0	1	0	1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-(2-chlorophenyl)- {Anilazine®, Dyrene®}
101-21-3	0	1	0	Carbamic acid, 3-chlorophenyl-, (1-methylethyl) ester {Chloropropham®}
101-39-3	0	1	0	2-Propenal, 2-methyl-3-phenyl-
101-41-7	1	1	1	Benzeneacetic acid, methyl ester {methyl phenylacetate}
101-53-1	1	0	0	Phenol, 4-phenylmethyl-
7563-63-5				
101-54-2	1	0	0	1,4-Benzenediamine, *N*-phenyl-
101-60-0	1	1	1	21*H*,23*H*-Porphine {porphyrin}
101-76-8	1	0	0	Benzene, 1,1′-methylenebis[4-chloro-
101-81-5	1	0	0	Benzene, 1,1′-methylenebis- {diphenylmethane}
101-82-6	1	0	0	Pyridine, 2-(phenylmethyl)-
101-84-8	0	1	0	Benzene, 1,1′-oxybis- {diphenyl ether}
101-94-0	0	1	0	Benzeneacetic acid, 4-methylphenyl ester {*p*-tolyl phenylacetate}
101-97-3	1	1	1	Benzeneacetic acid, ethyl ester {ethyl phenylacetate}
102-13-6	0	1	0	Benzeneacetic acid, 2-methylpropyl ester
102-16-9	0	1	0	Benzeneacetic acid, phenylmethyl ester {benzyl phenylacetate}
102-17-0	0	1	0	Benzenemethanol, 4-methoxy-, phenylacetate
102-19-2	1	1	1	Benzeneacetic acid, 3-methylbutyl ester
102-20-5	1	1	1	Benzeneacetic acid, 2-phenylethyl ester
102-22-7	0	1	0	Benzeneacetic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl phenylacetate}
102-27-2	0	1	0	Benzenamine, *N*-ethyl-3-methyl-
102-29-4	1	0	0	1,2-Benzenediol, monoacetate
102-32-9	1	1	1	Benzeneacetic acid, 3,4-dihydroxy-
102-61-4	0	1	0	Ethene, 1-(phenyl)-2-(3,5-dihydroxyphenyl)- {pinosylvin}
102-76-1	1	1	1	1,2,3-Propanetriol, triacetate {triacetin}
102-93-2	1	1	1	Benzenepropanamide
102-94-3	1	1	1	2-Propenoic acid, 3-phenyl-, (*Z*)- {*cis*-cinnamic acid}
103-17-3	0	1	0	Benzene, 1-chloro-4-((4-chlorophenyl)methyl)thio- {Chlorobenside®}
103-23-1	1	0	0	Hexanedioic acid, bis(2-ethylhexyl) ester
103-26-4	1	1	1	2-Propenoic acid, 3-phenyl-, methyl ester {methyl cinnamate}
103-28-6	1	1	1	Propanoic acid, 2-methyl-, phenylmethyl ester {benzyl isobutyrate}
103-29-7	1	0	0	Benzene, 1,1′-(1,2-ethanediyl)bis- {bibenzyl}
103-30-0	1	0	0	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*E*)-
103-33-3	0	1	0	Benzene, azobis- {azobenzene}
103-36-6	1	1	1	2-Propenoic acid, 3-phenyl-, ethyl ester {ethyl cinnamate}
103-37-7	1	1	1	Butanoic acid, phenylmethyl ester {benzyl butyrate}
103-38-8	0	1	0	Butanoic acid, 3-methyl-, phenylmethyl ester {benzyl isovalerate}
103-41-3	1	1	1	2-Propenoic acid, 3-phenyl-, phenylmethyl ester {benzyl cinnamate}
103-45-7	1	1	1	Acetic acid, 2-phenylethyl ester {2-phenethyl acetate}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
103-48-0	0	1	0	Propanoic acid, 2-methyl-, phenylethyl ester
103-50-4	1	0	0	Benzene, 1,1′-[oxybis(methylene)]bis- {dibenzyl ether}
103-52-6	0	1	0	Butanoic acid, phenylethyl ester
103-53-7	0	1	0	2-Propenoic acid, 3-phenyl-, phenylethyl ester
103-54-8	0	1	0	Acetic acid, 3-phenyl-2-propenyl ester {cinnamyl acetate}
103-56-0	1	1	1	Propanoic acid, 3-phenyl-2-propenyl ester {cinnamyl propionate}
103-59-3	0	1	0	Propanoic acid, 2-methyl-, 3-phenyl-2-propen-1-yl ester
103-65-1	1	1	1	Benzene, propyl-
103-69-5	1	0	0	Benzenamine, *N*-ethyl- {*N*-ethylaniline}
103-70-8	1	0	0	Formamide, *N*-phenyl-
103-73-1	1	0	0	Benzene, ethoxy-
103-74-2	1	0	0	2-Pyridineethanol
103-79-7	1	1	1	2-Propanone, 1-phenyl-
103-81-1	1	1	1	Benzeneacetamide {phenylacetamide}
103-82-2	1	1	1	Benzeneacetic acid {phenylacetic acid}
103-84-4	1	0	0	Acetamide, *N*-phenyl-
103-93-5	0	1	0	Propanoic acid, 2-methyl-, 4-methylphenyl ester {*p*-tolyl isobutyrate}
103-95-7	0	1	0	Benzenepropanal, α-methyl-4-(1-methylethyl)- {cyclamen aldehyde}
104-09-6	0	1	0	Benzeneacetaldehyde, 4-methyl-
104-20-1	0	1	0	2-Butanone, 4-(4-methoxyphenyl)-
104-21-2	1	1	1	Benzenemethanol, 4-methoxy-, acetate {anisyl acetate}
104-27-8	0	1	0	1-Penten-3-one, 1-(4-methoxyphenyl)-
104-45-0	0	1	0	Benzene, 1-methoxy-4-propyl- {dihydroanethole}
104-46-1	1	1	1	Benzene, 1-methoxy-4-(1-propenyl)- {anethole}
104-50-7	0	1	0	2(3*H*)-Furanone, 5-butyldihydro- {γ-octalactone}
104-51-8	1	0	0	Benzene, butyl-
104-53-0	0	1	0	Benzenepropanal
104-54-1	1	1	1	2-Propen-1-ol, 3-phenyl- {cinnamyl alcohol}
104-55-2	1	1	1	2-Propenal, 3-phenyl- {cinnamaldehyde}
104-57-4	1	1	1	Formic acid, phenylmethyl ester {benzyl formate}
104-61-0	1	1	1	2(3*H*)-Furanone, dihydro-5-pentyl- {γ-nonalactone}
104-62-1	1	1	1	Formic acid, 2-phenylethyl ester
104-66-5	0	1	0	Ethane, 1,2-diphenoxy-
104-67-6	0	1	0	2(3*H*)-Furanone, dihydro-5-heptyl- {γ-undecalactone}
104-76-7	1	1	1	1-Hexanol, 2-ethyl-
104-83-6	1	0	0	Benzene, 1-chloro-4-(chloromethyl)-
104-85-8	1	0	0	Benzonitrile, 4-methyl-
104-87-0	1	1	1	Benzaldehyde, 4-methyl- {*p*-tolualdehyde}
104-90-5	1	1	1	Pyridine, 5-ethyl-2-methyl-
104-93-8	1	1	1	Benzene, 1-methoxy-4-methyl- {*p*-methylanisole}
104-94-9	1	1	1	Benzenamine, 4-methoxy- {*p*-anisidine}
105-05-5	1	0	0	Benzene, 1,4-diethyl-
105-13-5	0	1	0	Benzenemethanol, 4-methoxy- {anisyl alcohol}
105-21-5	1	1	1	2(3*H*)-Furanone, dihydro-5-propyl- {γ-heptalactone}
105-30-6	0	1	0	1-Pentanol, 2-methyl-
105-37-3	1	1	1	Propanoic acid, ethyl ester {ethyl propionate}
105-38-4	0	1	0	Propanoic acid, ethenyl ester
105-42-0	1	0	0	2-Hexanone, 4-methyl-
105-43-1	1	1	1	Pentanoic acid, 3-methyl- {β-methylvaleric acid, 3-methylpentanoic acid}
105-45-3	0	1	0	Butanoic acid, 3-oxo-, methyl ester {methyl acetoacetate}
105-53-3	0	1	0	Propanedioic acid, diethyl ester
105-54-4	1	1	1	Butanoic acid, ethyl ester {ethyl butyrate}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
105-67-9	1	1	1	Phenol, 2,4-dimethyl- {2,4-xylenol}
105-68-0	0	1	0	Propanoic acid, 3-methylbutyl ester
105-86-2	0	1	0	Formic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl formate}
105-87-3	0	1	0	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl, (*E*)- ester {geranyl acetate}
106-02-5	0	1	0	Oxacyclohexadecan-2-one {ω-pentadecalactone, Exaltolide}
106-21-8	1	1	1	1-Octanol, 3,7-dimethyl-
106-22-9	1	1	1	6-Octen-1-ol, 3,7-dimethyl- {*dl*-citronellol}
106-23-0	1	1	1	6-Octenal, 3,7-dimethyl- {citronellal}
106-24-1	1	1	1	2,6-Octadien-1-ol, 3,7-dimethyl-, (*E*)- {geraniol}
106-25-2	1	1	1	2,6-Octadien-1-ol, 3,7-dimethyl-, (*Z*)- {nerol}
106-26-3	1	0	0	2,6-Octadienal, 3,7-dimethyl-
106-27-4	0	1	0	Butanoic acid, 3-methylbutyl ester
106-29-6	0	1	0	Butanoic acid, 3,7-dimethyl-2,6-octadien-1-yl ester {geranyl butyrate}
106-30-9	0	1	0	Heptanoic acid, ethyl ester
106-32-1	1	1	1	Octanoic acid, ethyl ester {ethyl caprylate}
106-33-2	0	1	0	Dodecanoic acid, ethyl ester {ethyl laurate}
106-34-3	1	0	0	2,5-Cyclohexadiene-1,4-dione, compd. with 1,4-benzenediol (1:1)
106-35-4	1	0	0	3-Heptanone {ethyl butyl ketone}
106-40-1	1	0	0	Benzenamine, 4-bromo-
106-42-3	1	1	1	Benzene, 1,4-dimethyl- {*p*-xylene}
106-44-5	1	1	1	Phenol, 4-methyl- {*p*-cresol}
106-46-7	1	0	0	Benzene, 1,4-dichloro-
106-47-8	1	0	0	Benzenamine, 4-chloro-
106-49-0	1	0	0	Benzenamine, 4-methyl- {*p*-toluidine, 4-toluidine}
106-50-3	1	0	0	1,4-Benzenediamine
106-51-4	1	0	0	2,5-Cyclohexadiene-1,4-dione {*p*-benzoquinone}
106-55-8	1	0	0	Piperazine, 2,5-dimethyl-
106-57-0	1	0	0	2,5-Piperazinedione
106-58-1	1	0	0	Piperazine, 1,4-dimethyl-
106-60-5	0	1	0	Pentanoic acid, 5-amino-4-oxo-
106-61-6	1	1	1	1,2,3-Propanetriol, monoacetate {monoacetin}
26446-35-5				
106-65-0	1	1	1	Butanedioic acid, dimethyl ester {dimethyl succinate}
106-68-3	0	1	0	3-Octanone {ethyl amyl ketone}
106-69-4	1	0	0	1,2,6-Hexanetriol
106-70-7	0	1	0	Hexanoic acid, methyl ester
106-73-0	0	1	0	Heptanoic acid, methyl ester
106-89-8	0	1	0	Oxirane, (chloromethyl)-
106-93-4	0	1	0	Ethane, 1,2-dibromo- {ethylene dibromide, EDB®, Bromofume®}
106-97-8	1	0	0	Butane
106-98-9	1	0	0	1-Butene
9003-28-5				
106-99-0	1	0	0	1,3-Butadiene
107-00-6	1	0	0	1-Butyne
107-01-7	1	0	0	2-Butene
107-02-8	1	1	1	2-Propenal {acrolein}
107-03-9	1	0	0	1-Propanethiol {propyl mercaptan}
107-06-2	1	0	0	Ethane, 1,2-dichloro-
107-07-3	1	1	1	Ethanol, 2-chloro- {chlorohydrin}
107-10-8	1	1	1	1-Propanamine
107-11-9	1	0	0	2-Propen-1-amine {allyl amine, acrylamine}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
107-12-0	1	1	1	Propanenitrile
107-13-1	1	0	0	2-Propenenitrile {acrylonitrile}
107-16-4	1	0	0	Acetonitrile, hydroxy-
107-18-6	1	1	1	2-Propen-1-ol {allyl alcohol}
107-21-1	1	1	1	1,2-Ethanediol {ethylene glycol}
107-22-2	1	1	1	Ethanedial {glyoxal}
107-31-3	1	1	1	Formic acid, methyl ester {methyl formate}
107-35-7	0	1	0	Ethanesulfonic acid, 2-amino- {taurine}
107-41-5	1	1	1	2,4-Pentanediol, 2-methyl-
107-43-7	0	1	0	Methanaminium, 1-carboxy-*N,N,N*-trimethyl-, inner salt {betaine}
107-49-3	0	1	0	Pyrophosphoric acid, tetraethyl ester {TEPP}
107-75-5	0	1	0	Octanal, 3,7-dimethyl-7-hydroxy- {hydroxycitronellal}
107-83-5	1	1	1	Pentane, 2-methyl-
107-85-7	1	1	1	1-Butanamine, 3-methyl-
107-86-8	1	0	0	2-Butenal, 3-methyl- {senecialdehyde}
107-87-9	1	1	1	2-Pentanone
107-88-0	1	1	1	1,3-Butanediol {1,3-butylene glycol}
107-89-1	1	0	0	Butanal, 3-hydroxy- {aldol}
107-91-5	1	0	0	Acetamide, 2-cyano-
107-92-6	1	1	1	Butanoic acid {butyric acid}
107-93-7	1	1	1	2-Butenoic acid, (*E*)- {*trans*-crotonic acid}
107-95-9	1	1	1	β-Alanine
107-98-2	0	1	0	2-Propanol, 1-methoxy-
108-01-0	1	0	0	Ethanol, 2-(dimethylamino)-
108-03-2	1	0	0	Propane, 1-nitro-
108-05-4	1	0	0	Acetic acid, ethenyl ester {vinyl acetate}
108-08-7	1	0	0	Pentane, 2,4-dimethyl-
108-10-1	1	1	1	2-Pentanone, 4-methyl-
108-11-2	1	1	1	2-Pentanol, 4-methyl-
108-18-9	1	0	0	2-Propanamine, *N*-(1-methylethyl)-
108-21-4	1	1	1	Acetic acid, 1-methylethyl ester
108-24-7	1	0	0	Acetic acid, anhydride
108-27-0	1	0	0	2-Pyrrolidinone, 5-methyl-
108-28-1	1	1	1	2(5*H*)-Furanone, 5-methylene- {protoanemonin}
108-29-2	1	1	1	2(3*H*)-Furanone, dihydro-5-methyl- {α-angelica lactone, γ-valerolactone}
108-30-5	1	1	1	2,5-Furandione, dihydro- {succinic anhydride}
108-31-6	1	1	1	2,5-Furandione {maleic anhydride}
108-32-7	1	1	1	1,3-Dioxalan-2-one, 4-methyl- {1,2-propylene glycol carbonate}
108-38-3	1	1	1	Benzene, 1,3-dimethyl- {*m*-xylene}
108-39-4	1	1	1	Phenol, 3-methyl- {*m*-cresol}
108-43-0	1	0	0	Phenol, 3-chloro-
108-44-1	1	0	0	Benzenamine, 3-methyl- {*m*-toluidine 3-toluidine}
108-46-3	1	1	1	1,3-Benzenediol {resorcinol}
108-47-4	1	1	1	Pyridine, 2,4-dimethyl- {2,4-lutidine}
108-48-5	1	1	1	Pyridine, 2,6-dimethyl- {2,6-lutidine}
108-50-9	1	1	1	Pyrazine, 2,6-dimethyl-
108-59-8	0	1	0	Propanedioic acid, dimethyl ester
108-61-2	1	0	0	1-Propanol, 2,2′-oxybis-
108-64-5	1	1	1	Butanoic acid, 3-methyl-, ethyl ester {ethyl isovalerate}
108-67-8	1	1	1	Benzene, 1,3,5-trimethyl- {mesitylene}
108-68-9	1	1	1	Phenol, 3,5-dimethyl- {3,5-xylenol}
108-69-0	1	1	1	Benzenamine, 3,5-dimethyl- {3,5-xylidine}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
108-75-8	1	1	1	Pyridine, 2,4,6-trimethyl- {2,4,6-collidine}
108-83-8	1	0	0	4-Heptanone, 2,6-dimethyl-
108-87-2	1	0	0	Cyclohexane, methyl-
108-88-3	1	1	1	Benzene, methyl- {toluene}
108-89-4	1	1	1	Pyridine, 4-methyl- {4-picoline}
108-90-7	1	0	0	Benzene, chloro-
108-93-0	1	0	0	Cyclohexanol
108-94-1	1	0	0	Cyclohexanone
108-95-2	1	1	1	Phenol
108-96-3	1	0	0	4-Pyridinol {4(1*H*)-pyridinone}
626-64-2				
108-97-4	1	0	0	4*H*-Pyran-4-one
108-98-5	1	0	0	Benzenethiol {phenyl mercaptan}
108-99-6	1	1	1	Pyridine, 3-methyl- {3-picoline}
109-00-2	1	1	1	3-Pyridinol
52536-09-1				
58064-43-0				
109-01-3	1	0	0	Piperazine, 1-methyl-
109-05-7	1	0	0	Piperidine, 2-methyl-
109-06-8	1	1	1	Pyridine, 2-methyl- {2-picoline}
109-07-9	1	0	0	Piperazine, 2-methyl-
109-08-0	1	1	1	Pyrazine, methyl- = pyrazine, 2-methyl-
109-15-9	0	1	0	Propanoic acid, 2-methyl-, octyl ester
109-19-3	0	1	0	Butanoic acid, 3-methyl-, butyl ester
109-21-7	0	1	0	Butanoic acid, butyl ester
109-42-2	0	1	0	10-Undecenoic acid, butyl ester
109-49-9	1	1	1	5-Hexen-2-one
109-52-4	1	1	1	Pentanoic acid {valeric acid}
109-60-4	0	1	0	Acetic acid, propyl ester {propyl acetate}
109-66-0	1	1	1	Pentane
109-67-1	1	0	0	1-Pentene
109-68-2	1	1	1	2-Pentene
109-73-9	1	1	1	1-Butanamine
109-74-0	1	0	0	Butanenitrile
109-75-1	1	0	0	3-Butenenitrile {allyl cyanide}
109-79-5	1	0	0	1-Butanethiol {butyl mercaptan}
109-83-1	0	1	0	Ethanol, 2-(methylamino)-
109-86-4	1	1	1	Ethanol, 2-methoxy-
109-89-7	1	1	1	Ethanamine, *N*-ethyl- {diethylamine}
109-94-4	1	0	0	Formic acid, ethyl ester
109-95-5	1	0	0	Nitrous acid, ethyl ester
109-96-6	1	1	1	1*H*-Pyrrole, 2,5-dihydro- {3-pyrroline}
109-97-7	1	1	1	1*H*-Pyrrole {azole}
109-99-9	1	1	1	Furan, tetrahydro-
110-00-9	1	0	0	Furan
110-02-1	1	1	1	Thiophene
110-12-3	1	0	0	2-Hexanone, 5-methyl-
110-13-4	1	1	1	2,5-Hexanedione {acetonylacetone}
110-14-5	1	0	0	Butanediamide {succinamide}
110-15-6	1	1	1	Butanedioic acid {succinic acid}
110-16-7	1	1	1	2-Butenedioic acid (*Z*)- {maleic acid}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
110-17-8	1	1	1	2-Butenedioic acid (*E*)- {fumaric acid}
110-19-0	0	1	0	Acetic acid, 2-methylpropyl ester {isobutyl acetate}
110-27-0	0	1	0	Tetradecanoic acid, 1-methylethyl ester
110-36-1	1	0	0	Tetradecanoic acid, butyl ester
110-38-3	1	1	1	Decanoic acid, ethyl ester {ethyl caprate}
110-40-7	0	1	0	Decanedioic acid, diethyl ester
110-42-9	0	1	0	Decanoic acid, methyl ester
110-43-0	1	1	1	2-Heptanone {methyl pentyl ketone}
110-44-1	1	1	1	2,4-Hexadienoic acid, (*E,E*)- {sorbic acid}
22500-92-1				
110-45-2	0	1	0	Formic acid, 3-methylbutyl ester
110-54-3	1	1	1	Hexane
110-58-7	1	1	1	1-Pentanamine
110-59-8	1	0	0	Pentanenitrile {valeronitrile}
110-60-1	0	1	0	1,4-Butanediamine {putrescine}
110-61-2	1	0	0	Butanedinitrile {succinonitrile}
110-62-3	1	1	1	Pentanal {valeraldehyde}
110-63-4	0	1	0	1,4-Butanediol {tetramethylene glycol}
110-66-7	1	0	0	1-Pentanethiol
110-68-9	1	1	1	1-Butanamine, *N*-methyl-
110-74-7	0	1	0	Formic acid, propyl ester
110-80-5	1	1	1	Ethanol, 2-ethoxy-
110-81-6	1	0	0	Disulfide, diethyl
110-82-7	1	1	1	Cyclohexane
110-83-8	1	0	0	Cyclohexene
110-86-1	1	1	1	Pyridine
110-87-2	1	1	1	2*H*-Pyran, 3,4-dihydro-
110-89-4	1	1	1	Piperidine {azacyclohexane}
110-91-8	0	1	0	Morpholine
110-93-0	1	1	1	5-Hepten-2-one, 6-methyl-
110-94-1	1	1	1	Pentanedioic acid {glutaric acid}
110-98-5	1	0	0	2-Propanol, 1,1′-oxybis-
111-02-4	1	1	1	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-*E*)- {squalene}
111-06-8	1	0	0	Hexadecanoic acid, butyl ester
111-11-5	0	1	0	Octanoic acid, methyl ester {methyl caprylate}
111-12-6	0	1	0	2-Octynoic acid, methyl ester
111-13-7	1	1	1	2-Octanone {hexyl methyl ketone}
111-14-8	1	1	1	Heptanoic acid {enanthic acid}
111-16-0	1	0	0	Heptanedioic acid {pimelic acid}
111-20-6	1	1	1	Decanedioic acid
111-21-7	1	1	1	Ethanol, 2,2′-[1,2-ethanediylbis(oxy)]bis-, diacetate
111-26-2	1	1	1	1-Hexanamine
111-27-3	1	1	1	1-Hexanol {caproyl alcohol}
111-31-9	1	0	0	1-Hexanethiol
111-42-2	1	1	1	Ethanol, 2,2′-iminobis- {diethanolamine}
111-43-3	1	0	0	Propane, 1,1′-oxybis- {dipropyl ether}
111-46-6	1	1	1	Ethanol, 2,2′-oxybis- {diethylene glycol}
111-47-7	1	0	0	Propane, 1,1′-thiobis- {dipropyl sulfide}
111-55-7	1	0	0	1,2-Ethanediol, diacetate
111-61-5	1	1	1	Octadecanoic acid, ethyl ester {ethyl stearate}
111-62-6	1	1	1	9-Octadecenoic acid (*Z*)-, ethyl ester {ethyl oleate}
111-65-9	1	1	1	Octane

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
111-66-0	1	0	0	1-Octene {caprylene}
111-67-1	1	0	0	2-Octene
111-68-2	1	1	1	Heptanamine
111-70-6	1	1	1	1-Heptanol
111-71-7	1	0	0	Heptanal
111-79-5	0	1	0	2-Nonenoic acid, methyl ester
111-82-0	1	1	1	Dodecanoic acid, methyl ester
111-84-2	1	1	1	Nonane
111-86-4	1	1	1	1-Octanamine
111-87-5	1	1	1	1-Octanol {caprylic alcohol}
111-92-2	1	1	1	1-Butanamine, *N*-butyl-
111-97-7	1	0	0	Propanenitrile, 3,3′-thiobis-
112-05-0	1	1	1	Nonanoic acid {pelargonic acid}
112-06-1	0	1	0	Acetic acid, heptyl ester
112-12-9	1	1	1	2-Undecanone {methyl nonyl ketone}
112-14-1	0	1	0	Acetic acid, octyl ester
112-18-5	1	0	0	Dodecanamine, *N*,*N*-dimethyl-
112-27-6	1	1	1	Ethanol, 2,2′-(1,2-ethanediylbis(oxy))bis- {triethylene glycol}
112-30-1	1	1	1	1-Decanol {capric alcohol}
112-31-2	1	1	1	Decanal {capraldehyde}
112-37-8	1	1	1	Undecanoic acid
112-38-9	0	1	0	10-Undecenoic acid
112-39-0	1	1	1	Hexadecanoic acid, methyl ester
112-40-3	1	1	1	Dodecane
112-41-4	1	0	0	1-Dodecene
112-42-5	1	1	1	1-Undecanol
112-44-7	1	1	1	Undecanal
112-45-8	0	1	0	10-Undecenal
112-53-8	1	1	1	1-Dodecanol {lauryl alcohol}
112-54-9	0	1	0	Dodecanal
112-60-7	0	1	0	Ethanol, 2,2′-[oxybis(2,1-ethanediyloxy)]bis- {tetraethylene glycol}
112-61-8	1	1	1	Octadecanoic acid, methyl ester
112-62-9	1	1	1	9-Octadecenoic acid (*Z*)-, methyl ester
112-63-0	1	1	1	9,12-Octadecadienoic acid (*Z*,*Z*)-, methyl ester {methyl linoleate}
112-66-3	0	1	0	Acetic acid, dodecyl ester
112-70-9	1	1	1	1-Tridecanol
112-72-1	1	1	1	1-Tetradecanol
112-79-8	1	1	1	Octadecenoic acid, (*E*)- {elaidic acid}
112-80-1	1	1	1	9-Octadecenoic acid (*Z*)- {oleic acid}
112-85-6	1	1	1	Docosanoic acid {behenic acid}
112-86-7	0	1	0	13-Docosenoic acid, (*Z*)-
112-88-9	1	0	0	1-Octadecene
112-92-5	1	1	1	1-Octadecanol {stearyl alcohol}
112-95-8	1	1	1	Eicosane
113-48-4	0	1	0	4,7-Methano-1*H*-isoindole-1,3(2*H*)-dione, 2-(2-ethylhexyl)-3a,4,7,7a-tetrahydro-
114-26-1	0	1	0	Phenol, 2-(1-methylethoxy)-, methylcarbamate {Undene®, Propoxur®}
114-33-0	1	1	1	3-Pyridinecarboxamide, *N*-methyl-
114-91-0	1	0	0	Pyridine, 2-(2-methoxyethyl)-
115-07-1	1	0	0	1-Propene
115-10-6	1	1	1	Methane, oxybis- {dimethyl ether}
115-11-7	1	0	0	1-Propene, 2-methyl- {isobutylene}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
115-18-4	1	0	0	3-Buten-2-ol, 2-methyl-
115-26-4	0	1	0	Phosphine oxide, bis(dimethylamino)fluoro- {Dimefox®}
115-29-7	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide {Thiodan®, Thiosulfan®, Endosulfan®}
115-32-2	0	1	0	Ethanol, 2,2,2-trichloro-1,1-bis(4-chlorophenyl)- {Dicofol®}
115-90-2	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylsulfinyl)phenyl] ester {Fensulfothion®}
115-95-7	0	1	0	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate {linalyl acetate}
115-99-1	0	1	0	1,6-Octadien-3-ol, 3,7-dimethyl-, formate {linalyl formate}
116-06-3	0	1	0	Propanal, 2-methyl-2-(methylthio)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb®}
116-09-6	1	1	1	2-Propanone, 1-hydroxy- {acetol}
116-26-7	0	1	0	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl- {safranal}
116-29-0	0	1	0	Benzene, 1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)- {Tetradifon®}
116-53-0	1	1	1	Butanoic acid, 2-methyl- {2-methylbutyric acid}
117-12-4	1	0	0	9,10-Anthracenedione, 1,5-dihydroxy-
117-39-5	1	1	1	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- {quercetin}
117-80-6	0	1	0	1,4-Naphthalenedione, 2,3-dichloro- {Diclone®}
117-81-7	1	1	1	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
117-84-0	1	1	1	1,2-Benzenedicarboxylic acid, dioctyl ester
118-58-1	0	1	0	Benzoic acid, 2-hydroxy-, phenylmethyl ester {benzyl salicylate}
118-61-6	0	1	0	Benzoic acid, 2-hydroxy-, ethyl ester {ethyl salicylate}
118-71-8	1	1	1	4*H*-Pyran-4-one, 3-hydroxy-2-methyl- {maltol}
118-74-1	0	1	0	Benzene, hexachloro-
118-79-6	0	1	0	Phenol, 2,4,6-tribromo-
118-90-1	1	1	1	Benzoic acid, 2-methyl- {*o*-toluic acid}
118-92-3	0	1	0	Benzoic acid, 2-amino-
118-93-4	1	1	1	Ethanone, 1-(2-hydroxyphenyl)-
119-33-5	1	0	0	Phenol, 4-methyl-2-nitro-
119-36-8	1	1	1	Benzoic acid, 2-hydroxy-, methyl ester {methyl salicylate}
119-53-9	0	1	0	Ethanone, 1,2-diphenyl-2-hydroxy
119-61-9	1	1	1	Methanone, diphenyl- {benzophenone}
119-64-2	1	1	1	Naphthalene, 1,2,3,4-tetrahydro- {tetralin}
119-65-3	1	1	1	Isoquinoline
119-84-6	1	1	1	2*H*-1-Benzopyran-2-one, 3,4-dihydro- {dihydrocoumarin}
120-12-7	1	1	1	Anthracene
120-14-9	1	1	1	Benzaldehyde, 3,4-dimethoxy- {veratraldehyde}
120-51-4	1	1	1	Benzoic acid, phenylmethyl ester {benzyl benzoate}
120-57-0	1	1	1	1,3-Benzodioxole-5-carboxaldehyde {piperonal, heliotropin}
120-72-9	1	1	1	1*H*-Indole {2,3-benzopyrrole}
120-73-0	0	1	0	1*H*-Purine
120-78-5	0	1	0	Benzothiazole, 2,2′-dithiobis- {Thiofide®}
120-80-9	1	1	1	1,2-Benzenediol {catechol, pyrocatechol}
120-92-3	1	1	1	Cyclopentanone {adipic ketone}
120-94-5	1	1	1	Pyrrolidine, 1-methyl-
121-20-0	0	1	0	Pyrethrins (natural)
121-21-1	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {Pyrethrin I®}
121-21-9	0	1	0	Pyrethrins (natural)
121-29-9	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester {Pyrethrin II®}
121-32-4	1	1	1	Benzaldehyde, 3-ethoxy-4-hydroxy- {ethylvanillin}
121-33-5	1	1	1	Benzaldehyde, 4-hydroxy-3-methoxy- {vanillin}
121-34-6	1	1	1	Benzoic acid, 4-hydroxy-3-methoxy- {vanillic acid}
121-44-8	1	1	1	Ethanamine, *N,N*-diethyl- {triethylamine}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
121-46-0	0	1	0	Bicyclo[2.2.1]hepta-2,5-diene {norbornadiene}
121-69-7	1	0	0	Benzenamine, *N*,*N*-dimethyl-
121-71-1	1	0	0	Ethanone, 1-(3-hydroxyphenyl)-
121-75-5	1	1	1	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester {Malathion®}
121-79-9	1	1	1	Benzoic acid, 3,4,5-trihydroxy-, propyl ester {propyl gallate}
121-91-5	1	0	0	1,3-Benzenedicarboxylic acid {isophthalic acid}
121-98-2	0	1	0	Benzoic acid, 4-methoxy-, methyl ester {methyl anisate}
122-00-9	1	1	1	Ethanone, 1-(4-methylphenyl)- {4-methylacetophenone}
122-03-2	1	1	1	Benzaldehyde, 4-(1-methylethyl)- {cuminaldehyde}
122-14-5	0	1	0	Phosphorothioic acid, *O*,*O*-dimethyl *O*-(3-methyl-4-nitrophenyl) ester {Fenitrothion®}
122-32-7	0	1	0	1,2,3-Propanetriol, tri-9-octadecenoate {triolein}
122-39-4	1	0	0	Benzenamine, *N*-phenyl- {diphenylamine}
122-40-7	0	1	0	2-Propenal, 3-phenyl-, α-pentyl-
122-43-0	0	1	0	Benzeneacetic acid, butyl ester
122-45-2	0	1	0	Benzeneacetic acid, octyl ester
122-57-6	1	1	1	3-Buten-2-one, 4-phenyl-
122-63-4	0	1	0	Propanoic acid, phenylmethyl ester {benzyl propionate}
122-67-8	0	1	0	2-Propenoic acid, 3-phenyl-, 2-methylpropyl ester
122-68-9	0	1	0	2-Propenoic acid, 3-phenyl-, 3-phenylpropyl ester {3-phenylpropyl cinnamate}
122-69-0	1	1	1	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester {cinnamyl cinnamate}
122-72-5	0	1	0	Acetic acid, phenylpropyl ester
122-78-1	1	1	1	Benzeneacetaldehyde {phenylacetaldehyde}
122-84-9	0	1	0	2-Propanone, 1-(4-methoxyphenyl)-
122-91-8	0	1	0	Benzenemethanol, 4-methoxy-, formate
122-97-4	1	1	1	Benzenepropanol {3-phenyl-1-propanol}
122-99-6	0	1	0	Ethanol, 2-phenoxy-
123-07-9	1	1	1	Phenol, 4-ethyl- {*p*-ethylphenol}
123-08-0	1	1	1	Benzaldehyde, 4-hydroxy-
123-11-5	1	1	1	Benzaldehyde, 4-methoxy- {*p*-anisaldehyde}
123-15-9	1	0	0	Pentanal, 2-methyl-
123-18-2	1	0	0	4-Nonanone, 2,6,8-trimethyl
123-19-3	1	1	1	4-Heptanone {butyrone, dipropyl ketone}
123-29-5	0	1	0	Nonanoic acid, ethyl ester
123-31-9	1	1	1	1,4-Benzenediol {hydroquinone}
123-32-0	1	1	1	Pyrazine, 2,5-dimethyl-
123-33-1	1	1	1	3,6-Pyridazinedione, 1,2-dihydro- {maleic hydrazide, MH, MH-30®}
123-35-3	1	1	1	1,6-Octadiene, 7-methyl-3-methylene- {myrcene}
123-38-6	1	1	1	Propanal {propionaldehyde}
123-39-7	1	0	0	Formamide, *N*-methyl-
123-41-1	0	1	0	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl- [2 CAS Nos.] {choline}
62-49-7				
123-42-2	1	1	1	2-Pentanone, 4-hydroxy-4-methyl- {diacetone alcohol}
123-51-3	1	1	1	1-Butanol, 3-methyl- {isoamyl alcohol}
123-54-6	1	1	1	2,4-Pentanedione
123-56-8	1	1	1	2,5-Pyrrolidinedione {succinimide}
123-63-7	1	0	0	1,3,5-Trioxane, 2,4,6-trimethyl- {paraldehyde, acetaldehyde trimer}
123-66-0	1	1	1	Hexanoic acid, ethyl ester {ethyl caproate}
123-68-2	1	1	1	Hexanoic acid, 2-propenyl ester
123-69-3	1	0	0	Oxacycloheptadec-8-en-2-one, (*Z*)- {ambrettolide}
123-72-8	1	1	1	Butanal {butyraldehyde}
123-73-9	1	1	1	2-Butenal (*E*)

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
123-75-1	1	1	1	Pyrrolidine
123-76-2	1	1	1	Pentanoic acid, 4-oxo- {levulinic acid}
123-79-5	1	0	0	Hexanedioic acid, dioctyl ester
123-86-4	1	1	1	Acetic acid, butyl ester {butyl acetate}
123-91-1	1	0	0	1,4-Dioxane
123-92-2	0	1	0	Acetic acid, 3-methylbutyl ester
123-96-6	1	0	0	2-Octanol
4128-31-8				
123-99-9	1	1	1	Nonanedioic acid {azelaic acid}
124-04-9	1	1	1	Hexanedioic acid {adipic acid}
124-06-1	0	1	0	Tetradecanoic acid, ethyl ester {ethyl myristate}
124-07-2	1	1	1	Octanoic acid {caprylic acid}
124-10-7	1	1	1	Tetradecanoic acid, methyl ester
124-11-8	1	0	0	1-Nonene
124-12-9	1	0	0	Octanenitrile
124-13-0	1	1	1	Octanal
124-18-5	1	1	1	Decane
124-19-6	1	1	1	Nonanal {pelargonaldehyde}
124-20-9	0	1	0	1,4-Butanediamine, *N*-(3-aminopropyl)- {spermidine}
124-25-4	1	1	1	Tetradecanal {myristaldehyde}
124-29-8	1	1	1	1-Hexadecanol [2 CAS Nos.]
36653-82-4				
124-38-9	1	1	1	Carbon dioxide
124-40-3	1	1	1	Methanamine, *N*-methyl- {dimethylamine}
124-76-5	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *exo*- {isoborneol}
125-12-2	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate {isobornyl acetate}
125-51-5	0	1	0	3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-isomethylionone}
125-67-7	0	1	0	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, potassium salt {gibberellic acid, potassium salt}
126-14-7	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, octaacetate
126-29-4	0	1	0	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S)- {violaxanthin}
126-30-7	1	0	0	1,3-Propanediol, 2,2-dimethyl-
126-33-0	1	0	0	Thiophene, tetrahydro-, 1,1-dioxide {Sulfolan®}
126-64-7	0	1	0	Benzoic acid, 3,7-dimethyl-1,6-octadien-6-yl ester {linalyl benzoate}
126-81-8	0	1	0	1,3-Cyclohexanedione, 5,5-dimethyl-
126-91-0	1	1	1	1,6-Octadien-3-ol, 3,7-dimethyl- {*l*-linalool}
126-98-7	1	0	0	2-Propenenitrile, 2-methyl- {methacrylonitrile}
127-00-4	1	0	0	2-Propanol, 1-chloro-
127-06-0	1	0	0	2-Propanone, oxime {acetone oxime}
127-08-2	0	1	0	Acetic acid, potassium salt
127-09-3	0	1	0	Acetic acid, sodium salt
127-17-3	1	1	1	Propanoic acid, 2-oxo- {pyruvic acid}
127-18-4	1	0	0	Ethene, tetrachloro-
127-19-5	1	1	1	Acetamide, *N,N*-dimethyl
127-40-2	0	1	0	β,ε-Carotene-3,3′-diol, (3R,3′R,6′R)- {xanthophyll, lutein}
127-41-3	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- [3 CAS Nos.] {α-ionone}
6901-97-9				
8013-90-9				
127-42-4	0	1	0	4-Penten-3-one, 5-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {methyl-α-ionone}
127-51-5	0	1	0	3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-isomethylionone}
127-91-3	1	1	1	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- [2 CAS Nos.] {β-pinene}
18172-67-3				

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
128-37-0	1	1	1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl- {BHT}
128-53-0	1	0	0	1*H*-Pyrrole-2,5-dione, 1-ethyl-
129-00-0	1	1	1	Pyrene {benzo[*def*]phenanthrene}
130-15-4	1	0	0	1,4-Naphthalenedione {1,4-naphthoquinone}
131-11-3	1	1	1	1,2-Benzenedicarboxylic acid, dimethyl ester {dimethyl phthalate}
131-16-8	1	1	1	1,2-Benzenedicarboxylic acid, dipropyl ester
131-20-4	1	1	1	1,2-Benzenedicarboxylic acid, bis(6-methylheptyl) ester [2 CAS Nos.] {diisooctyl phthalate}
27554-26-3				
132-64-9	1	1	1	Dibenzofuran {2,2′-biphenylene oxide}
132-65-0	1	1	1	Dibenzothiophene
132-75-2	1	0	0	1-Naphthaleneacetonitrile
133-06-2	1	1	1	1*H*-Isoindole-1,3(2*H*)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]- {Captan®}
133-07-3	0	1	0	1*H*-Isoindole-1,3(2*H*)-dione, 2-[(trichloromethyl)thio]- {Folpan®}
133-32-4	0	1	0	1*H*-Indole-3-butanoic acid
133-37-9	0	1	0	Butanedioic acid, 2,3-dihydroxy- {*dl*-tartaric acid}
133-89-1	0	1	0	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-glucopyranosyl ester
133-99-3	0	1	0	β-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {β-maltose}
134-20-3	0	1	0	Benzoic acid, 2-amino-, methyl ester {methyl anthranilate}
134-32-7	1	0	0	1-Naphthalenamine {naphthalene, 1-amino-, α-naphthylamine}
134-81-6	1	0	0	Ethanedione, diphenyl- {benzil}
134-96-3	1	1	1	Benzaldehyde, 3,5-dimethoxy-4-hydroxy- {syringaldehyde}
135-01-3	1	0	0	Benzene, 1,2-diethyl-
135-02-4	1	0	0	Benzaldehyde, 2-methoxy-
135-19-3	1	1	1	2-Naphthalenol {2-naphthol = β-naphthol}
135-48-8	1	0	0	Pentacene {benzo[*b*]naphthacene}
135-77-3	1	0	0	Benzene, 1,2,4-trimethoxy-
135-88-6	1	1	1	2-Naphthalenamine, *N*-phenyl-
136-60-7	1	0	0	Benzoic acid, butyl ester
137-00-8	0	1	0	Thiazole, 4-methyl-5-(2′-hydroxyethyl)-
137-08-8	0	1	0	β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (R)- [2 CAS Nos.] {pantothenic acid}
79-83-4				
137-18-8	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,5-dimethyl-
137-26-8	0	1	0	Thioformamide, 1,1′-dithiobis(*N*,*N*-dimethyl {Thiram®}
137-32-6	1	1	1	1-Butanol, 2-methyl-
137-40-6	0	1	0	Propanoic acid, sodium salt
137-42-8	0	1	0	Carbamic acid, *N*-methyldithio-, monosodium salt {Metham-sodium®}
138-08-9	0	1	0	2-Propenoic acid, 2-(phosphonooxy)-
138-22-7	1	0	0	Propanoic acid, 2-hydroxy-, butyl ester {butyl lactate}
138-52-3	0	1	0	β-*D*-Glucopyranoside, 2-(hydroxymethyl)phenyl-
138-59-0	0	1	0	1-Cyclohexene-1-carboxylic acid, 3,4,5-trihydroxy-, [3R-(3α,4α,5β)]- {shikimic acid}
138-86-3	1	1	1	Cyclohexene, 1-methyl-4-(1-methylethenyl)- {limonene, *p*-mentha-1,8-diene}
139-45-7	1	0	0	1,2,3-Propanetriol, tripropanoate
139-85-5	1	1	1	Benzaldehyde, 3,4-dihydroxy- {protocatechualdehyde}
140-10-3	1	1	1	2-Propenoic acid, 3-phenyl-, (*E*)- {*trans*-cinnamic acid}
140-11-4	1	1	1	Acetic acid, phenylmethyl ester {benzyl acetate}
140-26-1	1	1	1	Butanoic acid, 3-methyl-, 2-phenylethyl ester {phenethyl isovalerate}
140-27-2	1	1	1	Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester
140-29-4	1	1	1	Benzeneacetonitrile {benzyl cyanide}
140-56-7	0	1	0	Benzenediazosulfonate, dimethylamino-, sodium salt {Fenaminosulf®}
140-67-0	1	0	0	Benzene, 1-methoxy-4-(2-propenyl)- {estragole}
140-76-1	1	0	0	Pyridine, 5-ethenyl-2-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
141-05-9	1	0	0	2-Butenedioic acid (*Z*)-, diethyl ester {diethyl maleate}
141-10-6	1	1	1	3,5,9-Undecatrien-2-one, 6,10-dimethyl- {pseudoionone}
141-12-8	0	1	0	Acetic acid, 3,7-dimethyl-2,6-octadien-1-yl, (*Z*)- ester {neryl acetate}
141-16-2	0	1	0	Butanoic acid, 3,7-dimethyl-6-octenyl ester {citronellyl butyrate}
141-25-3	0	1	0	7-Octen-1-ol, 3,7-dimethyl- [2 CAS Nos.] {rhodinol}
6812-78-8				
141-27-5	1	1	1	2,6-Octadienal, 3,7-dimethyl- {citral}
5392-40-5				
141-43-5	0	1	0	Ethanol, 2-amino- {ethanolamine}
141-46-8	1	0	0	Acetaldehyde, hydroxy- {glycolaldehyde}
141-66-2	0	1	0	Phosphoric acid, 3-(dimethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Dicrotophos®}
141-78-6	1	1	1	Acetic acid, ethyl ester {ethyl acetate}
141-79-7	1	1	1	3-Penten-2-one, 4-methyl- {mesityl oxide}
141-82-2	1	1	1	Propanedioic acid {malonic acid}
141-93-5	1	0	0	Benzene, 1,3-diethyl-
141-97-9	0	1	0	Butanoic acid, 3-oxo-, ethyl ester
142-08-5	1	1	1	2-Pyridinol {2(1*H*)-pyridinone}
72762-00-6				
142-10-9	0	1	0	Propanal, 2,3-dihydroxy-, 3-phosphate
142-28-9	0	1	0	Propane, 1,3-dichloro-
142-29-0	1	0	0	Cyclopentene
142-50-7	0	1	0	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, [S-(*Z*)]-
142-62-1	1	1	1	Hexanoic acid {caproic acid}
142-68-7	1	1	1	2*H*-Pyran, tetrahydro-
142-72-3	0	1	0	Acetic acid, magnesium salt
142-82-5	1	0	0	Heptane
142-83-6	1	1	1	2,4-Hexadienal, (*E,E*)-
142-84-7	1	1	1	1-Propanamine, *N*-propyl-
142-91-6	1	1	1	Hexadecanoic acid, (1-methylethyl) ester
142-92-7	0	1	0	Acetic acid, hexyl ester {hexyl acetate}
143-07-7	1	1	1	Dodecanoic acid {lauric acid}
143-08-8	1	1	1	1-Nonanol
143-13-5	0	1	0	Acetic acid, nonyl ester
144-55-8	0	1	0	Carbonic acid, monosodium salt
144-62-7	1	1	1	Ethanedioic acid {oxalic acid}
144-68-3	0	1	0	β,β-Carotene-3,3′-diol, (3R,3′R)- {zeaxanthin}
145-13-1	0	1	0	Pregn-5-en-20-one, 3-hydroxy-, (3β)-
146-17-8	0	1	0	Riboflavin 5′-(dihydrogen phosphate)
147-71-7	0	1	0	Butanedioic acid, 2,3-dihydroxy- {*d*-tartaric acid}
147-73-9	0	1	0	Butanedioic acid, 2,3-dihydroxy- {meso-tartaric acid}
147-81-9	1	1	1	*DL*-Arabinose
147-85-3	1	1	1	*L*-Proline
148-03-8	1	1	1	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- {β-tocopherol}
148-24-3	1	1	1	8-Quinolinol
148-53-8	1	1	1	Benzaldehyde, 2-hydroxy-3-methoxy-
148-79-8	1	1	1	1*H*-Benzimidazole, 2-(4-thiazolyl)- {Thiabendazole®}
148-83-4	0	1	0	2*H*-1-Benzopyran-2-one, 7-hydroxy-6-(3,7-dimethyl-2,6-octadienyl)- {ostruthin}
149-32-6	1	1	1	1,2,3,4-Butanetetrol, (R*,S*)- {erythritol}
149-57-5	1	1	1	Hexanoic acid, 2-ethyl-
149-91-7	1	1	1	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}
150-19-6	1	1	1	Phenol, 3-methoxy-
150-68-5	0	1	0	Urea, 1,1-dimethyl-3-(4-chlorophenyl) {Monuron®}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
150-76-5	1	1	1	Phenol, 4-methoxy-
150-78-7	1	1	1	Benzene, 1,4-dimethoxy-
150-84-5	0	1	0	Acetic acid, 3,7-dimethyl-6-octen-1-yl ester {citronellyl acetate}
150-86-7	1	1	1	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(*E*)]]- {phytol}
150-96-9	0	1	0	Pentanoic acid, 3-hydroxy-3-methyl-
150-97-0	0	1	0	Pentanoic acid, 3,5-dihydroxy-5-methyl- {mevalonic acid}
151-05-3	0	1	0	Acetic acid, 1,1-dimethyl-2-phenylethyl ester
151-10-0	0	1	0	Benzene, 1,3-dimethoxy-
151-67-7	1	1	1	Ethane, 1,1,1-trifluoro-2-bromo-2-chloro- {Freon® 123b1, Halothane}
153-18-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl] oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {rutin}
153-78-6	1	0	0	9*H*-Fluoren-2-amine
154-17-6	0	1	0	*D*-Arabinohexose, 2-deoxy- {2-deoxy-*D*-glucose}
154-87-0	0	1	0	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, *P*,*P*′-dioxide
156-05-8	0	1	0	Benzenepropanoic acid, α-hydroxy- {phenyllactic acid}
156-06-9	0	1	0	Benzenepropanoic acid, α-oxo- {phenylpyruvic acid}
156-38-7	1	1	1	Benzeneacetic acid, 4-hydroxy-
156-39-8	1	0	0	Benzenepropanoic acid, 4-hydroxy-α-oxo-
156-62-7	0	1	0	Cyanamide, calcium salt
188-94-3	1	0	0	Diindeno[1,2,3-*cd*:1′,2′,3′-*lm*]perylene
189-01-5	1	0	0	Cyclopenta[*cd*]perylene
189-55-9	1	0	0	Benzo[*rst*]pentaphene {dibenzo[*a,i*]pyrene}
189-58-2	1	0	0	Anthra[9,1,2-*cde*]benzo[*h*]cinnoline
189-64-0	1	0	0	Dibenzo[*b,def*]chrysene {dibenzo[*a,h*]pyrene}
189-75-3	1	0	0	Dibenz[*j,mno*]aceanthrylene
190-26-1	1	0	0	Ovalene
190-99-8	1	0	0	1*H*-Naphtho[3,2,1,8-*defg*]chrysene {1,2,5,6-dibenzopyrene}
191-07-1	1	1	1	Coronene
191-24-2	1	1	1	Benzo[*ghi*]perylene
191-26-4	1	0	0	Dibenzo[*def,mno*]chrysene {anthanthrene}
191-30-0	1	0	0	Dibenzo[*def,p*]chrysene {dibenzo[*a,l*]pyrene}
191-37-7	1	0	0	Naphtho[2,1,8,7-*klmn*]xanthene
191-68-4	1	0	0	Dibenzo[*g,p*]chrysene
192-51-8	1	0	0	Dibenzo[*fg,op*]naphthacene {dibenzo[*e,l*]pyrene}
192-65-4	1	0	0	Naphtho[1,2,3,4-*def*]chrysene {dibenzo[*a,e*]pyrene}
192-97-2	1	1	1	Benzo[*e*]pyrene {B[*e*]P}
193-09-9	1	0	0	Dibenzo[*de,qr*]naphthacene {naphtho[2,3-*d*]pyrene}
193-39-5	1	1	1	Indeno[1,2,3-*cd*]pyrene {*o*-phenylenepyrene}
193-43-1	1	0	0	Indeno[1,2,3-*cd*]fluoranthene
193-54-4	1	0	0	Cyclopenta[*cd*]fluoranthene
194-03-6	1	0	0	Benzo[*lmn*]phenanthridine {thebenidine}
194-59-2	1	0	0	7*H*-Dibenzo[*c,g*]carbazole
195-19-7	1	0	0	Benzo[*c*]phenanthrene
195-84-6	1	0	0	Tricycloquinazoline
196-42-9	1	0	0	Naphtho[2,1,8-*qra*]naphthacene
197-61-5	1	0	0	Rubicene
197-70-6	1	0	0	Benzo[*b*]perylene
198-55-0	1	0	0	Perylene
199-94-0	1	0	0	7*H*-Benz[*de*]anthracene
201-06-9	1	0	0	Acephenanthrylene

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
202-03-9	1	0	0	Aceanthrylene
202-33-5	1	0	0	Benz[*j*]aceanthrylene {cholanthrylene}
202-98-2	1	0	0	4*H*-Cyclopenta[*def*]chrysene {4,5-methylenechrysene}
203-12-3	1	0	0	Benzo[*ghi*]fluoranthene
203-18-9	1	0	0	Dibenzo[*j,l*]fluoranthene
203-33-8	1	0	0	Benz[*a*]aceanthrylene {benzo[*a*]fluoranthene}
203-64-5	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene {4,5-methylenephenanthrene}
205-12-9	1	0	0	7*H*-Benzo[*c*]fluorene
205-25-4	1	0	0	7*H*-Benzo[*c*]carbazole
205-82-3	1	1	1	Benzo[*j*]fluoranthene
205-99-2	1	1	1	Benz[*e*]acephenanthrylene {benzo[*b*]fluoranthene}
206-44-0	1	1	1	Fluoranthene
206-49-5	1	0	0	Acenaphtho[1,2-b]pyridine {7-azafluoranthene}
206-56-4	1	0	0	Indeno[1,2,3-*ij*]isoquinoline {1-azafluoranthene}
207-08-9	1	1	1	Benzo[*k*]fluoranthene
207-84-1	0	1	0	7*H*-Dibenzo[*a,g*]carbazole
208-96-8	1	1	1	Acenaphthylene
211-95-0	1	0	0	Cyclopenta[*a*]phenalene
213-46-7	1	0	0	Picene {benzo[*a*]chrysene}
214-17-5	1	0	0	Benzo[*b*]chrysene {dibenzo[*b,h*]phenanthrene}
215-26-9	1	0	0	Naphtho[1,2-*b*]triphenylene {tribenz[*a,c,h*]anthracene}
215-58-7	1	0	0	Benzo[*b*]triphenylene {dibenz[*a,c*]anthracene}
216-00-2	1	0	0	Dibenzo[*a,c*]naphthacene
217-59-4	1	0	0	Triphenylene {9,10-benzophenanthrene}
218-01-9	1	1	1	Chrysene {1,2-benzophenanthrene}
219-07-8	1	0	0	15*H*-Cyclopenta[*a*]phenanthrene
219-08-9	1	0	0	17*H*-Cyclopenta[*a*]phenanthrene
219-86-3	1	0	0	7*H*-Cyclopent[*d*]acenaphthylene
220-97-3	1	0	0	11*H*-Indeno[2,1-*a*]phenanthrene {11*H*-naphtho[2,1-*a*]fluorene}
222-93-5	1	0	0	Pentaphene {dibenzo[*b,j*]phenanthrene, 2,3,6,7-dibenzophenanethrene}
224-41-9	1	0	0	Dibenz[*a,j*]anthracene
224-42-0	1	0	0	Dibenz[*a,j*]acridine
224-53-3	1	0	0	Dibenz[*c,h*]acridine
225-11-6	1	0	0	Benz[*a*]acridine
225-51-4	1	0	0	Benz[*c*]acridine
226-36-8	1	0	0	Dibenz[*a,h*]acridine
226-78-8	1	0	0	9*H* Benzo[*a*]cyclopenta[*i*]anthracene
226-88-0	1	0	0	Benzo[*a*]naphthacene
226-92-6	1	0	0	Dibenz[*a,i*]acridine
227-04-3	1	0	0	Dibenzo[*a,j*]naphthacene
229-87-8	1	0	0	Benzo[*c*]quinoline {phenanthridine, 9-azaphenanthrene}
230-27-3	1	0	0	Benzo[*h*]quinoline {4-azaphenanthrene}
232-54-2	1	0	0	1*H*-Benz[*e*]indene
232-85-9	1	0	0	3*H*-Pyrrolo[3,2-*f*]quinoline
232-95-1	1	0	0	Naphtho[2,1-*b*]furan
233-36-3	1	0	0	1*H*-Pyrrolo[2,3-*f*]quinoline
234-03-7	1	0	0	Naphtho[1,2-*b*]furan
235-92-7	1	0	0	1*H*-Cyclopenta[*l*]phenanthrene
238-79-9	1	0	0	5*H*-Benzo[*a*]fluorene
238-82-4	1	0	0	1*H*-Benzo[*a*]fluorine
238-84-6	1	0	0	11*H*-Benzo[*a*]fluorene
239-01-0	1	0	0	11*H*-Benzo[*a*]carbazole
239-30-5	1	0	0	Benzo[*b*]naphtho[2,1-*d*]furan

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
239-35-0	1	0	0	Benzo[*b*]naphtho[2,1-*d*]thiophene
239-60-1	1	0	0	13*H*-Dibenzo[*a,i*]fluorene
239-63-4	1	0	0	5*H*-Dibenzo[*a,i*]carbazole
239-64-5	1	0	0	13*H*-Dibenzo[*a,i*]carbazole
240-44-8	1	0	0	1*H*-Benzo[*a*]cyclopent[*h*]anthracene
243-17-4	1	0	0	11*H*-Benzo[*b*]fluorene
243-18-5	1	0	0	5*H*-Benzo[*b*]fluorene
30777-19-6				
243-28-7	1	0	0	5*H*-Benzo[*b*]carbazole
243-42-5	1	0	0	Benzo[*b*]naphtho[2,3-*d*]furan
244-63-3	1	1	1	9*H*-Pyrido[3,4-*b*]indole {norharman = β-carboline = 2-azacarbazole}
8001-81-8				
244-69-9	1	0	0	5*H*-Pyrido[4,3-*b*]indole
244-76-8	1	0	0	1*H*-Pyrido[2,3-*b*]indole
244-99-5	1	0	0	5*H*-Indeno[1,2-*b*]pyridine {4-azafluorene}
245-08-9	1	0	0	5*H*-Pyrido[3,2-*b*]indole
253-66-7	1	0	0	Cinnoline {1,2-diazanaphthalene}
253-69-0	1	0	0	1,7-Naphthyridine {1,7-diazanaphthalene, pyrido[3,4-*b*]pyridine}
253-72-5	1	0	0	1,6-Naphthyridine {1,6-diazanaphthalene, pyrido[4,3-*b*]pyridine}
253-82-7	1	0	0	Quinazoline {1,3-benzodiazine}
254-60-4	1	0	0	1,8-Naphthyridine {1,8-diazanaphthalene, pyrido[2,3-*b*]pyridine}
254-79-5	1	0	0	1,5-Naphthyridine {1,5-diazanaphthalene, pyrido[3,2-*b*]pyridine}
259-79-0	1	0	0	Biphenylene
260-36-6	1	0	0	Benzo[*g*]quinoline
260-94-6	1	0	0	Acridine {benzo[*b*]quinoline}
262-12-4	1	0	0	Dibenzo[*b,e*][1,4]dioxin
268-40-6	1	0	0	1*H*-Benz[*f*]indene
268-91-7	1	0	0	1*H*-Pyrrolo[2,3-*b*]quinoline
271-44-3	1	0	0	1*H*-Indazole
271-63-6	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine {7-azaindole}
271-89-6	1	0	0	Benzofuran {benzo[*b*]furan, coumarone}
273-53-0	1	0	0	Benzoxazole {1-oxa-3-azaindene}
274-40-8	1	0	0	Pyrrolo[1,2-*a*]pyridine
274-45-3	1	0	0	Pyrrolo[1,2-*a*]pyrazine
274-76-0	1	0	0	Imidazo[1,2-*a*]pyridine
275-51-4	1	0	0	Azulene {cyclopentacycloheptene}
279-19-6	1	0	0	Tricyclo[2.2.1.02,6]heptane
280-65-9	1	0	0	Bicyclo[3.3.1]nonane
287-92-3	1	0	0	Cyclopentane {pentamethylene}
288-13-1	1	1	1	1*H*-Pyrazole
288-14-2	0	1	0	Isoxazole
288-16-4	1	0	0	Isothiazole
288-32-4	1	1	1	1*H*-Imidazole {1,3-diazole}
288-42-6	1	0	0	Oxazole
288-47-1	1	1	1	Thiazole
289-80-5	1	0	0	Pyridazine
289-95-2	0	1	0	Pyrimidine {1,3-diazine}
290-37-9	1	1	1	Pyrazine
297-78-9	1	1	1	4,7-Methanoisobenzofuran, 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro- {Isobenzan®, Telodrin®}
297-97-2	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-pyrazinyl ester {Thionazine®, Zinophos®}
298-00-0	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-nitrophenyl) ester {Parathion-methyl®}
298-02-2	0	1	0	Phosphorodithioic acid, *O,O*-diethyl S-[2-(ethylthio)methyl] ester {Phorate®}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
298-04-4	1	1	1	Phosphorodithioic acid, *O*,*O*-diethyl S-[2-(ethylthio)ethyl] ester {Disulfoton®}
298-08-8	1	0	0	2-Propanone, 1-amino-
298-12-4	1	1	1	Acetic acid, oxo- {glyoxylic acid}
298-14-6	0	1	0	Carbonic acid, monopotassium salt
299-84-3	0	1	0	Phosphorothioic acid, *O*,*O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester {Fenchlorphos®, Phenchlorphos®}
300-57-2	1	0	0	Benzene, 2-propenyl- {allyl benzene}
300-76-5	0	1	0	Phosphate, 1,2-dibromo-2,2-dichloroethyl dimethyl {Naled®}
300-85-6	1	0	0	Butanoic acid, 3-hydroxy-
300-87-8	0	1	0	Isoxazole, 3,5-dimethyl-
301-00-8	1	1	1	9,12,15-Octadecatrienoic acid, methyl ester, (*Z,Z,Z*)- {methyl linolenate}
301-12-2	0	1	0	Phosphorodithioic acid, *O*,*O*-dimethyl S-[2-(ethylsulfinyl)ethyl] ester {Oxydemeton methyl®}
302-01-2	1	1	1	Hydrazine
302-04-5	1	0	0	Thiocyanate
303-07-1	1	1	1	Benzoic acid, 2,6-dihydroxy-
303-38-8	1	1	1	Benzoic acid, 2,3-dihydroxy-
303-43-5	0	1	0	Cholest-5-en-3-ol (3β)-, 9-octadecenoate, [3β(*Z*),22*E*]- {cholesteryl oleate}
303-98-0	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-(3,7,11,15,19,23,27,31,35,39-decamethyl-2,6,10,14,18,22,26,30,34,38-tetracontadecenyl)-6-methyl- {ubiquinone-10}
304-21-2	1	0	0	3*H*-Pyrido[3,4-*b*]indole, 4,9-dihydro-7-methoxy-1-methyl- {harmaline}
305-01-1	1	1	1	2*H*-1-Benzopyran-2-one, 6,7-dihydroxy- {esculetin}
306-08-1	1	0	0	Benzeneacetic acid, 4-hydroxy-3-methoxy- {homovanillic acid}
306-60-5	0	1	0	Guanidine, (4-aminobutyl)-
306-83-2	1	1	1	Ethane, 2,2-dichloro-1,1,1-trifluoro- {Freon 123}
309-00-2	1	1	1	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5α,8α,8aβ)- [endo, endo] {Aldrin®}
313-80-4	1	0	0	Naphtho[2,1,8-*def*]quinoline {1-azapyrene}
316-14-3	1	0	0	Benz[*a*]anthracene, 6-methyl-
316-49-4	1	0	0	Benz[*a*]anthracene, 4-methyl-
319-84-6	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {alpha-HCH, HCH-alpha, α-Lindane®}
319-85-7	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {β-Lindane®}
319-86-8	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro- {δ-Lindane®}
320-77-4	0	1	0	Pentaric acid, 3-carboxy-2,3-dideoxy-
327-57-1	0	1	0	Norleucine {2-aminohexanoic acid}
5157-09-5				
327-97-9	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]- [2 CAS Nos.]
93451-46-8				{chlorogenic acid, 3-*O*-caffeoylquinic acid}
328-42-7	0	1	0	Butanedioic acid, oxo- {oxalacetic acid}
328-50-7	1	1	1	Pentanedioic acid, 2-oxo- {α-ketoglutaric acid}
330-54-1	0	1	0	Urea, 1,1-dimethyl-3-(3,4-dichlorophenyl) {Diuron®}
330-55-2	1	1	1	Urea, *N*′-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methyl- {Monolinuron®, 20% of Molipan®}
331-39-5	1	1	1	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- {caffeic acid}
332-77-4	1	0	0	Furan, 2,5-dihydro-2,5-dimethoxy-
332-80-9	1	1	1	*L*-Histidine, 1-methyl-
333-41-5	1	1	1	Phosphorothioic acid, *O,O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester {Diazinon®}
334-48-5	1	1	1	Decanoic acid {capric acid}
340-99-8	1	0	0	Acenaphth[1,2-*a*]acenaphthylene
343-65-7	0	1	0	Benzenebutanoic acid, α,2-diamino-γ-oxo- {kynurenine}
350-03-8	1	1	1	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine or methyl 3-pyridyl ketone}
352-93-2	1	0	0	Ethane, 1,1′-thiobis-
354-38-1	1	0	0	Acetamide, 2,2,2-trifluoro-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
354-53-0	1	1	1	Ethane, 1-chloro-2-bromotetrafluoro- {Freon® 114b1}
366-18-7	1	1	1	2,2′-Bipyridine {nicotine}
367-47-5	1	1	1	Propanal, 2,3-dihydroxy- {glyceraldehyde}
368-16-1	1	1	1	*L*-Histidine, 3-methyl-
372-75-8	0	1	0	*L*-Ornithine, *N*5-(aminocarbonyl)- {citrulline}
373-49-9	1	1	1	9-Hexadecenoic acid, (*Z*)- {palmitoleic acid}
392-12-1	0	1	0	1*H*-Indole-3-propanoic acid, α-oxo-
409-02-9	0	1	0	Heptenone, methyl-
414-29-9	1	0	0	Dibenzanthracene
67775-07-9				
420-12-2	0	1	0	Thiacyclopropane {ethylene sulfide}
430-75-1	0	1	0	Oxyacetate {glyoxylate}
431-03-8	1	1	1	2,3-Butanedione [2 CAS Nos.] {diacetyl, biacetyl}
29350-67-2				
432-25-7	1	1	1	1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- {β-cyclocitral}
52844-21-0				
434-85-5	1	0	0	[9,9′-Bianthracene]-10,10′(9*H*,9′*H*)-dione {bianthrone, dianthraquinone}
442-51-3	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 7-methoxy-1-methyl- {harmine}
451-13-8	1	0	0	Benzeneacetic acid, 2,5-dihydroxy-
452-86-8	1	0	0	1,2-Benzenediol, 4-methyl-
454-29-5	0	1	0	*DL*-Homocysteine
454-41-1	0	1	0	Butanoic acid, 2-amino-4-(methylsulfinyl)-
458-35-5	1	1	1	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy- {coniferyl alcohol}
459-80-3	0	1	0	2,6-Octadienoic acid, 3,7-dimethyl- {geranic acid}
459-88-1	0	1	0	3,7-Nonadien-1-ol, 4,8-dimethyl-, (*E*)-
460-12-8	1	0	0	1,3-Butadiyne
460-19-5	1	0	0	Ethanedinitrile {cyanogen}
461-72-3	1	0	0	2,4-Imidazolidinedione {hydantoin}
462-08-8	1	0	0	3-Pyridinamine
462-10-2	0	1	0	Butanoic acid, 4,4′-dithiobis[2-amino]- {homocystine}
462-94-2	0	1	0	1,5-Pentanediamine {cadaverine}
463-40-1	1	1	1	9,12,15-Octadecatrienoic acid, (*Z,Z,Z*)- {linolenic acid}
463-49-0	1	0	0	1,2-Propadiene {allene}
463-51-4	1	0	0	Ethenone {ketene}
463-56-9	1	1	1	Thiocyanic acid
463-58-1	1	0	0	Carbon oxide sulfide (COS) {carbonyl sulfide}
463-79-6	0	1	0	Carbonic acid
464-45-9	1	1	1	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *endo*- {borneol} [2 CAS Nos.]
507-70-0				
465-73-6	0	1	0	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1α,4α,4aβ,5β,8β,8aβ)- [endo, exo] {Isodrin®}
468-44-0	0	1	0	Gibbane-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-,1,4a-lactone, (1α,2β,4aα,4bβ,10β)-.
468-84-8	1	1	1	3*H*-Naphtho[2,1-*b*]pyran-3-one, dodecahydro-4a,7,7,10a-tetramethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]- {ambreinolide}
469-38-5	1	0	0	9,19-Cyclolanost-24-en-3-ol, (3β)- {cycloartenol}
469-39-6	0	1	0	9,19-Cycloergost-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-
469-61-4	0	1	0	1*H*-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,7β,8aα)]- {cedrene}
11028-42-5				
470-55-3	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1 → 6)-*O*-α-*D*-galactopyranosyl-(1 → 6)-
470-57-5	0	1	0	α-*D*-Glucopyranoside, *O*-α-*D*-galactopyranosyl-(1 → 6)-β-*D*-fructofuranosyl- {theanderose}
470-82-6	1	1	1	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- {eucalyptol, 1.8-cineole}
470-90-6	0	1	0	Phosphoric acid, 2-chloro-1-(2-dichlorophenyl)ethenyl-, diethyl ester {Chlorfenvinphos®, Birlane®}
470-99-5	0	1	0	2-Cyclohexen-1-ol, 3,5,5-trimethyl- {isophorol}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
471-01-2	1	0	0	3-Cyclohexen-1-one, 3,5,5-trimethyl-
471-16-9	0	1	0	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, [1S-(1α,3β,5α)]- {sabinol}
471-34-1	1	0	0	Carbonic acid, calcium salt
471-53-4	1	0	0	Olean-12-en-29-oic acid, 3-hydroxy-11-oxo-, (3β,20β)-
471-90-9	0	1	0	1-Cyclohexene-1-carboxylic acid, 2,6,6-trimethyl- {cyclogeranic acid}
472-20-8	0	1	0	1 -Cyclohexene-1- methanol, 2,6,6-trimethyl- {β-cyclogeraniol}
472-65-1	0	1	0	1-Cyclohexene-1-ethanol, 2,6,6-trimethyl- {β-cyclohomogeraniol}
472-70-8	0	1	0	β,β-Caroten-3-ol, (3R)- {cryptoxanthin}
472-78-6	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-ionol}
25312-34-9				
472-80-0	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3*E*)- {β-ionol, (*E*)}
472-97-9	0	1	0	Tricyclo[6.3.1.02,5]dodecan-1-ol, 4,4,8-trimethyl-, [1R-(1α,2α,5β,8β)]-
473-08-5	1	1	1	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)- {bicyclo[4.4.0]dec-1-en-3-one, 2,6-dimethyl-9-isopropenyl-}
473-15-4	0	1	0	2-Naphthalenemethanol, 1,2α,3,4,4a,5,6,7,8,8aα-decahydro-α,α,4aβ-trimethyl-8-methylene- {β-eudesmol}
473-17-6	0	1	0	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl-, [2R-(2α,4aβ,8aβ)]-
473-81-4	1	1	1	Propanoic acid, 2,3-dihydroxy- {glyceric acid}
473-84-7	1	0	0	Cyclopentanone, 2-hydroxy-
474-40-8	1	1	1	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α,24*Z*)- {α-sitosterol}
474-58-8	1	1	1	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl- {β-sitosteryl glucoside}
20431-48-5				
474-60-2	0	1	0	Ergostan-3-ol,(3β,5α,24R)- {campestanol}
474-62-4	1	1	1	Ergost-5-en-3-ol, (3β,24*R*)- {campesterol}
474-63-5	0	1	0	Ergosta-5,24(28)-dien-3-ol, (3β)-
474-67-9	0	1	0	Ergosta-5,22-dien-3-ol, (3β,22*E*)-
474-68-0	0	1	0	Ergosta-7,24(28)-dien-3-ol, (3β,5α)-
474-77-1	0	1	0	Cholest-5-en-3-ol, (3α)- {epicholesterol}
475-03-6	1	1	1	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl- {α-ionene}
475-20-7	0	1	0	1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1α,3aβ,4α,8aβ)]-
479-23-2	1	0	0	Benz[*j*]aceanthrylene, 1,2-dihydro- {cholanthrene}
479-61-8 42617-16-3	0	1	0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-*N*23,*N*24,*N*25,*N*26]-, [*SP*-4-2-[3S-[3α(2*E*,7S*,11S*),4β,21β]]]- [2 CAS Nos.] {chlorophyll a}
479-79-8	1	0	0	11*H*-Benzo[*c*]fluoren-11-one
480-10-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-(β-*D*-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glycoside}
480-41-1	0	1	0	4*H*-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)- {naringenin}
480-90-0	1	0	0	1*H*-Inden-1-one
480-91-1	1	0	0	1*H*-Isoindol-1-one, 2,3-dihydro-
481-14-1	0	1	0	Stigmasta-5,24(28)-dien-3-ol, (3β,24*Z*)-
481-21-0	0	1	0	Cholestane, (5α)- {coprostane}
481-25-4	0	1	0	Cholest-7-en-3-ol, 4-methyl-, (3β,4α,5α)-
481-39-0	0	1	0	1,4-Naphthalenedione, 5-hydroxy- {juglone}
582-24-1	1	0	0	Ethanone, 2-hydroxy-1-phenyl-
482-66-6	1	0	0	15*H*-Cyclopenta[*a*]phenanthrene, 16,17-dihydro-
482-70-2	1	0	0	1,4-Naphthalenedione, 2,7-dimethyl-
483-17-0	0	1	0	Cephalin
483-76-1	0	1	0	Naphthalene, 4,7-dimethyl-1,2,3,5,6,8a-hexahydro-1-(1-methylethyl)-, (1S-*cis*)- {δ-cadinene}
483-77-2	0	1	0	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)- 1,2,3,4-tetrahydro-, (1S-*Z*)-
483-87-4	1	0	0	Phenanthrene, 1,7-dimethyl-
484-20-8	0	1	0	7*H*-Furo[3,2-*g*][1]benzopyran-7-one, 4-methoxy-
484-73-1	1	1	1	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione {pyrocoll}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
486-25-9	1	1	1	9*H*-Fluoren-9-one
486-34-0	1	1	1	Naphthalene, 1,2,7-trimethyl-
486-56-6	1	1	1	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, (S)- {cotinine}
486-84-0	1	1	1	9*H*-Pyrido[3,4-*b*]indole, 1-methyl- {harman}
487-11-6	0	1	0	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
487-19-4	1	1	1	Pyridine, 3-(1-methyl-1*H*-pyrrol-2-yl)- {nicotyrine}
487-68-3	1	0	0	Benzaldehyde, 2,4,6-trimethyl-
487-89-8	0	1	0	1*H*-Indole-3-carboxaldehyde
487-90-1	0	1	0	1*H*-Pyrrole-3-propanoic acid, 5-(aminomethyl)-4-(carboxymethyl)-
488-10-8	0	1	0	2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (*Z*)-
488-15-3	0	1	0	Pentanoic acid, 2-hydroxy-3-methyl-
488-17-5	1	0	0	1,2-Benzenediol, 3-methyl-
488-18-6	1	0	0	4*H*-Pyran-4-one, 3,5-dihydroxy-
488-21-1	0	1	0	2-Butenedioic acid, 2,3-dimethyl-, (*Z*)-
488-23-3	1	0	0	Benzene, 1,2,3,4-tetramethyl-
488-31-3	0	1	0	Pentaric acid
488-69-7	0	1	0	*D*-Fructose, 1,6-bis(dihydrogen phosphate)
488-81-3	1	0	0	Ribitol [pentahydroxypentane]
488-84-6	0	1	0	*D*-erythro-2-Pentulose = *D*-ribulose {xylulose}
488-87-9	1	0	0	1,3-Benzenediol, 2,5-dimethyl-
488-92-6	1	0	0	1*H*-Pyrrole, 3-ethyl-4-methyl-
488-93-7	1	0	0	3-Furancarboxylic acid
490-03-9	0	1	0	2-Cyclohexen-1-one, 2-hydroxy-3-methyl- {diosphenol}
490-78-8	1	0	0	Ethanone, 1-(2,5-dihydroxyphenyl)-
490-79-9	1	1	1	Benzoic acid, 2,5-dihydroxy- {gentisic acid}
490-83-5	0	1	0	*L*-threo-2,3-Hexodiulosonic acid, γ-lactone {*L*-2,3-diketogulonic acid, γ-lactone}
490-99-3	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5β)- {isomenthol}
23283-97-8				
491-01-0	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)- {*D*-neomenthol}
491-07-6	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethyl)-, (*E*)- {*dl*-isomenthone}
491-14-5	1	0	0	Pentonic acid, 5-C-[3,5-bis(1-methylpropyl)-1-cyclopenten-1-yl]-4-deoxy-
491-26-9	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, *N*-oxide, (2S)-
491-35-0	1	1	1	Quinoline, 4-methyl-
491-50-9	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-3,5-dihydroxy- {quercimeritrin}
492-27-3	1	0	0	2-Quinolinecarboxylic acid, 4-hydroxy-
492-37-5	1	0	0	Benzeneacetic acid, α-methyl- {hydratropic acid}
492-61-5	1	1	1	β-*D*-Glucopyranose
492-62-6	0	1	0	α-*D*-Glucopyranose
493-33-4	1	0	0	Ethanone, 1-(4-hydroxy-2-methoxyphenyl)-
494-04-2	1	1	1	3,2′:4′,3′-Terpyridine {nicotelline}
494-52-0	1	1	1	Pyridine, 3-(2-piperidinyl)-, (S)- {*l*-anabasine}
494-90-6	1	0	0	Benzofuran, 4,5,6,7-tetrahydro-3,6-dimethyl-
494-97-3	1	1	1	Pyridine, 3-(2-pyrrolidinyl)-, (S)- {*l*-nornicotine}
494-98-4	1	1	1	Pyridine, 3-(1*H*-pyrrol-2-yl)- {nornicotyrine}
494-99-5	1	0	0	Benzene, 1,2-dimethoxy-4-methyl-
495-40-9	1	0	0	1-Butanone, 1-phenyl-
495-45-4	0	1	0	2-Buten-1-one, 1,3-diphenyl-
495-62-5	0	1	0	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl- {bisabolene}
495-78-3	1	1	1	Benzenepropanoic acid, 2-hydroxy-
496-11-7	1	1	1	1*H*-Indene, 2,3-dihydro- {indane}
496-15-1	1	1	1	1*H*-Indole, 2,3-dihydro- {indoline}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
496-16-2	1	1	1	Benzofuran, 2,3-dihydro- {coumaran}
496-49-1	0	1	0	2-Propanone, 1-(1-methyl-2-pyrrolidinyl)-
496-63-9	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-
496-64-0	1	1	1	2*H*-Pyran-2-one, 3-hydroxy-
496-72-0	1	0	0	1,2-Benzenediamine, ethyl-
496-78-6	1	0	0	Phenol, 2,4,5-trimethyl- {pseudocumenol}
497-03-0	1	0	0	2-Butenal, 2-methyl-, (*E*)- {tiglicaldehyde}
497-06-3	1	0	0	3-Butene-1,2-diol
497-16-5	1	0	0	Propanedial, oxo-
497-19-8	0	1	0	Carbonic acid, disodium salt {sodium carbonate}
497-20-1	1	0	0	1,3-Cyclopentadiene, 5-methylene- {fulvene}
497-23-4	1	1	1	2(5*H*)-Furanone {crotonolactone}
498-00-0	1	1	1	Benzenemethanol, 4-hydroxy-3-methoxy-
498-02-2	1	1	1	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)- {acetovanillone}
498-07-7	1	1	1	β-*D*-Glucopyranose, 1,6-anhydro- {levoglucosan}
498-15-7	0	1	0	Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- {(+)-3-carene}
13466-78-9				
498-19-1	1	1	1	Homoserine [2 CAS Nos.] {2-amino-4-hydroxybutanoic acid}
672-15-1				
498-21-5	1	0	0	Butanedioic acid, methyl-
498-23-7	1	1	1	2-Butenedioic acid, 2-methyl-, (*Z*)- {citraconic acid}
498-24-8	1	0	0	2-Butenedioic acid, 2-methyl-, (*E*)- {mesaconic acid}
498-36-2	0	1	0	Pentanoic acid, 2-hydroxy-4-methyl-
498-40-8	0	1	0	Cysteic acid
498-60-2	1	1	1	3-Furancarboxaldehyde
498-66-8	1	0	0	Bicyclo[2.2.1]hept-2-ene {norbornene}
498-71-5	0	1	0	3-Cyclohexene-1-methanol, 5-hydroxy-α,α,4-trimethyl-
499-06-9	0	1	0	Benzoic acid, 3,5-dimethyl-
499-12-7	1	1	1	1-Propene-1,2,3-tricarboxylic acid {aconitic acid}
499-70-7	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethyl)-
59471-80-6				
499-74-1	1	0	0	2-Cyclohexen-1-one, 6-methyl-3-(1-methylethyl)-
499-75-2	1	1	1	Phenol, 2-methyl-5-(1-methylethyl)- {carvacrol}
499-78-5	1	0	0	4*H*-Pyran-4-one-2-carboxylic acid, 5-hydroxy-
499-84-3	0	1	0	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-
500-02-7	0	1	0	2-Cyclohexen-1-one, 4-(1-methylethyl)-
500-22-1	1	1	1	3-Pyridinecarboxaldehyde {nicotinaldehyde, 3-formylpyridine}
500-99-2	1	1	1	Phenol, 3,5-dimethoxy-
501-13-3	0	1	0	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxy-3-methoxyphenyl)-
501-16-6	1	1	1	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*E*)- {*trans*-caffeic acid}
501-36-0	0	1	0	Ethene, 1-(4-hydroxyphenyl)-2-(3,5-dihydroxyphenyl)- {*trans*-resveratrol}
501-52-0	1	1	1	Benzenepropanoic acid {3-phenylpropionic acid, hydrocinnamic acid}
501-92-8	1	1	1	Phenol, 4-(2-propenyl)-
501-94-0	1	1	1	Benzeneethanol, 4-hydroxy-
501-97-3	1	1	1	Benzenepropanoic acid, 4-hydroxy-
501-98-4	1	1	1	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*E*)- {*trans*-coumaric acid}
502-42-1	1	1	1	Cycloheptanone {suberone}
502-47-6	0	1	0	6-Octenoic acid, 3,7-dimethyl-
502-61-4	1	0	0	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (*E,E*)- {α-farnesene}
502-65-8	1	1	1	ψ,ψ-Carotene {lycopene}
502-69-2	1	1	1	2-Pentadecanone, 6,10,14-trimethyl- {phytone, hexahydrofarnesyl acetone}
502-73-8	1	1	1	16-Hentriacontanone
503-17-3	1	1	1	2-Butyne

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
503-29-7	1	1	1	Azetidine
503-45-7	1	0	0	Cyclohexene, 3,3,5-trimethyl-
503-48-0	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-4-methyl-
110053-65-1				
503-64-0	1	0	0	2-Butenoic acid, (*Z*)- {*cis*-crotonic acid}
503-66-2	1	1	1	Propanoic acid, 3-hydroxy-
503-74-2	1	1	1	Butanoic acid, 3-methyl- {isovaleric acid}
503-93-5	0	1	0	2,4-Cycloheptadien-1-one, 2,6,6-trimethyl- {eucarvone}
504-03-0	1	0	0	Piperidine, 2,6-dimethyl-
504-15-4	1	0	0	1,3-Benzenediol, 5-methyl- {orcinol}
504-20-1	0	1	0	2,5-Heptadien-4-one, 2,6-dimethyl-
504-24-5	1	0	0	4-Pyridinamine
504-29-0	1	1	1	2-Pyridinamine
504-31-4	1	0	0	2*H*-Pyran-2-one
504-60-9	1	1	1	1,3-Pentadiene {piperylene}
504-63-2	1	1	1	1,3-Propanediol {trimethylene glycol}
504-85-8	0	1	0	3-Pentenoic acid, 4-methyl-
504-96-1	1	1	1	1-Hexadecene, 3-methylene-7,11,15-trimethyl- {neophytadiene}
504-99-4	0	1	0	Octanoic acid, 6-methyl-
505-14-6	1	0	0	Thiocyanogen
15941-77-2				
505-22-6	1	0	0	1,3-Dioxane
505-32-8	1	1	1	1-Hexadecen-3-ol, 3,7,11,15-tetramethyl- {isophytol}
60046-87-9				
505-48-6	1	0	0	Octanedioic acid {suberic acid}
505-52-2	1	0	0	Tridecanedioic acid
505-54-4	0	1	0	Hexadecanedioic acid
505-57-7	1	1	1	2-Hexenal
505-84-0	1	0	0	Propane, 1,1′-[methylenebis(oxy)]bis- {dipropoxymethane}
506-12-7	1	1	1	Heptadecanoic acid
506-13-8	0	1	0	Hexadecanoic acid, 16-hydroxy-
506-21-8	1	1	1	9,12-Octadecadienoic acid, (*E*,*E*)- {linoleic acid}
506-30-9	1	1	1	Eicosanoic acid {arachidic acid}
506-32-1	1	1	1	5,8,11,14-Eicosatetraenoic acid, (all-*Z*)- {arachidonic acid}
506-37-6	1	0	0	15-Tetracosenoic acid, (*Z*)-
506-38-7	1	1	1	Pentacosanoic acid
506-43-4	0	1	0	9,12-Octadecadien-1-ol, (*Z,Z*)-
506-44-5	1	0	0	9,12,15-Octadecatrien-1-ol, (*Z,Z,Z*)-
506-46-7	1	1	1	Hexacosanoic acid {cerotinic acid}
506-48-9	1	1	1	Octacosanoic acid
506-50-3	1	0	0	Triacontanoic acid
506-51-4	1	1	1	1-Tetracosanol
506-52-5	0	1	0	1-Hexacosanol
507-70-0	1	1	1	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, *endo*- {borneol} [2 CAS Nos.]
464-45-9				
508-02-1	0	1	0	Olean-12-en-28-oic acid, 3-hydroxy-, (3β)-
509-11-5	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7-dimethyl-, (exo,anti)-
510-75-8	0	1	0	Gibb-3-ene-1,10-dicarboxylic acid, 2,4a-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-
511-61-5	0	1	0	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3β,24S)-
512-29-8	0	1	0	β,ε-Carotene-3,3′-diol, 5,8-epoxy-5,8-dihydro-, (3S,3′R,5R,6′R,8R)- {flavoxanthin}
512-69-6	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-galactopyranosyl-(1 → 6)- {raffinose}
513-35-9	1	1	1	2-Butene, 2-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
513-44-0	1	0	0	1-Propanethiol, 2-methyl- {isobutyl mercaptan}
513-53-1	1	0	0	2-Butanethiol
513-81-5	1	0	0	1,3-Butadiene, 2,3-dimethyl-
513-85-9	1	1	1	2,3-Butanediol
513-86-0	1	1	1	2-Butanone, 3-hydroxy- {acetoin}
514-96-5	0	1	0	1,3-Cyclohexadiene, 1,2,6,6-tetramethyl-
515-00-4	0	1	0	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-
36203-31-3				
515-03-7	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-α,2,5,5,8a-pentamethyl-, [1R-[1α(R*),2β,4aβ,8aα]]- {sclareol}
515-13-9	0	1	0	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-
516-05-2	0	1	0	Propanedioic acid, methyl-
517-23-7	1	0	0	2(3*H*)-Furanone, 3-acetyldihydro-
518-85-4	1	0	0	1*H*-Phenalen-1-one, 2,3-dihydro-
519-62-0	0	1	0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(2-)-*N*23,*N*24,*N*25,*N*26]-, [*SP*-4-2-[3S-[3α(2*E*,7S*,11S*),4β,21β]]]- {chlorophyll b}
520-18-3	1	1	1	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(4-hydroxyphenyl)- {kaempferol}
520-34-3	0	1	0	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)- {diosmetin}
521-03-9	0	1	0	Stigmast-7-en-3-ol, (3β,5α)-
522-12-3	1	1	1	4*H*-1-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- {quercetrin}
524-42-5	1	0	0	1,2-Naphthalenedione {1,2-naphthoquinone}
525-03-1	1	0	0	9*H*-Fluoren-9-amine
525-74-6	1	1	1	Pyridine, 3-(4,5-dihydro-1-methyl-2*H*-pyrrol-5-yl)- {*N*-methylmyosmine}
525-75-7	1	1	1	Pyridine, 2-(1-methyl-1*H*-pyrrol-2-yl)- {α-nicotyrine}
525-79-1	0	1	0	1*H*-Purin-6-amine, *N*-(2-furanylmethyl)-
526-55-6	0	1	0	1*H*-Indole-3-ethanol
526-73-8	1	1	1	Benzene, 1,2,3-trimethyl-
526-75-0	1	1	1	Phenol, 2,3-dimethyl- {2,3-xylenol}
526-83-0	1	1	1	Butanedioic acid, 2,3-dihydroxy- {tartaric acid}
526-85-2	1	1	1	Phenol, 2,3,4-trimethyl-
526-86-3	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethyl-
526-91-0 D	1	0	0	Pentanoic acid, 2,3,4,5-tetrahydroxy- [4 CAS Nos.]
4172-43-4				
4172-44-5 L				
17828-56-7 DL				
526-99-8	0	1	0	Galactaric acid
527-17-3	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl-
527-35-5	1	1	1	Phenol, 2,3,5,6-tetramethyl- {durenol}
527-53-7	1	0	0	Benzene, 1,2,3,5-tetramethyl-
527-54-8	1	0	0	Phenol, 3,4,5-trimethyl-
527-60-6	1	1	1	Phenol, 2,4,6-trimethyl- {mesitol}
527-61-7	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl-
528-50-7	0	1	0	Cellobiose
528-53-0	0	1	0	1-Benzopyrylium, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-, chloride
528-58-5	0	1	0	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride
529-00-0	0	1	0	Cyclohexanone, 5-methyl-2-(1-methylethenyl)- {isopulegone}
529-05-5	1	0	0	Azulene, 1,4-dimethyl-7-ethyl-
529-19-1	1	1	1	Benzonitrile, 2-methyl-
529-20-4	1	1	1	Benzaldehyde, 2-methyl- {*o*-tolualdehyde}
529-21-5	1	0	0	Pyridine, 3-ethyl-4-methyl-
529-33-9	1	0	0	1-Naphthalenol, 1,2,3,4-tetrahydro-
529-34-0	1	0	0	1(2*H*)-Naphthalenone, 3,4-dihydro- {1-tetralone}
529-44-2	0	1	0	4*H*-1-Benzopyran-4-one, 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricetin}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
530-45-0	0	1	0	Ethane, bis(4-methylphenyl)-
530-57-4	1	1	1	Benzoic acid, 4-hydroxy-3,5-dimethoxy- {syringic acid}
530-59-6	1	0	0	2-Propenoic acid, 3-(4-hydroxy-3,5-dimethoxyphenyl)-
530-91-6	1	0	0	2-Naphthalenol, 1,2,3,4-tetrahydro-
531-44-2	0	1	0	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-methoxy- {scopolin}
531-58-8	0	1	0	2*H*-1-Benzopyran-2-one, 7-(β-*D*-glucopyranosyloxy)-6-hydroxy- {cichoriin}
531-59-9	0	1	0	2*H*-1-Benzopyran-2-one, 7-methoxy-
531-67-9	0	1	0	2,2′-Bipiperidine
531-75-9	1	1	1	2*H*-1-Benzopyran-2-one, 6-(β-*D*-glucopyranosyloxy)-7-hydroxy- {esculin}
532-12-7	1	1	1	Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)- {*l*-myosmine}
532-32-1	0	1	0	Benzoic acid, sodium salt
533-37-9	1	0	0	5*H*-1-Pyrindine, 6,7-dihydro-
533-67-5	0	1	0	*D*-erythro-Pentose, 2-deoxy- {deoxyribose}
533-73-3	1	0	0	1,2,4-Benzenetriol {hydroxyhydroquinone}
533-74-4	0	1	0	1,3,5-Thiadiazine, 2-thio-3,5-dimethyl-tetrahydro- {Dazomet®, Mylone®}
534-15-6	1	0	0	Ethane, 1,1-dimethoxy-
534-22-5	1	1	1	Furan, 2-methyl-
534-61-2	1	0	0	Cyclohexanecarboxylic acid, 3-[[3-(3,4- dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-[1S-(1α,3β,4β,5 α)]- {isochlorogenic acid}
534-82-7	0	1	0	1,2-Ethanediol, 1-(4-hydroxy-3-methoxyphenyl)-
535-24-0	0	1	0	Heptanedioic acid, 2,6-diamino-3-hydroxy-
535-75-1	1	1	1	2-Piperidinecarboxylic acid {pipecolic acid}
535-77-3	1	1	1	Benzene, 1-methyl-3-(1-methylethyl)- {*m*-cymene}
535-83-1	0	1	0	Pyridinium, 3-carboxy-1-methyl-, hydroxide, inner salt
536-30-1	0	1	0	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethyl)-, (1S-*Z*)-
536-50-5	0	1	0	Benzenemethanol, α,4-dimethyl-
536-74-3	1	0	0	Benzene, ethynyl- {phenylacetylene}
536-75-4	1	1	1	Pyridine, 4-ethyl-
536-78-7	1	1	1	Pyridine, 3-ethyl-
536-90-3	1	1	1	Benzenamine, 3-methoxy- {*m*-anisidine}
537-33-7	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)-2,6-dimethoxy- {sinapyl alcohol}
537-40-6	0	1	0	1,2,3-Propanetriol, tri-9,12-octadecadienoate {trilinolein}
537-73-5	1	0	0	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-
537-98-4	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*E*)- {*trans*-ferulic acid}
538-68-1	1	1	1	Benzene, pentyl-
538-79-4	1	1	1	3-Buten-1-amine, *N*-methyl-4-(3-pyridinyl)- {metanicotine}
538-86-3	0	1	0	Benzene, (methoxymethyl)- {benzyl methyl ether}
538-93-2	1	0	0	Benzene, (2-methylpropyl)-
539-12-8	1	0	0	Phenol, 4-(1-propen-1-yl)-
539-32-2	1	1	1	Pyridine, 3-butyl-
539-47-9	1	0	0	2-Propenoic acid, 3-(2-furanyl)-
539-82-2	1	1	1	Pentanoic acid, ethyl ester {ethyl valerate}
539-88-8	1	1	1	Pentanoic acid, 4-oxo-, ethyl ester {ethyl levulinate}
539-90-2	0	1	0	Butanoic acid, 2-methylpropyl ester
540-04-5	0	1	0	ψ,ψ-Carotene, 7,7′,8,8′,11,11′,12,12′-octahydro- {phytoene}
13920-14-4				
540-05-6	0	1	0	ψ,ψ-Carotene, 7,7′,8,8′,11,12-hexahydro- {phytofluene}
27664-65-9				
540-07-8	0	1	0	Hexanoic acid, pentyl ester
540-09-0	1	1	1	12-Tricosanone
540-10-3	1	1	1	Hexadecanoic acid, hexadecyl ester

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
540-18-1	0	1	0	Butanoic acid, pentyl ester
540-67-0	1	0	0	Ethane, methoxy-
541-31-1	1	0	0	1-Butanethiol, 3-methyl-
541-35-5	1	0	0	Butanamide
541-46-8	1	0	0	Butanamide, 3-methyl-
541-47-9	1	1	1	2-Butenoic acid, 3-methyl-
541-50-4	0	1	0	Butanoic acid, 3-oxo- {acetoacetic acid}
541-58-2	1	0	0	Thiazole, 2,4-dimethyl-
541-59-3	1	1	1	1*H*-Pyrrole-2,5-dione {maleimide}
541-73-1	1	0	0	Benzene, 1,3-dichloro-
541-85-5	0	1	0	3-Heptanone, 5-methyl-
541-91-3	0	1	0	Cyclopentadecanone, 3-methyl-
542-10-9	1	0	0	1,1-Ethanediol, diacetate
542-28-9	1	1	1	2*H*-Pyran-2-one, tetrahydro- {δ-valerolactone}
542-32-5	0	1	0	Hexanedioic acid, 2-amino-
542-50-7	0	1	0	14-Heptacosanone
542-54-1	1	0	0	Pentanenitrile, 4-methyl-
542-59-6	1	0	0	1,2-Ethanediol, monoacetate {acetic acid, 2-hydroxyethyl ester}
542-75-6	0	1	0	1-Propene, 1,3-dichloro- {1,3-D}
542-78-9	1	0	0	Propanedial
542-92-7	1	1	1	1,3-Cyclopentadiene {pyropentylene}
543-49-7	0	1	0	2-Heptanol
544-12-7	0	1	0	3-Hexen-1-ol
544-25-2	1	0	0	1,3,5-Cycloheptatriene {tropilidene}
544-35-4	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, ethyl ester {ethyl linoleate}
544-40-1	1	0	0	Butane, 1,1′-thiobis- {dibutyl sulfide}
544-63-8	1	1	1	Tetradecanoic acid {myristic acid}
544-76-3	1	1	1	Hexadecane
544-85-4	1	1	1	Dotriacontane
545-47-1	0	1	0	Lup-20(29)-en-3-ol, (3β)-
545-97-1	0	1	0	Gibbane-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,4aα,4bβ,10β)-
547-63-7	0	1	0	Propanoic acid, 2-methyl-, methyl ester
547-64-8	1	0	0	Propanoic acid, 2-hydroxy-, methyl ester
548-35-6	1	0	0	5*H*-Tribenzo[*a,f,l*]trindene, 10,15-dihydro- {5*H*-diindeno[1,2-*a*:1′,2′-*c*]fluorene, truxene}
27096-03-3				
550-44-7	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, *N*-methyl-
551-08-6	0	1	0	1(3*H*)-Isobenzofuranone, 3-butylidene-
551-68-8	0	1	0	*D*-Psicose
552-82-9	1	0	0	Benzenamine, *N*-methyl-*N*-phenyl-
553-26-4	1	1	1	4,4′-Bipyridine
553-86-6	1	0	0	2(3*H*)-Benzofuranone
553-97-9	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2-methyl-
554-12-1	1	1	1	Propanoic acid, methyl ester
554-14-3	1	0	0	Thiophene, 2-methyl-
554-15-4	1	1	1	1*H*-Pyrrole, 2,5-dihydro-1-methyl-
554-62-1	0	1	0	1,3,4-Octadecanetriol, 2-amino-, [2S-(2R*,3R*,4S*)]-
554-84-7	1	0	0	Phenol, 3-nitro-
554-91-6	0	1	0	Gentiobiose
555-44-2	0	1	0	1,2,3-Propanetriol, trihexadecanoate {tripalmitin}
555-45-3	0	1	0	1,2,3-Propanetriol, tritetradecanoate {trimyristin}
556-24-1	0	1	0	Butanoic acid, 3-methyl-, methyl ester {methyl isovalerate}
556-48-9	0	1	0	1,4-Cyclohexanediol

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
556-52-5	1	0	0	Oxiranemethanol {glycidol}
556-61-6	0	1	0	Isothiocyanic acid, methyl- {Trapex®}
556-64-9	1	0	0	Thiocyanic acid, methyl ester
556-82-1	0	1	0	2-Buten-1-ol, 3-methyl-
557-31-3	1	1	1	1-Propene, 3-ethoxy- {allyl ethyl ether}
557-48-2	0	1	0	2,6-Nonadienal, (*E,Z*)-
557-59-5	1	1	1	Tetracosanoic acid {lignoceric acid}
557-61-9	1	1	1	1-Octacosanol {montanyl alcohol}
558-30-5	1	0	0	Oxirane, 2,2-dimethyl- {isobutylene oxide}
558-37-2	1	0	0	1-Butene, 3,3-dimethyl-
559-70-6	1	1	1	Olean-12-en-3-ol, (3β)- {β-amyrin}
561-56-8	0	1	0	Gibb-2-ene-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,4aα,4bβ,10β)-
562-73-2	1	1	1	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy- [2 CAS Nos.] {quinic acid}
77-95-2				
562-74-3	1	1	1	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- {4-carvomenthol}
563-45-1	1	0	0	1-Butene, 3-methyl-
563-46-2	1	0	0	1-Butene, 2-methyl-
563-72-4	0	1	0	Ethanedioic acid, calcium salt [2 CAS Nos.]
25454-23-3				
563-78-0	1	1	1	1-Butene, 2,3-dimethyl-
563-79-1	1	0	0	2-Butene, 2,3-dimethyl-
563-80-4	1	1	1	2-Butanone, 3-methyl-
563-83-7	1	0	0	Propanamide, 2-methyl-
564-20-5	1	1	1	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {1,5,5,9-tetramethyl-13-oxatricyclo[8,3,0,0(4,9)]tridecane} {sclareolide}
565-60-6	0	1	0	2-Pentanol, 3-methyl-
565-61-7	1	1	1	2-Pentanone, 3-methyl-
565-62-8	1	0	0	3-Penten-2-one, 3-methyl-
565-67-3	1	0	0	3-Pentanol, 2-methyl-
565-69-5	1	1	1	3-Pentanone, 2-methyl-
565-70-8	1	1	1	Butanoic acid, 2-hydroxy-
565-80-0	1	0	0	3-Pentanone, 2,4-dimethyl-
569-41-5	1	1	1	Naphthalene, 1,8-dimethyl-
571-58-4	1	1	1	Naphthalene, 1,4-dimethyl-
571-61-9	1	1	1	Naphthalene, 1,5-dimethyl-
573-98-8	1	1	1	Naphthalene, 1,2-dimethyl-
574-06-1	1	0	0	Ethanone, 1,2-diphenyl-2-(acetyloxy)- {benzoin acetate}
575-37-1	1	1	1	Naphthalene, 1,7-dimethyl-
575-41-7	1	1	1	Naphthalene, 1,3-dimethyl-
575-43-9	1	1	1	Naphthalene, 1,6-dimethyl-
576-26-1	1	1	1	Phenol, 2,6-dimethyl- {2,6-xylenol}
576-37-4	1	1	1	Glucuronic acid
577-16-2	1	1	1	Ethanone, 1-(2-methylphenyl)- {2-methylacetophenone}
578-54-1	1	1	1	Benzenamine, 2-ethyl-
578-58-5	1	0	0	Benzene, 1-methoxy-2-methyl- {*o*-methylanisole}
579-07-7	1	0	0	1,2-Propanedione, 1-phenyl-
579-66-8	1	1	1	Benzenamine, 2,6-diethyl-
579-75-9	0	1	0	Benzoic acid, 2-methoxy- {*o*-anisic acid}
580-22-3	1	0	0	2-Quinolinamine
581-40-8	1	1	1	Naphthalene, 2,3-dimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
581-42-0	1	1	1	Naphthalene, 2,6-dimethyl-
581-46-4	1	1	1	3,3′-Bipyridine
581-47-5	1	1	1	2,4′-Bipyridine
581-49-7	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (S)- {*l*-anatabine}
581-50-0	1	1	1	2,3′-Bipyridine {isonicoteine}
582-16-1	1	1	1	Naphthalene, 2,7-dimethyl-
582-22-9	1	0	0	Benzeneethanamine, β-methyl-
582-60-5	1	0	0	1*H*-Benzimidazole, 5,6-dimethyl-
583-04-0	0	1	0	Benzoic acid, 2-propenyl ester
583-17-5	1	1	1	2-Propenoic acid, 3-(2-hydroxyphenyl)- [2 CAS Nos.] {*o*-coumaric acid}
614-60-8				
583-52-8	0	1	0	Ethanedioic acid, dipotassium salt
583-58-4	1	1	1	Pyridine, 3,4-dimethyl- {3,4-lutidine}
583-60-8	0	1	0	Cyclohexanone, 2-methyl-
583-61-9	1	1	1	Pyridine, 2,3-dimethyl- {2,3-lutidine}
583-63-1	1	1	1	3,5-Cyclohexadiene-1,2-dione {*o*-benzoquinone}
583-92-6	0	1	0	Butanoic acid, 4-(methylthio)-2-oxo-
584-02-1	0	1	0	3-Pentanol
584-08-7	0	1	0	Carbonic acid, dipotassium salt
584-79-2	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, 2-(1-propenyl)-4-hydroxy-3-methyl-2-cyclopenten-1-one ester {Allethrin®}
585-09-1	0	1	0	Butanedioic acid, hydroxy-, dipotassium salt
585-25-1	1	1	1	2,3-Octanedione
585-34-2	1	0	0	Phenol, 3-(1,1-dimethylethyl)-
585-74-0	1	1	1	Ethanone, 1-(3-methylphenyl)- {3-methylacetophenone}
585-88-6	0	1	0	Hexane, hexahydroxy-, 4-*O*-β-*D*-glucopyranosyl- {maltitol, 4-*O*-β-*D*-glucopyranosyl-*D*-glucitol}
585-99-9	0	1	0	Melibiose
586-30-1	1	1	1	Benzoic acid, 3-hydroxy-4-methyl-
586-37-8	1	0	0	Ethanone, 1-(3-methoxyphenyl)-
586-38-9	1	1	1	Benzoic acid, 3-methoxy-
586-62-9	0	1	0	Cyclohexene, 1-methyl-4-(1-methylethylidene)- {terpinolene}
586-67-4	1	0	0	Cyclohexene, 4-methyl-1-(1-methylethenyl)- {3,8-menthadiene}
586-81-2	0	1	0	Cyclohexanol, 1-methyl-4-(1-methylethylidene)-
587-02-0	1	0	0	Benzenamine, 3-ethyl-
587-45-1	0	1	0	Tyrosine, 3-hydroxy-
588-30-7	0	1	0	2-Propenoic acid, 3-(3-hydroxyphenyl)-
588-59-0	1	1	1	Benzene, 1,1′-(1,2-ethenediyl)bis- {stilbene}
589-08-2	1	1	1	Benzeneethanamine, *N*-methyl-
589-16-2	1	0	0	Benzenamine, 4-ethyl-
589-18-4	0	1	0	Benzenemethanol, 4-methyl-
589-33-3	1	0	0	1*H*-Pyrrole, 1-butyl-
589-34-4	1	0	0	Hexane, 3-methyl-
589-35-5	0	1	0	1-Pentanol, 3-methyl-
589-38-8	1	1	1	3-Hexanone {ethyl propyl ketone}
589-43-5	1	0	0	Hexane, 2,4-dimethyl-
116502-44-4				
589-59-3	0	1	0	Butanoic acid, 3-methyl-, 2-methylpropyl ester
589-81-1	1	0	0	Heptane, 3-methyl-
589-92-4	1	0	0	Cyclohexanone, 4-methyl-
589-93-5	1	1	1	Pyridine, 2,5-dimethyl- {2,5-lutidine}
589-98-0	0	1	0	3-Octanol
590-00-1	0	1	0	2,4-Hexadienoic acid, potassium salt [2 CAS Nos.]
24624-61-5				

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
590-01-2	0	1	0	Propanoic acid, butyl ester
590-18-1	1	0	0	2-Butene, (*Z*)-
590-19-2	1	0	0	1,2-Butadiene
590-28-3	0	1	0	Cyanic acid, potassium salt
590-36-3	0	1	0	2-Pentanol, 2-methyl-
590-66-9	1	0	0	Cyclohexane, 1,1-dimethyl-
590-86-3	1	1	1	Butanal, 3-methyl- {3-methylbutyraldehyde, isovaleraldehyde}
590-90-9	1	1	1	2-Butanone, 4-hydroxy-
591-11-7	1	1	1	2(5*H*)-Furanone, 5-methyl- {β-angelica lactone}
591-12-8	1	1	1	2(3*H*)-Furanone, 5-methyl- {4-hydroxy-3-pentenoic acid lactone, α-angelica lactone}
591-21-9	1	0	0	Cyclohexane, 1,3-dimethyl-
591-22-0	1	1	1	Pyridine, 3,5-dimethyl- {3,5-lutidine}
591-24-2	1	0	0	Cyclohexanone, 3-methyl-
591-27-5	1	0	0	Phenol, 3-amino-
591-31-1	1	0	0	Benzaldehyde, 3-methoxy-
591-47-9	1	0	0	Cyclohexene, 4-methyl-
591-48-0	1	0	0	Cyclohexene, 3-methyl-
591-49-1	1	0	0	Cyclohexene, 1-methyl-
591-68-4	0	1	0	Pentanoic acid, butyl ester
591-76-4	1	0	0	Hexane, 2-methyl-
591-78-6	1	1	1	2-Hexanone {butyl methyl ketone}
591-80-0	1	1	1	4-Pentenoic acid
591-93-5	1	0	0	1,4-Pentadiene
591-95-7	1	1	1	1,2-Pentadiene {ethylallene}
592-13-2	1	0	0	Hexane, 2,5-dimethyl-
592-20-1	1	1	1	2-Propanone, 1-(acetyloxy)-
592-27-8	1	0	0	Heptane, 2-methyl-
592-41-6	1	0	0	1-Hexene
592-42-7	1	0	0	1,5-Hexadiene
592-43-8	1	0	0	2-Hexene
592-45-0	1	0	0	1,4-Hexadiene
592-46-1	1	0	0	2,4-Hexadiene
592-47-2	1	0	0	3-Hexene
592-48-3	1	0	0	1,3-Hexadiene
592-51-8	1	0	0	4-Pentenenitrile
592-57-4	1	0	0	1,3-Cyclohexadiene
592-65-4	1	0	0	Propane, 1,1′-thiobis[2-methyl- {diisobutyl sulfide}
592-76-7	1	0	0	1-Heptene
592-77-8	1	0	0	2-Heptene
592-84-7	0	1	0	Formic acid, butyl ester
592-88-1	1	0	0	1-Propene, 3,3′-thiobis-
592-99-4	1	0	0	4-Octene
593-08-8	0	1	0	2-Tridecanone
593-45-3	1	1	1	Octadecane
593-47-5	0	1	0	9-Octadecen-1-ol
593-49-7	1	1	1	Heptacosane
593-50-0	1	1	1	1-Triacontanol
593-67-9	1	1	1	Ethenamine
594-07-0	0	1	0	Carbamodithioic acid
594-61-6	0	1	0	Propanoic acid, 2-hydroxy-2-methyl-
596-84-9	0	1	0	1*H*-Naphtho[2,1-*b*]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aβ,6aα,10aβ,10bα)]-
596-85-0	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-α,5,5,8a-tetramethyl-2-methylene-, [1S-[1α(S*),4aβ,8aα]]- {manool}
597-04-6	0	1	0	Butanoic acid, 2,2-dimethyl-3-oxo-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
598-55-0	0	1	0	Carbamic acid, methyl ester
598-58-3	1	0	0	Nitric acid, methyl ester
598-75-4	1	0	0	2-Butanol, 3-methyl-
598-82-3	1	1	1	Propanoic acid, 2-hydroxy- [2 CAS Nos.] {lactic acid}
50-21-5				
599-04-2	1	1	1	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (R)-
600-14-6	1	1	1	2,3-Pentanedione
600-18-0	1	1	1	Butanoic acid, 2-oxo-
600-22-6	1	1	1	Propanoic acid, 2-oxo-, methyl ester
600-24-8	1	0	0	Butane, 2-nitro-
600-28-2	1	0	0	1*H*-Pyrrole, 2,3-dimethyl-
601-77-4	1	0	0	2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso
603-17-8	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2*E*,7S*,11S*),4β,21β]]- {pheophytin A}
603-32-7	1	0	0	Arsine, triphenyl-
603-76-9	1	0	0	1*H*-Indole, 1-methyl-
603-79-2	1	0	0	Benzoic acid, 2,3-dimethyl-
604-35-3	1	0	0	Cholest-5-en-3-ol (3β)-, acetate {cholesteryl acetate}
604-53-5	1	0	0	1,1′-Binaphthalene
604-98-8	0	1	0	Coenzyme A, S-(hydrogen butanedioate)
605-02-7	1	1	1	Naphthalene, 1-phenyl-
605-83-4	1	0	0	Anthracene, 9-ethyl-
606-06-4	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2-(3,7-dimethyl-2,6-octadienyl)-5,6-dimethoxy-3-methyl-, (*E*)-
606-23-5	1	0	0	1*H*-Indene-1,3(2*H*)-dione
607-81-8	1	0	0	Propanedioic acid, (phenylmethyl)-, diethyl ester
607-91-0	1	1	1	1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)- {myristicin}
608-25-3	1	0	0	1,3-Benzenediol, 2-methyl-
608-34-4	1	0	0	2,4(1*H*,3*H*)-Pyrimidinedione, 3-methyl-
608-43-5	1	0	0	1,4-Benzenediol, 2,3-dimethyl-
608-73-1	1	1	1	Cyclohexane, 1,2,3,4,5,6-hexachloro-
609-38-1	1	1	1	2-Furancarboxamide
609-41-6	1	0	0	1*H*-Pyrrole, 1-acetyl-
610-02-6	1	0	0	Benzoic acid, 2,3,4-trihydroxy-
610-48-0	1	0	0	Anthracene, 1-methyl-
610-49-1	1	1	1	1-Anthracenamine
610-72-0	1	0	0	Benzoic acid, 2,5-dimethyl-
610-99-1	1	0	0	1-Propanone, 1-(2-hydroxyphenyl)-
611-13-2	1	1	1	2-Furancarboxylic acid, methyl ester {methyl 2-furoate}
1334-76-5				
611-14-3	1	1	1	Benzene, 1-ethyl-2-methyl-
611-15-4	1	0	0	Benzene, 1-ethenyl-2-methyl-
611-21-2	1	0	0	Benzenamine, *N*,2-dimethyl-
611-32-5	1	0	0	Quinoline, 8-methyl-
611-34-7	1	0	0	Quinoline, 5-amino-
612-19-1	1	0	0	Benzoic acid, 2-ethyl-
612-20-4	1	0	0	Benzoic acid, 2-(hydroxymethyl)-
612-58-8	1	0	0	Quinoline, 3-methyl-
612-60-2	1	0	0	Quinoline, 7-methyl-
612-78-2	1	0	0	2,2′-Binaphthalene
612-94-2	1	1	1	Naphthalene, 2-phenyl-
613-12-7	1	0	0	Anthracene, 2-methyl-
613-13-8	1	1	1	2-Anthracenamine

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
613-31-0	1	0	0	Anthracene, 9,10-dihydro-
613-33-2	1	0	0	1,1′-Biphenyl, 4,4′-dimethyl-
613-45-6	0	1	0	Benzaldehyde, 2,4-dimethoxy-
613-46-7	1	0	0	2-Naphthalenecarbonitrile
614-00-6	1	1	1	Benzenamine, *N*-methyl-*N*-nitroso-
614-60-8	1	1	1	2-Propenoic acid, 3-(2-hydroxyphenyl)- [2 CAS Nos.] {*o*-coumaric acid}
583-17-5				
614-18-6	1	1	1	3-Pyridinecarboxylic acid, ethyl ester
614-75-5	1	1	1	Benzeneacetic acid, 2-hydroxy-
614-82-4	1	0	0	Benzeneacetic acid, 2,4-dihydroxy-
614-96-0	1	0	0	1*H*-Indole, 5-methyl-
614-99-3	0	1	0	2-Furancarboxylic acid, ethyl ester {ethyl 2-furoate}
615-13-4	1	0	0	2*H*-Inden-2-one, 1,3-dihydro-
615-15-6	1	0	0	1*H*-Benzimidazole, 2-methyl-
615-22-5	0	1	0	Benzothiazole, 2-methylthio-
615-90-7	1	0	0	1,4-Benzenediol, 2,5-dimethyl-
616-02-4	1	1	1	2,5-Furandione, 3-methyl-
616-03-5	1	1	1	2,4-Imidazolidinedione, 5-methyl-
616-04-6	1	0	0	2,4-Imidazolidinedione, 1-methyl-
616-12-6	1	0	0	2-Pentene, 3-methyl-, (*E*)-
616-24-0	1	0	0	3-Pentanamine
616-25-1	1	1	1	1-Penten-3-ol
616-43-3	1	0	0	1*H*-Pyrrole, 3-methyl-
616-44-4	1	0	0	Thiophene, 3-methyl-
616-45-5	1	1	1	2-Pyrrolidinone {γ-butyrolactam}
616-47-7	1	0	0	1*H*-Imidazole, 1-methyl-
617-05-0	0	1	0	Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester
617-12-9	0	1	0	1,5-Cyclohexadiene-1-carboxylic acid, 3-[(1-carboxyethenyl)oxy]-4-hydroxy-, (3R-*E*)- {chorismic acid}
617-31-2	0	1	0	Pentanoic acid, 2-hydroxy-
617-35-6	1	0	0	Propanoic acid, 2-oxo-, ethyl ester
617-62-9	0	1	0	Pentanedioic acid, 2-methyl-
617-90-3	1	0	0	2-Furancarbonitrile
617-92-5	1	1	1	1*H*-Pyrrole, 1-ethyl-
617-94-7	1	1	1	Benzenemethanol, α,α-dimethyl-
618-45-1	1	1	1	Phenol, 3-(1-methylethyl)-
619-01-2	0	1	0	2-Cyclohexanol, 1-methyl-4-(1-methylethylene)-
619-04-5	1	0	0	Benzoic acid, 3,4-dimethyl-
699-17-2	1	1	1	2-Butanone, 4-(2-furanyl)-
619-20-5	1	0	0	Benzoic acid, 3-ethyl-
619-64-7	1	0	0	Benzoic acid, 4-ethyl-
620-02-0	1	1	1	2-Furancarboxaldehyde, 5-methyl-
620-14-4	1	1	1	Benzene, 1-ethyl-3-methyl-
620-17-7	1	1	1	Phenol, 3-ethyl-
620-18-8	1	0	0	Phenol, 3-ethenyl-
620-22-4	1	0	0	Benzonitrile, 3-methyl-
620-23-5	1	1	1	Benzaldehyde, 3-methyl- {*m*-tolualdehyde}
620-24-6	1	1	1	Benzenemethanol, 3-hydroxy-
621-23-8	1	0	0	Benzene, 1,3,5-trimethoxy-
621-27-2	1	0	0	Phenol, 3-propyl-
621-34-1	1	0	0	Phenol, 3-ethoxy-
621-37-4	1	1	1	Benzeneacetic acid, 3-hydroxy-
621-42-1	0	1	0	Acetamide, 3-hydroxyphenyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
621-54-5	1	1	1	Benzenepropanoic acid, 3-hydroxy-
33393-93-0				
621-64-7	1	1	1	1-Propanamine, *N*-nitroso-*N*-propyl- {NDPA}
621-79-4	1	0	0	2-Propenamide, 3-phenyl-
621-82-9	1	1	1	2-Propenoic acid, 3-phenyl- {cinnamic acid}
622-24-2	0	1	0	Benzene, 2-chloroethyl-
622-39-9	1	0	0	Pyridine, 2-propyl-
622-78-6	0	1	0	Benzene, (isothiocyanatomethyl)-
622-96-8	1	1	1	Benzene, 1-ethyl-4-methyl-
622-97-9	1	0	0	Benzene, 1-ethenyl-4-methyl-
623-05-2	1	1	1	Benzenemethanol, 4-hydroxy- {benzyl alcohol, 4-hydroxy-}
623-08-5	1	0	0	Benzenamine, *N*,4-dimethyl-
623-09-6	1	0	0	1,4-Benzenediamine, *N*-methyl-
623-15-4	1	1	1	3-Buten-2-one, 4-(2-furanyl)-
623-17-6	1	1	1	2-Furanmethanol, acetate
623-26-7	1	0	0	1,4-Benzenedicarbonitrile
623-36-9	1	0	0	2-Pentenal, 2-methyl-
623-37-0	1	1	1	3-Hexanol
623-42-7	0	1	0	Butanoic acid, methyl ester
623-50-7	1	0	0	Acetic acid, hydroxy-, ethyl ester
623-56-3	1	0	0	3-Hexanone, 5-methyl-
623-91-6	0	1	0	2-Butenedioic acid (*E*)-, diethyl ester {diethyl fumarate}
624-24-8	0	1	0	Pentanoic acid, methyl ester {methyl valerate}
624-29-3	1	0	0	Cyclohexane, 1,2-dimethyl-, (*Z*)-
624-41-9	0	1	0	Acetic acid, 2-methylbutyl ester
624-45-3	1	1	1	Pentanoic acid, 4-oxo-, methyl ester {methyl levulinate}
624-48-6	1	0	0	2-Butenedioic acid (*Z*)-, dimethyl ester
624-51-1	1	0	0	3-Nonanol
624-64-6	1	0	0	2-Butene, (*E*)
624-78-2	1	1	1	Ethanamine, *N*-methyl-
624-80-6	1	0	0	Hydrazine, ethyl-
624-83-9	1	0	0	Methane, isocyanato- {methyl isocyanate}
624-89-5	1	0	0	Ethane, (methylthio)-
624-91-9	1	1	1	Nitrous acid, methyl ester
624-92-0	1	1	1	Disulfide, dimethyl
625-08-1	1	1	1	Butanoic acid, 3-hydroxy-3-methyl-
625-23-0	1	1	1	2-Hexanol, 2-methyl-
625-27-4	1	0	0	2-Pentene, 2-methyl-
625-28-5	1	1	1	Butanenitrile, 3-methyl-
625-30-9	1	1	1	2-Pentanamine
625-33-2	1	1	1	3-Penten-2-one
625-37-6	1	0	0	2-Butenamide, (*E*)- [2 CAS Nos.] {crotonamide}
23350-58-5				
625-38-7	1	0	0	3-Butenoic acid
625-43-4	1	1	1	1-Propanamine, *N*,2-dimethyl-
625-45-6	0	1	0	Acetic acid, methoxy-
625-50-3	1	0	0	Acetamide, *N*-ethyl-
625-55-8	1	0	0	Formic acid, 1-methylethyl ester
625-82-1	1	1	1	1*H*-Pyrrole, 2,4-dimethyl-
625-84-3	1	1	1	1*H*-Pyrrole, 2,5-dimethyl-
625-86-5	1	1	1	Furan, 2,5-dimethyl-
626-06-2	0	1	0	2(1*H*)-Pyridinone, 6-hydroxy- {2,6-pyridinediol}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
626-17-5	1	0	0	1,3-Benzenedicarbonitrile
626-23-3	0	1	0	2-Butanamine, *N*-(1-methylpropyl)-
626-51-7	1	0	0	Pentanedioic acid, 3-methyl-
626-56-2	1	0	0	Piperidine, 3-methyl-
626-58-4	1	0	0	Piperidine, 4-methyl-
626-64-2	1	0	0	4-Pyridinol {4(1*H*)-pyridinone}
108-96-3				
626-67-5	0	1	0	Piperidine, 1-methyl-
626-77-7	0	1	0	Hexanoic acid, propyl ester
626-82-4	0	1	0	Hexanoic acid, butyl ester
626-89-1	0	1	0	1-Pentanol, 4-methyl-
626-93-7	1	1	1	2-Hexanol
626-96-0	1	0	0	Pentanal, 4-oxo-
626-97-1	1	0	0	Pentanamide {valeramide}
626-98-2	1	1	1	2-Pentenoic acid
627-05-4	1	0	0	Butane, 1-nitro-
627-20-3	1	0	0	2-Pentene, (*Z*)-
627-21-4	1	0	0	2-Pentyne
627-27-0	1	0	0	3-Buten-1-ol
627-35-0	1	1	1	1-Propanamine, *N*-methyl-
627-59-8	1	1	1	2-Hexanol, 5-methyl-
627-69-0	1	1	1	1,2-Propanediol, 1-acetate
627-98-5	0	1	0	1-Hexanol, 5-methyl-
628-02-4	1	0	0	Hexanamide
628-05-7	1	0	0	Pentane, 1-nitro-
628-29-5	1	0	0	Butane, 1-(methylthio)- {butyl methyl sulfide}
628-41-1	0	1	0	1,4-Cyclohexadiene
628-46-6	0	1	0	Hexanoic acid, 5-methyl-
628-63-7	0	1	0	Acetic acid, pentyl ester
628-71-7	1	0	0	1-Heptyne
628-73-9	1	0	0	Hexanenitrile {capronitrile}
628-97-7	1	1	1	Hexadecanoic acid, ethyl ester {ethyl palmitate}
628-99-9	1	0	0	2-Nonanol
629-06-1	1	0	0	Heptane, 1-chloro-
629-08-3	1	0	0	Heptanenitrile
629-20-9	1	0	0	1,3,5,7-Cyclooctatetraene
629-33-4	0	1	0	Formic acid, hexyl ester
629-50-5	1	1	1	Tridecane
629-59-4	1	1	1	Tetradecane
629-62-9	1	1	1	Pentadecane
629-70-9	0	1	0	Acetic acid, 1-hexadecyl ester
629-73-2	1	0	0	1-Hexadecene {1-cetene}
629-76-5	1	1	1	1-Pentadecanol
629-78-7	1	1	1	Heptadecane
629-80-1	0	1	0	Hexadecanal
629-87-8	1	1	1	Pentacosane, 2-methyl-
629-90-3	0	1	0	Heptadecanal
629-92-5	1	1	1	Nonadecane
629-94-7	1	1	1	Heneicosane
629-96-9	1	1	1	1-Eicosanol {arachic alcohol}
629-97-0	1	1	1	Docosane
629-99-2	1	1	1	Pentacosane

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
630-01-3	1	1	1	Hexacosane
630-02-4	1	1	1	Octacosane
630-03-5	1	1	1	Nonacosane
630-04-6	1	1	1	Hentriacontane
630-05-7	1	1	1	Tritriacontane
630-06-8	1	1	1	Hexatriacontane
630-07-9	1	1	1	Pentatriacontane
630-08-0	1	0	0	Carbon monoxide
630-19-3	1	0	0	Propanal, 2,2-dimethyl- {pivalaldehyde}
631-57-2	1	0	0	Propanenitrile, 2-oxo-
631-66-3	1	0	0	Propanamide, 2-oxo- {pyruvamide}
634-36-6	1	1	1	Benzene, 1,2,3-trimethoxy-
634-97-9	1	0	0	1*H*-Pyrrole-2-carboxylic acid
635-46-1	1	0	0	Quinoline, 1,2,3,4-tetrahydro-
635-90-5	1	0	0	1*H*-Pyrrole, 1-phenyl-
636-38-4	0	1	0	2-Propenal, 2,3-dihydroxy-
636-41-9	1	0	0	1*H*-Pyrrole, 2-methyl-
636-44-2	1	0	0	3-Furancarboxylic acid, 2,5-dimethyl-
636-58-8	0	1	0	*L*-Cysteine, *N*-*L*-γ-glutamyl-
636-60-2	1	0	0	Butanedioic acid, methyl-, (±)-
637-50-3	1	1	1	Benzene, 1-propenyl-
637-69-4	1	0	0	Benzene, 1-ethenyl-4-methoxy-
637-88-7	1	1	1	1,4-Cyclohexanedione
638-00-6	1	0	0	Thiophene, 2,4-dimethyl-
638-25-5	0	1	0	Octanoic acid, pentyl ester
638-31-3	1	0	0	1*H*-Pyrrole, 2,3-dihydro-
638-36-8	1	1	1	Hexadecane, 2,6,10,14-tetramethyl- {phytane}
638-37-9	1	0	0	Butanedial {succinaldehyde}
638-49-3	0	1	0	Formic acid, pentyl ester
638-53-9	1	1	1	Tridecanoic acid
638-67-5	1	1	1	Tricosane
638-68-6	1	1	1	Triacontane
638-95-9	1	1	1	Urs-12-en-3-ol, (3β)- {α-amyrin}
639-99-6	0	1	0	Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)-, [1R-(1α,3α,4β)]-
640-06-2	1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy- {Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, γ-lactone, quinic acid lactone, quinide}
640-15-3	0	1	0	Phosphorodithioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Thiometon®}
641-38-3	0	1	0	6*H*-Dibenzo[*b,d*]pyran-6-one, 1-methyl-3,7,9-trihydroxy-
641-48-5	1	0	0	Aceanthrylene, 1,2-dihydro-
643-13-0	0	1	0	*D*-Fructose, 6-(dihydrogen phosphate)
643-38-9	0	1	0	2,3-Quinolinedicarboxylic acid
643-57-2	0	1	0	4*H*-1-Benzopyran-4-one, 2,7-dihydroxy-3-(3,7,11-trimethyldodeca-2,6,10-trienyl)- {ammoresinol}
643-58-3	1	0	0	1,1′-Biphenyl, 2-methyl-
643-93-6	1	0	0	1,1′-Biphenyl, 3-methyl-
644-00-8	1	0	0	21*H*,23*H*-Porphine-2-propanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-
644-08-6	1	0	0	1,1′-Biphenyl, 4-methyl-
644-30-4	0	1	0	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-
644-35-9	1	0	0	Phenol, 2-propyl-
644-46-2	1	0	0	4*H*-Pyran-4-one, 5-hydroxy-2-methyl- = 4*H*-pyran-4-one, 3-hydroxy-6-methyl- {allomaltol}
644-76-8	1	0	0	β-*D*-Galactopyranose, 1,6-anhydro-
644-98-4	1	0	0	Pyridine, 2-(1-methylethyl)-
645-08-9	1	0	0	Benzoic acid, 3-hydroxy-4-methoxy- {isovanillic acid}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
645-49-8	1	0	0	Benzene, 1,1′-(1,2-ethenediyl)bis-, (*Z*)-
645-56-7	1	0	0	Phenol, 4-propyl-
645-59-0	1	0	0	Benzenepropanenitrile
645-72-7	1	1	1	1-Hexadecanol, 3,7,11,15-tetramethyl- {dihydrophytol}
646-04-8	1	0	0	2-Pentene, (*E*)-
646-07-1	1	1	1	Pentanoic acid, 4-methyl- {isocaproic acid}
646-20-8	1	0	0	Heptanedinitrile
646-30-0	1	1	1	Nonadecanoic acid
646-31-1	1	1	1	Tetracosane
652-67-5	1	0	0	*D*-Glucitol, 1,4:3,6-dianhydro-
656-53-1	1	0	0	Thiazole, 4-methyl-5-(2-acetoxyethyl)-
659-70-1	1	1	1	Butanoic acid, 3-methyl-, 3-methylbutyl ester {isoamyl isovalerate}
661-19-8	1	1	1	1-Docosanol {behenyl alcohol}
665-27-0	1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy-, [1S-(exo,exo)]-
668-30-4	1	0	0	Indeno[1,2,3,4-*defg*]chrysene {also known as indeno[3,2,1,7-*defg*]chrysene, dibenzo[*b,mno*]fluoranthene, naphtho[1,2,3,4-*ghi*]fluoranthene}
672-15-1	1	1	1	Homoserine [2 CAS Nos.] {2-amino-4-hydroxybutanoic acid}
498-19-1				
673-32-5	1	0	0	Benzene, 1-propynyl-
673-84-7	1	0	0	2,4,6-Octatriene, 2,6-dimethyl- {alloöcimene}
674-76-0	1	0	0	2-Pentene, 4-methyl-, (*E*)-
675-20-7	1	1	1	2-Piperidinone {5-pentanelactam}
676-46-0	0	1	0	Butanedioic acid, hydroxy-, disodium salt
685-73-4	1	1	1	*D*-Galacturonic acid
685-91-6	1	0	0	Acetamide, *N,N*-diethyl-
688-31-3	1	0	0	1-Pentanamine, 2-ethyl-*N,N*-dimethyl-
689-67-8	0	1	0	5,9-Undecadien-2-one, 6,10-dimethyl-
689-97-4	1	0	0	1-Buten-3-yne
691-37-2	1	0	0	1-Pentene, 4-methyl-
691-38-3	1	0	0	2-Pentene, 4-methyl-, (*Z*)-
692-31-9	1	0	0	2-Buten-1-amine, *N,N*-dimethyl-
692-33-1	1	0	0	Acetamide, *N*-2-propenyl-
692-45-5	1	0	0	Formic acid, ethenyl ester {vinyl formate}
692-73-0	1	0	0	Ethanone, 1-(hydroxymethylphenyl)-
692-86-4	0	1	0	10-Undecenoic acid, ethyl ester
693-02-7	1	0	0	1-Hexyne
693-19-6	0	1	0	Octanoic acid, 7-methyl-
693-23-2	1	0	0	Dodecanedioic acid
693-54-9	1	1	1	2-Decanone {methyl octyl ketone}
693-89-0	1	0	0	Cyclopentene, 1-methyl-
693-95-8	1	0	0	Thiazole, 4-methyl-
693-98-1	1	0	0	1*H*-Imidazole, 2-methyl-
694-05-3	1	1	1	Pyridine, 1,2,3,6-tetrahydro- {Δ^3-piperidine}
694-81-5	1	0	0	Pyrimidine, 4,5-dimethyl-
694-85-9	1	1	1	2(1*H*)-Pyridinone, 1-methyl-
695-06-7	1	1	1	2(3*H*)-Furanone, dihydro-5-ethyl- {γ-hexalactone}
695-34-1	1	0	0	2-Pyridinamine, 4-methyl- {2-amino-4-picoline}
695-84-1	1	0	0	Phenol, 2-ethenyl-
695-98-7	1	1	1	Pyridine, 2,3,5-trimethyl- {2,3,5-collidine}
696-30-0	1	0	0	Pyridine, 4-(1-methylethyl)-
697-82-5	1	0	0	Phenol, 2,3,5-trimethyl- {isopseudocumenol}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
698-10-2	0	1	0	2(5*H*)-Furanone, 5-ethyl-3-hydroxy-4-methyl-
698-27-1	0	1	0	Benzaldehyde, 2-hydroxy-4-methyl-
698-71-5	1	1	1	Phenol, 3-ethyl-5-methyl-
698-76-0	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-propyl- {δ-octalactone}
699-02-5	0	1	0	Benzeneethanol, 4-methyl-
699-22-9	1	1	1	1*H*-Pyrrole, 1-pentyl-
1551-12-8				
699-83-2	1	0	0	Ethanone, 1-(2,6-dihydroxyphenyl)-
700-13-0	1	0	0	1,4-Benzenediol, 2,3,5-trimethyl-
700-46-9	1	0	0	Quinazoline, 4-methyl-
700-79-8	1	0	0	Quinazoline, 2-methyl-
703-23-1	1	0	0	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-
703-98-0	1	0	0	Ethanone, 1-(2-hydroxy-3-methoxyphenyl)-
705-86-2	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-pentyl- {δ-decalactone}
706-14-9	0	1	0	2(3*H*)-Furanone, dihydro-5-hexyl- {γ-decalactone}
707-35-7	0	1	0	Tricyclo[3.3.1.1]decane, 1,3,5-trimethyl-
708-76-9	1	1	1	Benzaldehyde, 4,6-dimethoxy-2-hydroxy-
710-04-3	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-hexyl- {δ-undecalactone}
711-79-5	1	1	1	Ethanone, 1-(1-hydroxy-2-naphthalenyl)-
713-68-8	1	0	0	Phenol, 3-phenoxy-
713-95-1	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-heptyl- {δ-dodecalactone}
723-98-8	1	0	0	1*H*-Cyclopenta[*l*]phenanthrene, 2,3-dihydro-
732-26-3	1	1	1	Phenol, 2,4,6-tris(1,1-dimethylethyl)-
747-90-0	1	0	0	Cholesta-3,5-diene
759-94-4	0	1	0	Carbamothioic acid, dipropyl-, *S*-ethyl ester {EPTC®}
760-20-3	1	0	0	1-Pentene, 3-methyl-
760-21-4	1	0	0	Pentane, 3-methylene- {2-ethyl-1-butene}
762-29-8	1	1	1	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl- {three isomers} {farnesyl acetone}
763-29-1	1	0	0	1-Pentene, 2-methyl-
763-30-4	1	0	0	1,4-Pentadiene, 2-methyl-
763-89-***3***	0	1	0	3-Penten-1-ol, 4-methyl-
763-93-9	1	0	0	3-Hexen-2-one
764-13-6	1	0	0	2,4-Hexadiene, 2,5-dimethyl-
764-35-2	1	0	0	2-Hexyne
764-39-6	0	1	0	2-Pentenal
764-40-9	1	1	1	2,4-Pentadienal
765-38-8	1	0	0	Pyrrolidine, 2-methyl-
765-43-5	1	0	0	Ethanone, 1-cyclopropyl-
765-69-5	1	0	0	1,3-Cyclopentanedione, 2-methyl-
765-70-8	1	1	1	1,2-Cyclopentanedione, 3-methyl- {cyclotene}
765-87-7	0	1	0	1,2-Cyclohexanedione
766-09-6	1	0	0	Piperidine, 1-ethyl-
766-36-9	1	0	0	2*H*-Pyrrol-2-one, 3-ethyl-1,5-dihydro-4-methyl-
766-39-2	1	1	1	2,5-Furandione, 3,4-dimethyl-
766-45-0	1	0	0	2*H*-Pyrrol-2-one, 4-ethyl-1,5-dihydro-3-methyl-
767-00-0	1	0	0	Benzonitrile, 4-hydroxy-
767-10-2	1	0	0	Pyrrolidine, 1-butyl-
767-58-8	1	0	0	1*H*-Indene, 2,3-dihydro-1-methyl-
767-59-9	1	0	0	1*H*-Indene, 1-methyl-
767-60-2	1	0	0	1*H*-Indene, 3-methyl-
769-92-6	0	1	0	Benzenamine, 4-(1,1-dimethylethyl)- {parvoline}
770-39-8	1	0	0	2-Propanone, 1-(4-hydroxyphenyl)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
771-50-6	0	1	0	1*H*-Indole-3-carboxylic acid
771-51-7	0	1	0	1*H*-Indole-3-acetonitrile
774-64-1	1	1	1	2(5*H*)-Furanone, 3,4-dimethyl-5-pentylidene- {bovolide}
776-35-2	1	0	0	Phenanthrene, 9,10-dihydro-
779-02-2	1	0	0	Anthracene, 9-methyl-
779-03-3	1	0	0	9-Anthracenamine
779-90-8	0	1	0	Ethanone, 1,1′,1″-(1,3,5-benzenetriyl)tris- {1,3,5-triacetylbenzene}
781-43-1	1	0	0	Anthracene, 9,10-dimethyl-
782-08-1	1	0	0	Methane, chlorobis(4-chlorophenyl)-
789-02-6	1	1	1	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]- {*o,p′*-DDT}
811-97-2	1	1	1	Ethane, 1,1,1,2-tetrafluoro- {Freon® 134a}
813-94-5	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, calcium salt
814-78-8	1	0	0	3-Buten-2-one, 3-methyl-
817-88-9	0	1	0	3,7-Nonadien-2-one, 4,8-dimethyl-
818-49-5	0	1	0	1-Hexanol, 4-methyl-
820-11-1	0	1	0	Propanoic acid, 2-hydroxy-3-(phosphonooxy)-
821-08-9	1	0	0	1,5-Hexadien-3-yne {divinylacetylene}
821-38-5	1	0	0	Tetradecanedioic acid
821-41-0	1	0	0	5-Hexen-1-ol
821-55-6	1	1	1	2-Nonanone
821-95-4	1	0	0	1-Undecene
822-36-6	1	0	0	1*H*-Imidazole, 4-methyl-
822-50-4	1	0	0	Cyclopentane, 1,2-dimethyl-, *trans*-
822-51-5	1	0	0	1*H*-Pyrrole, 3,4-dimethyl-
822-67-3	1	1	1	2-Cyclohexen-1-ol
822-90-2	1	0	0	1*H*-Imidazole, 2,4,5-trimethyl-
823-22-3	1	1	1	2*H*-Pyran-2-one, tetrahydro-6-methyl- {δ-hexalactone, δ–caprolactone}
26991-67-3				
823-36-9	1	0	0	1,3-Cyclopentanedione, 2-ethyl-
823-40-5	1	0	0	1,3-Benzenediamine, 2-methyl-
823-76-7	0	1	0	Ethanone, 1-cyclohexyl-
823-82-5	1	1	1	2,5-Furandicarboxaldehyde
824-22-6	1	0	0	1*H*-Indene, 2,3-dihydro-4-methyl-
824-46-4	1	1	1	1,4-Benzenediol, 2-methoxy-
824-63-5	1	0	0	1*H*-Indene, 2,3-dihydro-2-methyl-
824-90-8	1	0	0	Benzene, 1-butenyl-
826-74-4	1	0	0	Naphthalene, 1-ethenyl-
827-54-3	1	0	0	Naphthalene, 2-ethenyl-
828-82-0	1	0	0	4*H*-1-Benzopyran-4-one, 3-ethyl-
829-26-5	1	1	1	Naphthalene, 2,3,6-trimethyl-
830-96-6	0	1	0	1*H*-Indole-3-propanoic acid
831-82-3	1	0	0	Phenol, 4-phenoxy-
832-64-4	1	0	0	Phenanthrene, 4-methyl-
832-69-9	1	0	0	Phenanthrene, 1-methyl-
832-71-3	1	0	0	Phenanthrene, 3-methyl-
834-24-2	1	0	0	Benzenamine, 4-(2-phenylethenyl)-
866-84-2	1	1	1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripotassium salt
868-57-5	0	1	0	Butanoic acid, 2-methyl-, methyl ester
869-06-7	0	1	0	Butanedioic acid, hydroxy-, magnesium salt
870-23-5	1	0	0	2-Propene-1-thiol
871-71-6	1	0	0	Formamide, *N*-butyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
871-83-0	1	0	0	Nonane, 2-methyl-
872-05-9	1	1	1	1-Decene
872-50-4	1	1	1	2-Pyrrolidinone, 1-methyl-
872-55-9	1	0	0	Thiophene, 2-ethyl-
873-64-3	1	0	0	Thiazole, 4,5-dimethyl-2-ethyl-
873-62-1	1	0	0	Benzonitrile, 3-hydroxy-
874-35-1	1	0	0	1*H*-Indene, 2,3-dihydro-5-methyl-
874-41-9	1	0	0	Benzene, 1,3-dimethyl-4-ethyl-
874-63-5	1	0	0	Benzene, 3,5-dimethyl-1-methoxy-
874-66-8	1	0	0	2-Propenal, 3-(2-furanyl)-2-methyl-
875-30-9	1	0	0	1*H*-Indole, 1,3-dimethyl-
875-79-6	1	0	0	1*H*-Indole, 1,2-dimethyl-
875-80-9	1	0	0	Imidazo[1,2-*a*]pyridine, 2,3-dimethyl-
877-43-0	1	1	1	Quinoline, 2,6-dimethyl-
877-95-2	1	0	0	Acetamide, *N*-(2-phenylethyl)-
883-20-5	1	0	0	Phenanthrene, 9-methyl-
886-66-8	1	0	0	Benzene, 1,1′-(1,3-butadiyne-1,4-diyl)bis-
905-99-7	0	1	0	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-, (1α,3α,4α,5β)-
906-33-2	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-(1α,3α,4α,5β)]- {neochlorogenic acid, 5-*O*-caffeoylquinic acid} Also listed as cyclohexanecarboxylic acid, 5-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-
919-86-8	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *S*-[2-(ethylthio)ethyl] ester {Demeton-S-methyl®}
921-53-9	0	1	0	Butanedioic acid, 2,3-dihydroxy- [R-(R*,R*)]-, dipotassium salt
922-61-2	1	0	0	2-Pentene, 3-methyl- (*Z*)
923-16-0	0	1	0	*D*-Alanine, *N*-*D*-alanyl-
924-16-3	1	1	1	1-Butanamine, *N*-butyl-*N*-nitroso- {NDBA}
924-46-9	1	1	1	1-Propanamine, *N*-methyl-*N*-nitroso- {NMPA}
926-56-7	0	1	0	1,3-Pentadiene, 4-methyl-
926-64-7	1	0	0	Acetonitrile, (dimethylamino)-
927-20-8	0	1	0	1,2,3-Propanetriol, 1-(dihydrogen phosphate), magnesium salt (1:1)
927-49-1	0	1	0	6-Undecanone
927-56-0	1	0	0	Pentanenitrile, 4-oxo-
927-97-9	1	0	0	1,4-Hexadiene, 2,5-dimethyl-
928-49-4	1	0	0	3-Hexyne
928-68-7	1	1	1	2-Heptanone, 6-methyl-
928-95-0	0	1	0	2-Hexen-1-ol
928-96-1	1	1	1	3-Hexen-1-ol, (*Z*)- {leaf alcohol}
928-97-2	0	1	0	3-Hexen-1-ol, (*E*)-
929-10-2	0	1	0	Heptanoic acid, 6-methyl-
929-20-4	1	0	0	1,3,6-Octatriene
930-18-7	1	0	0	Cyclopropane, 1,2-dimethyl-, (*Z*)-
930-27-8	1	1	1	Furan, 3-methyl-
930-30-3	1	0	0	2-Cyclopenten-1-one {cyclopenten-3-one}
930-36-9	1	0	0	1*H*-Pyrazole, 1-methyl-
930-55-2	1	1	1	Pyrrolidine, 1-nitroso- {NPYR}
930-60-9	0	1	0	4-Cyclopentene-1,3-dione
930-62-1	1	0	0	1*H*-Imidazole, 2,4-dimethyl-
930-68-7	1	1	1	2-Cyclohexen-1-one
931-17-9	0	1	0	1,2-Cyclohexanediol, (*E*)-
931-20-4	1	1	1	2-Piperidinone, 1-methyl-
931-22-6	1	1	1	2-Cyclopenten-1-one, 3,5-dimethyl-
931-35-1	0	1	0	1*H*-Imidazole, 4,5-dihydro-2-ethyl-4-methyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
931-36-2	1	0	0	1*H*-Imidazole, 2-ethyl-4-methyl-
931-40-8	1	0	0	1,3-Dioxalan-2-one, 4-(hydroxymethyl)- {glycerol carbonate}
932-16-1	1	1	1	Ethanone, 1-(1-methyl-1*H*-pyrrol-2-yl)-
932-17-2	1	0	0	2-Pyrrolidinone, 1-acetyl-
932-53-6	0	1	0	6-Azathymine
932-62-7	1	1	1	Ethanone, 1-(1-methyl-1*H*-pyrrol-3-yl)-
932-66-1	1	0	0	Ethanone, 1-(1-cyclohexen-1-yl)-
933-40-4	1	0	0	Cyclohexane, 1,1-dimethoxy-
933-67-5	1	0	0	1*H*-Indole, 7-methyl-
933-99-3	1	0	0	1,2-Benzenediol, 3-ethyl-
934-00-9	1	1	1	1,2-Benzenediol, 3-methoxy-
934-34-9	0	1	0	2(3*H*)-Benzothiazolone
934-80-5	1	0	0	Benzene, 1,2-dimethyl-4-ethyl-
935-13-7	1	0	0	Propanoic acid, 3-(2-furanyl)-
935-92-2	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2,3,5-trimethyl-
936-12-9	1	0	0	1*H*-Pyrrole-3-carboxylic acid, 2-methyl-, ethyl ester
937-30-4	1	0	0	Ethanone, 1-(4-ethylphenyl)-
937-61-1	1	0	0	Benzene, propoxymethyl- {benzyl propyl ether}
938-22-7	0	1	0	Benzene, 1,2,3,5-tetrachloro-4-methoxy-
938-33-0	1	0	0	Quinoline, 8-methoxy-
939-23-1	1	1	1	Pyridine, 4-phenyl-
939-27-5	1	1	1	Naphthalene, 2-ethyl-
941-98-0	1	0	0	Ethanone, 1-(1-naphthalenyl) {1′-acetonaphthone}
942-24-5	0	1	0	1*H*-Indole-3-carboxylic acid, methyl ester
942-43-8	0	1	0	1*H*-Indene, 2,3-dihydro-1,1,5,6-tetramethyl-
944-22-9	0	1	0	Phosphonodithioic acid, ethyl-, *O*-ethyl S-phenyl ester {Fonofos®}
946-18-9	1	0	0	1*H*-Benzimidazole, 2-(3-methylbutyl)-
947-02-4	0	1	0	Dithiolan-2-ylidenephosphoramidic acid, diethyl ester {Cyolane®, Phosfolan®}
947-73-9	1	0	0	9-Phenanthrenamine
948-65-2	1	1	1	1*H*-Indole, 2-phenyl-
950-37-8	0	1	0	Phosphorodithioic acid, *O,O*-dimethyl-*S*-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl ester {Supracide®, Methidathion®}
954-21-2	1	1	1	Benzeneacetamide, *N*-methyl-α-phenyl- {desmethyl diphenamid}
957-51-7	1	1	1	Benzeneacetamide, *N,N*-dimethyl-α-phenyl- {diphenamid, Enide®}
959-98-8	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aβ,6α,9α,9aβ)- {α-Endosulfan®}
961-22-8	0	1	0	Phosphorothioic acid, *O*,*O*-dimethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl) methyl] ester
963-89-3	1	0	0	Benz[*c*]acridine, 7,9-dimethyl-
970-73-0	0	1	0	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*E*)-
970-74-1	0	1	0	2*H*-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R-*Z*)-
997-10-4	0	1	0	Propanal, 2-oxo-3-hydroxy- {reductone}
997-68-2	0	1	0	*L*-Glutamic acid, *N*-(5-amino-5-carboxypentyl)-, (S)-
1001-43-0	1	1	1	Tetracosanoic acid, tetracosyl ester
1002-43-3	1	1	1	Undecane, 3-methyl-
1002-84-2	1	1	1	Pentadecanoic acid
1003-28-7	1	1	1	Pyrrolidine, 2-ethyl-
1003-29-8	1	1	1	1*H*-Pyrrole-2-carboxaldehyde
1003-56-1	1	0	0	2-Pyridinol, 3-methyl- {2(1*H*)-pyridinone, 3-methyl-}
91914-04-4				
1003-68-5	1	0	0	2-Pyridinol, 5-methyl- {2(1*H*)-pyridinone, 5-methyl-}
91914-06-6				

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
1003-73-2	1	0	0	Pyridine, 3-methyl-*N*-oxide
1004-36-0	1	0	0	4*H*-Pyran-4-one, 2,6-dimethyl-
1004-66-6	1	0	0	Benzene, 1,3-dimethyl-2-methoxy-
1006-59-3	1	0	0	Phenol, 2,6-diethyl-
1007-26-7	0	1	0	Benzene, (2,2-dimethylpropyl)-
1007-32-5	1	0	0	2-Butanone, 1-phenyl-
1008-88-4	1	0	0	Pyridine, 3-phenyl-
1008-89-5	1	0	0	Pyridine, 2-phenyl-
1009-14-9	1	0	0	1-Pentanone, 1-phenyl-
1009-20-6	0	1	0	Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadieny-1-yl ester
1012-72-2	1	1	1	Benzene, 1,4-bis(1.1-dimethylethyl)-
1014-60-4	1	1	1	Benzene, 1,3-bis(1.1-dimethylethyl)-
1014-83-1	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, (*Z*)- {*cis*-ferulic acid}
1022-22-6	1	1	1	Benzene, 1,1′-(chloroethenylidene)bis[4-chloro- {DDM}
1024-57-3	1	1	1	2,5-Methano-2*H*-indeno[1,2-*b*]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)- {Heptachlor® epoxide}
1031-07-8	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3,3-dioxide {Thiodan® sulfate, Endosulfan® sulfate}
1066-33-7	1	1	1	Carbonic acid, monoammonium salt {ammonium hydrogen carbonate}
1067-20-5	1	0	0	Pentane, 3,3-diethyl-
1069-09-6	0	1	0	Arginine, *N*2-(1-carboxyethyl)- [2 CAS Nos.]
34522-32-2				
1070-68-4	0	1	0	Heptanoic acid, 5-methyl-
1070-83-3	0	1	0	Butanoic acid, 3,3-dimethyl-
1071-23-4	0	1	0	Ethanol, 2-amino-, dihydrogen phosphate (ester)
1071-73-4	1	1	1	2-Pentanone, 5-hydroxy-
1071-81-4	1	0	0	Hexane, 2,2,5,5-tetramethyl-
1071-83-6	0	1	0	Glycine, *N*-(phosphonomethyl)-
1072-62-4	1	0	0	1*H*-Imidazole, 2-ethyl-
1072-82-8	1	1	1	Ethanone, 1-(1*H*-pyrrol-3-yl)- {3-acetylpyrrole, methyl 3-pyrrolyl ketone}
1072-83-9	1	1	1	Ethanone, 1-(1*H*-pyrrol-2-yl)- {2-acetylpyrrole, methyl 2-pyrrolyl ketone}
1072-87-3	1	0	0	1*H*-Pyrrole-2,5-dione, 3-methyl-
1072-91-9	1	0	0	1*H*-Pyrazole, 1,3,5-trimethyl-
1073-11-6	0	1	0	2(3*H*)-Furanone, dihydro-5-ethenyl-5-methyl-
1073-13-8	1	0	0	2-Cyclohexen-1-one, 4,4-dimethyl-
1073-26-3	1	1	1	1-Propanone, 1-(1*H*-pyrrol-2-yl)-
1073-96-7	1	1	1	4*H*-Pyran-4-one, 3,5-dihydroxy-2-methyl- {5-hydroxymaltol}
1074-43-7	1	0	0	Benzene, 1-methyl-3-propyl-
1074-55-1	1	0	0	Benzene, 1-methyl-4-propyl-
1075-38-3	1	0	0	Benzene, 1-(1,1-dimethylethyl)-3-methyl-
1076-26-2	1	0	0	2-Naphthalenol, 1-methyl-
1076-56-8	0	1	0	Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-
1077-16-3	1	0	0	Benzene, hexyl-
1078-61-1	1	1	1	Benzenepropanoic acid, 3,4-dihydroxy- {dihydrocaffeic acid}
1086-80-2	0	1	0	Benzo[*g*]pteridine-2,4(1*H*,3*H*)-dione, 7,8-dimethyl-
1088-56-8	0	1	0	Benzo[*g*]pteridine-2,4(3*H*,10*H*)-dione, 7,8,10-trimethyl-
1113-57-1	1	0	0	Butanamide, 2-methyl-
1113-60-6	0	1	0	Propanoic acid, 3-hydroxy-2-oxo-
1113-68-4	1	1	1	Acetamide, *N*-acetyl-*N*-methyl
1114-34-7	1	1	1	Lyxose
1114-71-2	0	1	0	Carbamothioic acid, butylethyl-, *S*-propyl ester {Tillam®, Pebulate®}
1115-08-8	1	0	0	1,4-Pentadiene, 3-methyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
1115-11-3	1	1	1	2-Butenal, 2-methyl-
1116-22-9	0	1	0	*L*-Glutamic acid, *N*-*L*-γ-glutamyl-
1116-54-7	1	1	1	Ethanol, 2,2′-(nitrosoimino)bis- {NDELA}
1117-52-8	1	1	1	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (*E,E*)-
1117-74-4	1	1	1	Hexanoic acid, 4-oxo-
1118-58-7	1	1	1	1,3-Pentadiene, 2-methyl-
1118-66-7	1	0	0	3-Penten-2-one, 4-amino-
1118-68-9	0	1	0	Glycine, *N,N*-dimethyl-
1118-77-0	0	1	0	Hexadecanoic acid, 3,7,11,15-tetramethyl-, methyl ester
1118-85-0	0	1	0	Butanoic acid, 2-amino-4-(methylsulfonyl)- [2 CAS Nos.] {methionine sulfone, methionine *S*-oxide}
3226-65-1				
1119-16-0	1	0	0	Pentanal, 4-methyl-
1119-19-3	1	0	0	2-Butynal
1119-29-5	1	0	0	Pentanamide, 4-methyl-
1119-44-4	0	1	0	3-Hepten-2-one
1119-49-9	1	0	0	Acetamide, *N*-butyl-
1119-60-4	0	1	0	6-Heptenoic acid
1120-21-4	1	1	1	Undecane
1120-25-8	0	1	0	9-Hexadecenoic acid, methyl ester, (*Z*)-
1120-28-1	1	0	0	Eicosanoic acid, methyl ester
1120-36-1	1	1	1	1-Tetradecene
1120-62-3	1	0	0	Cyclopentene, 3-methyl-
1120-72-5	1	0	0	Cyclopentanone, 2-methyl-
1120-73-6	1	0	0	2-Cyclopenten-1-one, 2-methyl-
1121-05-7	1	1	1	2-Cyclopenten-1-one, 2,3-dimethyl-
1121-07-9	1	1	1	2,5-Pyrrolidinedione, 1-methyl-
1121-18-2	1	0	0	2-Cyclohexen-1-one, 2-methyl-
1121-19-3	1	0	0	3-Pyridinol, 4-methyl-
1121-25-1	1	1	1	3-Pyridinol, 2-methyl-
1121-33-1	1	0	0	Cyclopentanone, 2,4-dimethyl-
1121-55-7	1	1	1	Pyridine, 3-ethenyl-
1121-60-4	1	0	0	2-Pyridinecarboxaldehyde
1121-66-0	1	0	0	2-Cyclohepten-1-one
1121-78-4	1	0	0	3-Pyridinol, 6-methyl-
1121-84-2	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-methyl-
1121-89-7	1	0	0	2,6-Piperidinedione {glutarimide}
1122-39-0	1	0	0	Pyridine, 2,4,5-trimethyl- {2,4,5-collidine}
1122-43-6	1	0	0	3-Pyridinol, 2,6-dimethyl-
1122-45-8	1	0	0	Pyridine, 2,4-dimethyl-1-oxide
1122-54-9	1	1	1	Ethanone, 1-(4-pyridinyl)- {4-acetylpyridine}
1122-62-9	1	1	1	Ethanone, 1-(2-pyridinyl)- {2-acetylpyridine}
1122-69-6	1	0	0	Pyridine, 2-ethyl-6-methyl-
1122-70-9	1	0	0	Pyridine, 2-ethenyl-6-methyl-
1123-73-5	1	0	0	Phenol, 3-ethyl-2-methyl-
1123-94-0	1	0	0	Phenol, 4-ethyl-3-methyl-
1123-96-2	1	0	0	Pyridine, 2-ethyl-3,5-dimethyl- = pyridine, 2,4-dimethyl-6-ethyl-
1124-11-4	1	1	1	Pyrazine, tetramethyl-
1124-20-5	1	0	0	Benzene, 1-methyl-3-(1-methylethenyl)-
1124-35-2	1	0	0	Pyridine, 2-ethyl-4,6-dimethyl-
1124-39-6	1	0	0	1,2-Benzenediol, 4-ethyl-
1125-21-9	1	1	1	2-Cyclohexene-1,4-dione, 2,6,6-trimethyl- {4-ketoisophorone, 4-oxoisophorone}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
1125-78-6	1	0	0	2-Naphthalenol, 5,6,7,8-tetrahydro-
1125-80-0	1	0	0	Isoquinoline, 3-methyl-
1125-88-8	1	1	1	Benzene, dimethoxy-methyl-
1126-61-0	1	1	1	1,2-Benzenediol, 4-(2-propenyl)-
1127-76-0	1	1	1	Naphthalene, 1-ethyl-
1128-67-2	1	0	0	2(3*H*)-Benzothiazolone, 3-methyl-, hydrazone
1131-16-4	1	0	0	1*H*-Pyrazole, 3,5-dimethyl-1-phenyl-
1131-62-0	1	0	0	Ethanone, 1-(3,4-dimethoxyphenyl)-
1133-03-5	0	1	0	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-
1133-63-7	1	0	0	1,1′-Biphenyl, 2,3-dihydroxy-
1133-64-8	1	1	1	Pyridine, 3-(1-nitroso-2-piperidinyl)-, (S)- [2 CAS Nos.] {NAB}
37620-20-5				
1135-23-5	1	0	0	Benzenepropanoic acid, 4-hydroxy-3-methoxy- {hydroferulic acid}
1135-24-6	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, {ferulic acid}
1139-30-6	0	1	0	5-Oxatricyclo[8.2.0.04,6]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- {β-caryophyllene oxide}
1139-49-7	1	0	0	Benzene, 1-methyl-3-(2,2,6-trimethylcyclohexyl)- {toluene, *m*-(2,2,6-trimethylcyclohexyl)}
1148-79-4	1	1	1	2,2′:6′,2′-Terpyridine
1162-65-8	0	1	0	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,9a-tetrahydro-4-methoxy-, (6aR-*cis*)- {aflatoxin B_1}
1171-63-0	0	1	0	Pyrethrins (natural)
1176-52-9	0	1	0	Ergosta-7,24(28)-dien-3-ol, 4-methyl-, (3β,4α,5α)-
1180-71-8	1	0	0	11*H*,13*H*-Oxireno[d]pyrano[4′,3′:3,3a]isobenzofuro[5,4-f][2]benzopyran-4,6,13(2*H*,5a*H*)-trione,8-(3-furyl) decahydro-2,2,4a,8a-tetramethyl- {limonin}
1185-39-3	0	1	0	Pentanoic acid, 2,2-dimethyl-
1187-41-3	1	0	0	2-Butenamide, *N*,2-dimethyl-
72693-06-2				
1187-58-2	1	0	0	Propanamide, *N*-methyl-
1188-02-9	0	1	0	Heptanoic acid, 2-methyl-
1189-05-5	1	0	0	Acetamide, *N*-(1-methylpropyl)-
1190-63-2	1	1	1	Octadecanoic acid, hexadecyl ester
1190-76-7	1	0	0	2-Butenenitrile [*cis* or *trans*]
1190-94-9	0	1	0	Lysine, hydroxy-
28902-93-4				
1191-04-4	0	1	0	2-Hexenoic acid
1191-16-8	0	1	0	Acetic acid, 3-methyl-2-butenyl ester
1191-25-9	1	0	0	Hexanoic acid, 6-hydroxy-
1191-41-9	0	1	0	9,12,15-Octadecatrienoic acid, ethyl ester, (*Z,Z,Z*)-
1191-99-7	1	0	0	Furan, 2,3-dihydro-
1192-20-7	1	0	0	2(3*H*)-Furanone, 3-aminodihydro-
1192-42-3	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-3-methyl-
1192-51-4	1	0	0	2,4(3*H*,5*H*)-Furandione, 3-methyl-
1192-58-1	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 1-methyl-
1192-62-7	1	1	1	Ethanone, 1-(2-furanyl)- {2-acetylfuran}
1192-79-6	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 5-methyl-
1192-88-7	1	0	0	1-Cyclohexene-1-carboxaldehyde
1193-18-6	1	0	0	2-Cyclohexen-1-one, 3-methyl-
1193-55-1	1	1	1	1,3-Cyclohexanedione, 2-methyl-
1193-62-0	1	1	1	1*H*-Pyrrole-2-carboxylic acid, methyl ester
1193-79-9	1	1	1	Ethanone, 1-(5-methyl-2-furanyl)- {2-acetyl-5-methylfuran}
1194-97-4	1	0	0	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, methyl ester
1194-98-5	1	0	0	Benzaldehyde, 2,5-dihydroxy-
1195-09-1	1	1	1	Phenol, 2-methoxy-5-methyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
1195-32-0	1	0	0	Benzene, 1-methyl-4-(1-methylethenyl)- {*p*,α-dimethylstyrene}
1195-79-5	0	1	0	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-
1196-79-8	1	0	0	1*H*-Indole, 2,5-dimethyl-
1197-01-9	1	1	1	Benzenemethanol, α,α,4-trimethyl- {*p*,α,α-trimethylbenzyl alcohol}
1197-09-7	1	0	0	Ethanone, 1-(3,4-dihydroxyphenyl)-
1197-20-2	1	1	1	1,2-Propanedione, 1-(5-methyl-2-furanyl)-
1197-40-6	1	1	1	Furan, 2,2′-methylenebis-
1197-92-8	0	1	0	Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
1198-30-7	1	0	0	1-Isoquinolinecarbonitrile
1198-37-4	1	0	0	Quinoline, 2,4-dimethyl-
1198-84-1	1	0	0	Benzeneacetic acid, α,4-dihydroxy-
1202-08-0	0	1	0	Ethanone, 1-[2-methyl-5-(1-methylethyl)phenyl]-
1202-34-2	1	0	0	2-Pyridinamine, *N*-2-pyridinyl-
1202-41-1	0	1	0	2-Propenamide, 3-(3,4-dihydroxyphenyl)-
1203-08-3	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- {dehydro-β-ionone}
1207-20-1	1	0	0	9*H*-Fluorene, 2-ethyl-
1210-35-1	1	0	0	5*H*-Dibenzo[*a,d*]cycloheptен-5-one, 10,11-dihydro-
1211-29-6	0	1	0	Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester {methyl jasmonate}
1214-39-7	0	1	0	1*H*-Purin-6-amine, *N*-(phenylmethyl)-
1235-78-5	1	1	1	Spiro[furan-2(5*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5-one, 3′a,4′,5′,5′a,6′,7′,8′,9′,9′a,9′b-decahydro-3,3′a,6′,6′,9′a-pentamethyl-, [2′S-(2′α,3′aα,5′aβ,9′aα,9′bβ)]- {β-levantenolide}
1253-88-9	0	1	0	Cholest-5-en-3-ol, 4,4-dimethyl-, (3β)-
1289-40-3	1	0	0	Hexenoic acid
1289-45-8	1	0	0	Dodecenoic acid
1300-71-6	1	1	1	Phenol, dimethyl- {xylenol}
1305-62-0	0	1	0	Calcium hydroxide
1305-78-8	0	1	0	Calcium oxide
1309-37-1	0	1	0	Iron oxide (ferric oxide)
1332-37-2				
1309-48-4	0	1	0	Magnesium oxide
1310-73-2	0	1	0	Sodium hydroxide
1313-59-3	0	1	0	Sodium oxide
1314-56-3	0	1	0	Phosphorus oxide
1314-62-1	0	1	0	Vanadium pentoxide
1317-39-1	0	1	0	Copper oxide
1318-74-7	0	1	0	Kaolinite
1318-94-1	0	1	0	Muscovite
1319-77-3	1	1	1	Phenol, methyl- {cresol}
1321-16-0	1	0	0	Cyclohexenecarboxaldehyde
1321-27-3	1	1	1	Benzeneethanol (60-12-8) {phenethyl alcohol} Occasionally listed as 1321-27-3 Ethanol, phenyl-
60-12-8				
1321-48-8	1	0	0	1-Propanone, 1-phenyl-3-hydroxy-
1321-67-1	1	0	0	Naphthalenol
1321-94-4	1	1	1	Naphthalene, methyl-
1322-01-6	0	1	0	Benzoic acid, 4-hydroxy-, butyl ester
94-26-8				
1322-20-9	1	0	0	[1,1′-Biphenyl]-ol
1327-53-3	0	1	0	Arsenic oxide {arsenious oxide}
1329-97-1	1	0	0	Phenol, dimethyl-methoxy-
1329-99-3	1	1	1	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- {α-phellandrene}
99-83-2				
1330-20-7	1	1	1	Benzene, dimethyl- {xylene}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
1330-70-7	0	1	0	Octadecanoic acid, hydroxy-
1331-81-3	0	1	0	Benzenemethanol, ar-methoxy-
1332-37-2	0	1	0	Iron oxide (ferric oxide)
1309-37-1				
1332-40-7	0	1	0	Copper oxychloride [2 CAS Nos.] {RAME}
1332-65-6				
1332-82-7	0	1	0	Cobalt chloride
1333-22-8	0	1	0	Copper oxysulfate
1333-41-1	1	1	1	Pyridine, methyl- {picoline}
1333-52-4	1	1	1	Ethanone, 1-(2-naphthalenyl)- {methyl naphthyl ketone}
93-08-3				
1333-53-5	1	0	0	Quinoline, (1-methylethyl)-
1333-74-0	1	0	0	Hydrogen (molecular)
1334-78-7	1	0	0	Benzaldehyde, methyl-
1335-09-7	0	1	0	Heptenol, methyl-
1334-76-5	1	1	1	2-Furancarboxylic acid, methyl ester {methyl 2-furoate}
611-13-2				
1335-30-4	1	1	1	Aluminum silicate
1335-34-8	0	1	0	1,2,3-Propanetriol, mono(dihydrogen phosphate), potassium salt
1335-39-3	0	1	0	Hexenal
1336-21-6	0	1	0	Ammonium hydroxide
1337-81-1	1	0	0	Pyridine, ethenyl-
1338-24-5	0	1	0	Naphthenic acid
1344-13-4	0	1	0	Tin chloride (stannic chloride)
1344-28-1	0	1	0	Aluminum oxide
1398-61-4	0	1	0	*D*-Glucose, β-(1,4)-2-acetamido-2-deoxy-
1401-55-4	0	1	0	Tannins {tannic acid}
1405-86-3	0	1	0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl- {glycyrrhizic acid, glycyrrhizin}
1406-65-1	0	1	0	Chlorophylls a + b
1406-66-2	1	1	1	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl) {tocopherol}
1415-93-6	0	1	0	Humic acids
1430-97-3	1	0	0	9*H*-Fluorene, 2-methyl-
1438-90-0	1	0	0	1,2-Butanedione, 1-(2-furanyl)-
1438-92-2	1	1	1	1,2-Propanedione, 1-(2-furanyl)-
1438-94-4	1	1	1	1*H*-Pyrrole, 1-(2-furanylmethyl)-
1445-73-4	1	1	1	4-Piperidone, *N*-methyl-
1449-09-8	0	1	0	9,19-Cyclolanostan-3-ol, 24-methylene-, (3β)-
1450-72-2	1	1	1	Ethanone, 1-(2-hydroxy-5-methylphenyl)-
1452-77-3	1	0	0	2-Pyridinecarboxamide
1453-58-3	1	0	0	1*H*-Pyrazole, 3-methyl-
1453-82-3	0	1	0	4-Pyridinecarboxamide {isonicotinamide}
1454-84-8	1	1	1	1-Nonadecanol
1454-85-9	1	1	1	1-Heptadecanol
1456-08-2	1	0	0	Propanoic acid, 3-(5-methyl-2-furanyl)-
1460-18-0	1	0	0	Pentadecanedioic acid
1461-27-4	0	1	0	Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)-
1462-11-9	1	0	0	1,5-Hexanediol, 5-methyl-
1462-84-6	1	1	1	Pyridine, 2,3,6-trimethyl- {2,3,6-collidine}
1463-03-2	1	0	0	Pyridine, 2,6-dimethyl-3-phenyl-
1463-17-8	1	0	0	Quinoline, 2,8-dimethyl-
1464-44-4	0	1	0	β-*D*-Glucopyranoside, phenyl-
1467-79-4	1	1	1	Cyanamide, dimethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
1470-50-4	0	1	0	2-Octenoic acid
1470-94-6	1	0	0	1*H*-Inden-5-ol, 2,3-dihydro-
1484-12-4	1	0	0	9*H*-Carbazole, 9-methyl-
1484-19-1	1	0	0	1*H*-Indole, 3-ethyl-
1484-80-6	1	0	0	Piperidine, 2-ethyl-
1486-70-0	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-methoxy-
1487-18-9	1	1	1	Furan, 2-ethenyl-
1490-04-6	1	1	1	Cyclohexanol, 5-methyl-2-(1-methylethyl)- {menthol}
1500-94-3	1	0	0	Ethanone, 1-(2,5-dimethyl-1*H*-pyrrol-3-yl)-
1504-06-9	1	0	0	2*H*-Indol-2-one, 1,3-dihydro-3-methyl-
1504-16-1	1	0	0	1*H*-Indole, 3-phenyl-
1504-55-8	0	1	0	3-Buten-2-ol, 4-phenyl-
1504-74-1	0	1	0	2-Propenal, 3-(2-methoxyphenyl)- = 2-propenal, 3-phenyl-2′-methoxy-
1509-34-8	0	1	0	Isoleucine, allo-
1520-21-4	1	1	1	Benzenamine, 4-ethenyl- {4-aminostyrene}
1532-84-9	1	0	0	1-Isoquinolinamine
1530-88-7	1	0	0	1-Pyrrolidinecarbonitrile
1540-94-9	1	1	1	Acetamide, *N*-(2-methylpropyl)-
1551-08-2	0	1	0	1*H*-Pyrrole, 2-propyl-
1551-12-8	1	1	1	1*H*-Pyrrole, 1-pentyl-
699-22-9				
1551-16-***2***	1	0	0	1*H*-Pyrrole, 2-ethyl-
1556-99-6	1	0	0	9*H*-Fluorene, 4-methyl-
1558-17-4	1	0	0	Pyrimidine, 4,6-dimethyl-
1559-81-5	1	1	1	Naphthalene, 1-methyl-1,2,3,4-tetrahydro-
1560-72-1	1	1	1	Triacontane, 2-methyl-
1560-75-4	1	1	1	Nonacosane, 2-methyl-
1560-78-7	0	1	0	Tetracosane, 2-methyl-
1560-81-2	1	1	1	Docosane, 2-methyl-
1560-82-3	1	1	1	Heneicosane, 2-methyl-
1560-84-5	0	1	0	Eicosane, 2-methyl-
52845-08-6				
1560-88-9	0	1	0	Octadecane, 2-methyl-
1560-89-0	1	1	1	Heptadecane, 2-methyl-
1560-92-5	1	1	1	Hexadecane, 2-methyl-
1560-93-6	1	1	1	Pentadecane, 2-methyl-
1560-95-8	0	1	0	Tetradecane, 2-methyl-
1560-96-9	0	1	0	Tridecane, 2-methyl-
1560-97-0	1	0	0	Dodecane, 2-methyl-
1560-98-1	1	1	1	Octacosane, 2-methyl-
1561-00-8	1	1	1	Heptacosane, 2-methyl-
1561-02-0	1	1	1	Hexacosane, 2-methyl-
1561-11-1	0	1	0	Hexanoic acid, 4-methyl-
1563-38-8	0	1	0	7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-
1563-66-2	1	1	1	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester Sometimes listed as 7-benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate {Furadan®, Carbofuran®}
1567-93-7	1	0	0	2-Pentanone, 5-hydroxy-3-methyl-
1569-60-4	0	1	0	5-Hepten-2-ol, 6-methyl-
1570-48-5	1	1	1	1-Propanone, 1-(3-pyridinyl)- {pyridyl ethyl ketone}
1574-41-0	1	1	1	1,3-Pentadiene, (*Z*)-
1575-46-8	1	0	0	2(5*H*)-Furanone, 3,4-dimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
1575-57-1	1	1	1	2-Butanone, 1-(acetyloxy)-
1575-74-2	0	1	0	4-Pentenoic acid, 2-methyl-
1576-67-6	1	0	0	Phenanthrene, 3,6-dimethyl-
1576-69-8	1	0	0	Phenanthrene, 2,7-dimethyl-
1576-87-0	1	0	0	2-Pentenal, (*E*)-
1576-95-0	0	1	0	2-Penten-1-ol, (Z)
1577-20-4	1	1	1	4-Hexenoic acid, (*E*)-
1577-22-6	0	1	0	5-Hexenoic acid
1579-40-4	1	0	0	Benzene, 1.1′-oxybis(4-methyl-di-
1582-09-8	0	1	0	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)- {Trifluralin®}
1587-15-1	1	0	0	Butanedioic acid, hydroxy-, dimethyl ester {dimethyl malate, malic acid dimethyl ester}
1599-67-3	1	0	0	1-Docosene
1599-68-4	1	0	0	1-Heneicosene
1603-03-8	1	1	1	Hexadecanoic acid, 15-methyl-
1603-40-3	1	0	0	2-Pyridinamine, 3-methyl-
1603-41-4	1	0	0	2-Pyridinamine, 5-methyl-
1604-28-0	1	1	1	3,5-Heptadien-2-one, 6-methyl-, (*E*)-
1604-34-8	1	1	1	2-Undecanone, 6,10-dimethyl- {tetrahydrogeranylacetone}
1606-67-3	1	0	0	1-Pyreneamine
1608-63-5	0	1	0	2(3*H*)-Furanone, dihydro-3-(1-methylethyl)-
1611-21-8	1	0	0	Cyclohexene, 5-ethenyl-1,5-dimethyl-
1613-34-9	1	0	0	Quinoline, 2-ethyl-
1613-46-3	1	0	0	Butane, 1-(propylthio)-
1616-86-0	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-(1α,2β,4aβ,8aα)]- {*Z*-abienol}
1617-31-8	1	1	1	3-Butenoic acid, 3-methyl-
1617-32-9	1	0	0	3-Pentenoic acid, (*E*)-
1619-28-9	1	0	0	2-Cyclopenten-1-one, 3-(1-methylethyl)-
1620-76-4	1	0	0	2-Pyridinecarbonitrile, 4-methyl-
1620-98-0	0	1	0	Benzaldehyde, 3,5-di(1,1-dimethylethyl)-4-hydroxy-
1628-89-3	1	0	0	Pyridine, 2-methoxy-
1629-58-9	1	1	1	1-Penten-3-one
1630-94-0	1	0	0	Cyclopropane, 1,1-dimethyl-
1632-16-2	0	1	0	Heptane, 3-methylene-
1632-83-3	1	0	0	1*H*-Benzimidazole, 1-methyl-
1637-39-4	0	1	0	2-Buten-1-ol, 2-methyl-4-(1*H*-purin-6-ylamino)-, (*E*)-
1641-41-4	1	0	0	1*H*-Indenol, 2,3-dihydro- [1*H*-Inden-4-ol, 2,3-dihydro-]
1646-87-3	0	1	0	Propanal, 2-methyl-2-(methylsulfinyl)-, *O*-[(methylamino)carbonyl]oxime {Aldicarb Sulfoxide®}
1646-88-4	0	1	0	Propanal, 2-methyl-2-(methylsulfonyl)-, *O*-[(methylamino)carbonyl]oxime {Aldoxycarb®}
1652-97-7	1	0	0	2-Tetradecene
1653-40-3	0	1	0	1-Heptanol, 6-methyl-
1657-56-3	1	1	1	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-, (*E*)- {*trans*-DCS}
1667-01-2	0	1	0	Ethanone, 1-(2,4,6-trimethylphenyl)-
1669-44-9	0	1	0	3-Octen-2-one
1674-37-9	1	0	0	1-Octanone, 1-phenyl- {octanophenone}
1676-63-7	1	0	0	Ethanone, 1-(4-ethoxyphenyl)-
1678-91-7	1	0	0	Cyclohexane, ethyl-
1678-92-8	1	0	0	Cyclohexane, propyl-
1679-47-6	0	1	0	2(3*H*)-Furanone, dihydro-3-methyl-
1679-49-8	1	1	1	2(3*H*)-Furanone, dihydro-4-methyl-
1680-51-9	1	1	1	Naphthalene, 6-methyl-1,2,3,4-tetrahydro- {naphthalene, 2-methyl-5,6,7,8-tetrahydro-}
1680-58-6	1	1	1	Naphthalene, 1-(1-methylpropyl)-
1686-10-8	0	1	0	3-Hexadecenoic acid, (*E*)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
1687-61-2	1	0	0	Phenol, 2-ethyl-5-methyl-
1687-64-5	1	0	0	Phenol, 2-ethyl-6-methyl-
1687-65-6	1	0	0	Phenol, 5-ethyl-2-methyl-
1701-69-5	1	0	0	1-Propanone, 1-(4-pyridinyl)-
1701-70-8	1	1	1	1-Butanone, 1-(3-pyridinyl)- {propyl pyridyl ketone}
1703-51-1	1	1	1	Heptane-2,5-dione
1703-52-2	1	0	0	Furan, 2-ethyl-5-methyl-
1705-85-7	1	0	0	Chrysene, 6-methyl-
1705-89-1	1	0	0	9*H*-Fluoren-9-one, 3-methyl-
1706-01-0	1	0	0	Fluoranthene, 3-methyl-
1708-25-4	1	0	0	Furan, 2,3-dihydro-2-methyl-
1708-29-8	1	1	1	Furan, 2,5-dihydro-
1708-30-1	1	0	0	Furan, 2,5-dihydro-2-methyl-
1708-82-3	0	1	0	3-Hexen-1-ol, acetate
1720-11-2	1	1	1	Dotriacontane, 2-methyl-
1720-12-3	1	1	1	Hentriacontane, 2-methyl-
1721-93-3	1	0	0	Isoquinoline, 1-methyl-
1724-02-3	0	1	0	2-Pentenedioic acid {glutaconic acid}
1730-37-6	1	0	0	9*H*-Fluorene, 1-methyl-
1731-81-3	0	1	0	1-Undecanol, acetate
1731-84-6	0	1	0	Nonanoic acid, methyl ester
1731-86-8	0	1	0	Undecanoic acid, methyl ester
1731-88-0	0	1	0	Tridecanoic acid, methyl ester
1731-92-6	1	1	1	Heptadecanoic acid, methyl ester
1731-94-8	0	1	0	Nonadecanoic acid, methyl ester
1738-25-6	1	0	0	Propanenitrile, 3-(dimethylamino)-
1739-84-0	1	0	0	1*H*-Imidazole, 1,2-dimethyl-
1740-97-2	1	0	0	Phenol, 2-methyl-4-(1-methylethyl)-
1745-81-9	1	0	0	Phenol, 2-(2-propenyl)-
1746-01-6	1	1	1	Dibenzo[*b,e*][1,4]dioxin, 2,3,7,8-tetrachloro-
1746-11-8	0	1	0	Benzofuran, 2,3-dihydro-2-methyl-
1746-81-2	1	1	1	Urea, *N′*-(4-chlorophenyl)-*N*-methoxy-*N*-methyl- {Linuron®, 30% of Molipan®}
1754-58-1	1	1	1	Phosphorodiamidic acid, *N,N′*-dimethyl-, phenyl ester {Diamidafos®}
1757-42-2	1	0	0	Cyclopentanone, 3-methyl-
1758-51-6	0	1	0	Butanal, 2,3,4-trihydroxy-, (R*,R*)- {erythrose}
1758-88-9	1	0	0	Benzene, 1,4-dimethyl-2-ethyl-
1759-28-0	1	0	0	Thiazole, 5-ethenyl-4-methyl-
1759-81-5	1	0	0	Cyclopentene, 4-methyl-
1761-10-0	0	1	0	Indolizine, 3-methyl-
1761-11-1	1	0	0	Indolizine, 6-methyl-
1767-84-6	0	1	0	Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-
1775-43-5	0	1	0	3-Hexenoic acid, (*Z*)-
1782-55-4	0	1	0	2-Propenoic acid, 3-(4,5-dihydroxy-3-methoxyphenyl)- {5-hydroxyferulic acid}
1786-12-5	0	1	0	Cyclotetradecane, 1,7,11-trimethyl-4-(1-methylethyl)-
1802-20-6	1	1	1	Pyridine, 3-pentyl-
1812-51-7	1	0	0	1,1′-Biphenyl, 2-ethyl-
1817-47-6	1	0	0	Benzene, 1-(1-methylethyl)-4-nitro- {4-nitrocumene}
1821-29-0	0	1	0	3-Hexen-2-one, 5-methyl-, (*E*)-
1821-38-1	1	1	1	Benzenamine, 2-ethyl-*N*-methyl-
1822-74-8	1	0	0	Methyl ethenyl sulfide
1823-90-1	1	0	0	2-Butanone, 4-hydroxy-3,3-dimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
1824-81-3	1	0	0	2-Pyridinamine, 6-methyl-
1842-56-4	0	1	0	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, methyl ester
1842-63-3	1	0	0	1*H*-Imidazole, 1,2,4-trimethyl-
1848-84-6	1	0	0	1*H*-Benzimidazole, 2-ethyl-
1852-04-6	1	1	1	Undecanedioic acid
1859-92-3	1	0	0	1*H*-Indole, 3-propyl-
1861-32-1	0	1	0	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester {Dichlorthal-dimethyl®, DCPA®}
1861-40-1	0	1	0	Benzenamine, *N*-butyl-2,6-dinitro-*N*-ethyl-4-(trifluoromethyl)- {Benefin®, Benfluralin®}
1873-54-7	1	0	0	Quinoline, 3-ethyl-
1885-29-6	1	0	0	Benzonitrile, 2-amino- {anthranilonitrile}
1892-54-2	1	0	0	3-Phenanthrenamine
1897-45-6	0	1	0	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro {Chlorothalonil®}
1898-13-1	0	1	0	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(*E,Z,E,E*)]-
1899-29-2 27044-07-1	0	1	0	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)- [2 CAS Nos.] {3-*O*-feruloylquinic acid} Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-
1899-30-5	0	1	0	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]-, [1S-(1α,3α,4α,5β)]- {*p*-coumaroylquinic acid}
1912-33-0	0	1	0	1*H*-Indole-3-acetic acid, methyl ester
1917-15-3	1	0	0	2-Furancarboxylic acid, 5-methyl-
1917-64-2	1	0	0	2-Furancarboxaldehyde, 5-(methoxymethyl)-
1918-00-9	1	1	1	Benzoic acid, 3,6-dichloro-2-methoxy- {Dicamba®}
1918-02-1	0	1	0	2-Pyridinecarboxylic acid, 4-amino-3,5,6-trichloro- {Picloram®}
1919-64-8	0	1	0	1,3-Cyclohexanedione, 5,5-dimethyl-2-propyl-
1921-70-6	1	0	0	Pentadecane, 2,6,10,14-tetramethyl- {pristane}
1928-30-9	1	1	1	Tricosane, 2-methyl-
1929-77-7	0	1	0	Carbamothioic acid, dipropyl-, *S*-propyl ester {Vernolate®}
1929-82-4	0	1	0	Pyridine, 2-chloro-6-(trichloromethyl)- {Nitrapyrin®}
1932-50-9	0	1	0	Acetic acid, hydroxy-, potassium salt
1937-54-8	1	1	1	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [S-(*E*)]- {solanone}
1948-54-5	0	1	0	Galactose, 2-amino-2-deoxy-
1949-89-9	0	1	0	*D*-Galactose, 2-deoxy-
1961-72-4	1	1	1	Tetradecanoic acid, 3-hydroxy-
1963-26-8 21963-26-8	0	1	0	2(5*H*)-Furanone, 5-pentyl- [2 CAS Nos.]
1971-46-6	1	0	0	1*H*-Indole, 1,2,3-trimethyl-
1976-85-8	0	1	0	21*H*,23*H*-Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetrakis(carboxymethyl)-5,10,15,20,22,24-hexahydro-
1988-89-2	0	1	0	Phenol, 4-(1phenylethyl)-
1992-50-3	1	0	0	Benzenepropanol, α-ethyl-
2004-39-9	0	1	0	1-Heptacosanol
2004-70-8	1	1	1	1,3-Pentadiene, (*E*)-
2009-74-7	1	1	1	3-Hepten-2-one, 6-methyl-
2016-57-1	1	0	0	1-Decanamine
2027-17-0	0	1	0	Naphthalene, 2 (1-methylethyl)-
2027-19-2	1	0	0	Naphthalene, 2-propyl-
2028-39-9	1	0	0	1-Propene-3-thiol
2032-59-9	0	1	0	Methylcarbamic acid, 4-(dimethylamino)-3-methylphenyl ester {Aminocarb®}
2032-65-7	0	1	0	Methylcarbamic acid, 3,5-dimethyl-4-(methylthio)phenyl ester {Methiocarb®}
2033-89-8	1	0	0	Phenol, 3,4-dimethoxy-
2034-60-8	0	1	0	1,2-Propanedione, 1-(4-hydroxy-3-methoxyphenyl)-
2035-99-6	0	1	0	Octanoic acid, 3-methylbutyl ester
2039-89-6	1	1	1	Benzene, 1,4-dimethyl-2-ethenyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
2040-64-4	1	1	1	Tetradecanoic acid, dodecyl ester
2040-96-2	1	0	0	Cyclopentane, propyl-
2042-14-0	1	0	0	Phenol, 4-methyl-3-nitro-
2043-08-1	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, 3-acetate, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-
2043-61-0	0	1	0	Cyclohexanecarboxaldehyde
2049-95-8	1	0	0	Benzene, (1,1-dimethylpropyl)-
2049-96-9	1	0	0	Benzoic acid, pentyl ester {amyl benzoate}
2050-01-3	0	1	0	Propanoic acid, 2-methyl-, 3-methylbutyl ester
2050-67-1	1	0	0	1,1′-Biphenyl, 3,3′-dichloro-
2050-68-2	1	0	0	1,1′-Biphenyl, 4,4′-dichloro-
2051-24-3	1	1	1	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6,6′-decachloro- {1,1′-biphenyl, decachloro-}
2051-28-7	1	0	0	Quinoline, decahydro-
2051-49-2	0	1	0	Hexanoic anhydride
2051-60-7	1	0	0	1,1′-Biphenyl, 2-chloro-
2052-14-4	0	1	0	Benzoic acid, 2-hydroxy-, butyl ester
2055-23-4	0	1	0	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)- {pseudooxynicotine}
2055-29-0	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, *N*,1-dioxide, (S)-
2057-39-8	1	0	0	Pyridine, 3-(4-methyl-3-pentenyl)-
2068-02-2	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5-hydroxy-3,7-dimethoxy-
2088-07-5	1	1	1	1-Penten-3-ol, 2-methyl-
2091-29-4	1	1	1	9-Hexadecenoic acid, (*E*)- [2 CAS Nos.] {palmitelaidic acid}
10030-73-6				
2104-96-3	0	1	0	Phosphorothioic acid, *O,O*-dimethyl *O*-(4-bromo-2,5-dichlorophenyl) ester {Bromophos®}
2109-98-0	1	0	0	Butanal, 2,3-dimethyl-
2116-65-6	0	1	0	Pyridine, 4-(phenylmethyl)-
2122-46-5	1	0	0	Phenoxyl radical
2131-39-7	1	1	1	Naphthalene, 1,3,5-trimethyl-
2131-41-1	1	0	0	Naphthalene, 1,4,5-trimethyl-
2131-42-2	1	1	1	Naphthalene, 1,4,6-trimethyl-
2134-29-4	1	0	0	Propanal, 3-hydroxy-
2138-43-4	1	0	0	1,2-Benzenediol, 4-(1-methylethyl)-
2138-48-9	1	0	0	1,2-Benzenediol, 3-(1-methylethyl)-
2140-82-1	1	1	1	1-Pentadecene, 2,6,10,14-tetramethyl- [3 CAS Nos.] {norphytene}
60976-73-0				
100404-00-0				
2143-68-2	1	0	0	Methoxy radical
2146-38-5	1	0	0	Cyclopentene, 1-ethyl-
2150-18-7	1	0	0	Pyridine, 2-ethyl-4-methyl-
2154-50-9	1	0	0	Ethoxyl radical
2157-98-4	0	1	0	1-Propene, 1-methyl-3-(methylamino)-3-oxo-, dimethyl phosphate {Monocrotophos®}
2167-14-8	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 1-ethyl-
2177-47-1	1	0	0	1*H*-Indene, 2-methyl-
2177-78-8	1	1	1	Pentanoic acid, 3-methyl-, methyl ester
2177-83-5	0	1	0	Hexanoic acid, 5-methyl-, methyl ester
2179-58-0	1	0	0	Disulfide, methyl2-propen-1-yl-
2179-59-1	1	0	0	Disulfide, propyl2-propen-1-yl-
2179-60-4	1	0	0	Disulfide, methyl propyl
2180-43-0	1	0	0	3-Hexanol, 1-phenyl-
2189-60-8	1	0	0	Benzene, octyl- [2 CAS Nos.] {phenyloctane}
71607-64-2				
2197-57-1	1	0	0	1,4-Naphthalenedione, 2,3-dimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
2198-23-4	1	0	0	4-Nonene
2198-61-0	0	1	0	Hexanoic acid, 3-methylbutyl ester
2203-80-7	1	0	0	1-Hexyne, 5-methyl-
2207-04-7	1	0	0	Cyclohexane, 1,2-dimethyl-, (*E*)-
2213-23-2	0	1	0	Heptane, 2,4-dimethyl-
2216-33-3	1	0	0	Octane, 3-methyl-
2216-34-4	0	1	0	Octane, 4-methyl-
2216-39-8	1	0	0	2-Nonene
2216-51-5	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, [1R-(1α,2β,5α)]-
2216-69-5	1	0	0	Naphthalene, 1-methoxy-
2216-70-8	1	0	0	2,4-Octadiene, 7-methyl-
2219-73-0	1	0	0	Phenol, 4-ethyl-2-methyl-
2219-79-6	1	0	0	Phenol, 4,6-dimethyl-2-ethyl-
2229-07-4	1	0	0	Methyl radical
2233-29-6	1	0	0	Pyridine, 2,3,4-trimethyl- {2,3,4-collidine}
2234-20-0	1	0	0	Benzene, 1,4-dimethyl-2-ethenyl-
2235-12-3	1	0	0	1,3,5-Hexatriene
2243-35-8	0	1	0	Ethanone, 1-phenyl-2-(acetyloxy)-
2243-47-2	1	0	0	[1,1′-Biphenyl]-3-amine
2243-53-0	1	1	1	3-Butenoic acid, 4-phenyl- {styrylacetic acid}
2244-02-2	1	0	0	2-Undecene
2244-16-8	0	1	0	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*d*-carvone}
2245-38-7	1	1	1	Naphthalene, 1,6,7-trimethyl- {naphthalene, 2,3,5-trimethyl-}
2246-44-8	1	0	0	1-Naphthalenamine, 2-methyl-
2257-09-2	0	1	0	Benzene, (2-isothiocyanatoethyl)-
2275-23-2	0	1	0	Phosphorothioic acid, *O,O*-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]thio]ethyl] ester {Vamidothion®}
2277-19-2	0	1	0	6-Nonenal, (*Z*)-
2278-53-7	0	1	0	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, [R-(*E*)]-
2294-76-0	1	1	1	Pyridine, 2-pentyl-
2294-82-8	1	0	0	9*H*-Fluorene, 9-ethyl-
2298-99-9	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2,6-dimethyl-
2302-39-8	1	0	0	1*H*-Imidazole, 4,5-dimethyl-
2303-17-5	0	1	0	Carbamothioic acid, *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl) ester {Triallate®}
2305-05-7	0	1	0	2(*3H*)-Furanone, dihydro-5-octyl- {γ-dodecalactone}
2305-21-7	0	1	0	2-Hexen-1-ol, (*E*)-
2305-25-1	0	1	0	Hexanoic acid, 3-hydroxy-, ethyl ester
2308-84-1	1	1	1	Stigmasta-5,22-dien-3-ol, hexadecanoate, (3β,22*E*)- {stigmasteryl palmitate}
2308-85-2	1	1	1	Stigmast-5-en-3-ol, hexadecanoate, (3β)- {β-sitosteryl palmitate}
2309-07-1	1	1	1	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester {ferulic acid, methyl ester}
2310-17-0	0	1	0	Phosphorodithioic acid, S-[(6-chloro-2-oxo-3(2*H*)-benzoxazolyl)methyl] *O,O*-diethyl ester {Phosalone®}
2315-09-5	0	1	0	3-Hexen-1-ol, formate
2315-68-6	1	1	1	Benzoic acid, propyl ester
2316-26-9	0	1	0	2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-
2319-96-2	1	0	0	Benz[*a*]anthracene, 5-methyl-
2338-03-6	0	1	0	Butanoic acid, 2-amino-4-oxo-, (S)-
2338-45-6	0	1	0	Butanedioic acid, (1-methylethyl)-
2345-28-0	0	1	0	2-Pentadecanone
2346-26-1	1	0	0	2,4-Oxazolidinedione
2349-70-4	1	0	0	1,4-Benzenediol, 2-ethyl- = 1,4-benzenediol, ethyl-
2349-71-5	0	1	0	1,4-Benzenediol, 2-(1-methylethyl)-
2363-71-5	1	1	1	Heneicosanoic acid
2363-84-0	1	0	0	Hexanal, 2-oxo-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
2363-85-1	1	0	0	Heptanal, 2-oxo-
2363-88-4	0	1	0	2,4-Decadienal
2364-23-0	0	1	0	Stigmasta-5,25-dien-3-ol, (3β,24S)-
2365-40-4	0	1	0	1*H*-Purin-6-amine, *N*-(3-methyl-2-butenyl)-
2380-78-1	1	1	1	Benzeneethanol, 4-hydroxy-3-methoxy-
2381-15-9	1	0	0	Benz[*a*]anthracene, 10-methyl-
2381-16-0	1	0	0	Benz[*a*]anthracene, 9-methyl-
2381-21-7	1	1	1	Pyrene, 1-methyl-
2381-31-9	1	0	0	Benz[*a*]anthracene, 8-methyl-
2381-40-0	1	0	0	Benz[*c*]acridine, 7,10-dimethyl-
2381-87-5	1	1	1	2*H*-Pyran-2-one, 5,6-dihydro-4-methyl-
2385-85-5	0	1	0	1,3,4-Metheno-1*H*-cyclobuta[*cd*])pentalene, 1,1a,2,2,3,3a,4,5,5,5a,5b,6-dodecachlorooctahydro- {Mirex®}
2396-61-4	1	0	0	1-Propanol, 3,3′-oxybis-
2396-78-3	0	1	0	3-Hexenoic acid, methyl ester
2400-66-0	0	1	0	Eicosanal
2402-06-4	1	0	0	Cyclopropane, 1,2-dimethyl-, (*E*)-
2407-43-4	1	1	1	2(5*H*)-Furanone, 5-ethyl-
2408-37-9	1	1	1	Cyclohexanone, 2,2,6-trimethyl- {2,6,6-trimethylcyclohexanone}
2412-80-8	1	0	0	Pentanoic acid, 4-methyl-, methyl ester
2416-94-6	1	0	0	Phenol, 2,3,6-trimethyl-
2417-10-9	1	0	0	Phenol, 2-phenoxy-
2422-79-9	1	0	0	Benz[*a*]anthracene, 12-methyl-
2429-94-9	0	1	0	2(3*H*)-Furanone, dihydro-5-(3-methylbutyl)-
2431-51-1	1	0	0	Butanethioic acid, *S*-methyl ester
2432-11-3	1	0	0	1,1′,3′-Terphenyl-2′-ol
2433-57-0	1	0	0	3-Buten-2-one, 4-(1*H*-pyrrol-2-yl)-, (*E*)-
2433-66-1	0	1	0	1*H*-Pyrrole, 2-ethenyl-
2433-96-7	1	1	1	Tricosanoic acid
2433-97-8	0	1	0	Tricosanoic acid, methyl ester
2437-56-1	1	1	1	1-Tridecene
2437-79-8	1	0	0	1,1′-Biphenyl, 2,2′,4,4′-tetrachloro-
2437-92-5	0	1	0	Phytodienes
2438-80-4	0	1	0	Fucose
2439-01-2	0	1	0	1,3-Dithiolo[4,5-*b*]quinoxalin-2-one, 6-methyl- {Quinomethionate®}
2445-69-4	0	1	0	Propanoic acid, 2-methyl-, 2-methylbutyl ester
2445-77-4	0	1	0	Butanoic acid, 3-methyl-, 2-methylbutyl ester
2445-78-5	0	1	0	Butanoic acid, 2-methyl-, 2-methylbutyl ester
2445-82-1	1	0	0	2*H*-1-Benzopyran-2-one, 3-methyl-
2346-00-1	1	0	0	Thiazole, 4,5-dihydro-2-methyl-
2450-53-5	0	1	0	Cyclohexanecarboxylic acid, 3,5-bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4-dihydroxy-, [1R-(1α,3α,4α,5β)]-
2451-01-6	1	0	0	Cyclohexanemethanol, 4-hydroxy-α,α,4-trimethyl-, monohydrate, *cis*-{terpin hydrate}
2452-99-5	1	0	0	Cyclopentane, 1,2-dimethyl-, *cis*-
2456-73-7	0	1	0	*L*-Aspartic acid, *N*-(1*H*-indol-3-ylacetyl)-
2462-84-2	0	1	0	9-Octadecenoic acid, methyl ester
2462-85-3	0	1	0	9,12-Octadecadienoic acid, methyl ester
2463-53-8	1	1	1	2-Nonenal
2463-63-0	0	1	0	2-Heptenal
2466-76-4	0	1	0	1*H*-Imidazole, 1-acetyl-
2471-84-3	1	0	0	1*H*-Indene, 1-methylene-
2474-72-8	1	0	0	2,5-Cyclohexadiene-1,4-dione, 2-hydroxy-
2478-38-8	1	0	0	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
2485-71-4	0	1	0	Tetradecanoic acid, 13-methyl-
2490-01-9	0	1	0	1-Octadecanol, 16-methyl-
2490-43-9	0	1	0	1-Hexadecanol, 14-methyl-
2490-49-5	1	1	1	Hexadecanoic acid, 14-methyl-, methyl ester
2497-06-5	0	1	0	Phosphorodithioic acid, *O*,*O*-diethyl S-[2-(ethylsulfonyl)ethyl] ester (Thiodemeton sulfone®)
2497-18-9	0	1	0	2-Hexen-1-ol, acetate, (*E*)-
2497-25-8	0	1	0	2-Decenal, (*Z*)-
2498-75-1	1	0	0	Benz[*a*]anthracene, 3-methyl-
2498-76-2	1	0	0	Benz[*a*]anthracene, 2-methyl-
2498-77-3	1	0	0	Benz[*a*]anthracene, 1-methyl-
2503-46-0	1	1	1	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-
110053-51-5				
2504-18-9	1	1	1	1-Propanamine, *N*,2-dimethyl-*N*-nitroso- [2 CAS Nos.]
34419-76-6				
2510-74-9	1	0	0	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro-, (*Z*)- {*cis*-DCS}
2511-95-7	1	0	0	Cyclopropane, 1,2-dimethyl-
2516-33-8	0	1	0	Cyclopropanemethanol
2517-04-6	0	1	0	2-Azetidinecarboxylic acid
2523-37-7	1	0	0	9*H*-Fluorene, 9-methyl-
2523-39-9	1	0	0	9*H*-Fluorene, 3-methyl-
2524-49-4	1	0	0	3-Buten-1-amine
2524-90-5	1	0	0	Ethanone, 1-(4-methyl-1*H*-imidazol-2-yl)-
2525-02-2	1	0	0	1,2-Benzenediol, 4-propyl-
2531-84-2	1	0	0	Phenanthrene, 2-methyl-
2539-53-9	0	1	0	Benzaldehyde, 4-ethoxy-3-hydroxy-
2540-82-1	0	1	0	Phosphorodithioic acid, S-[2-(formylmethylamino)-2-oxoethyl] *O,O*-dimethyl ester {Formothion®}
2543-54-6	0	1	0	Hexanoic acid, 2-(1-methylethyl)-5-oxo-
2544-06-1	0	1	0	Propanoic acid, 3-methoxy-
2548-87-0	0	1	0	2-Octenal
2550-21-2	0	1	0	2-Hexanone, 3-methyl-
2550-26-7	1	0	0	2-Butanone, 4-phenyl-
2551-62-4	0	1	0	Sulfur hexafluoride
2553-59-5	0	1	0	Propanoic acid, 3-hydroxy-2-(phosphonooxy)-
2555-05-7	1	0	0	2-Pyrrolidinone, 3-methyl-
2571-52-0	1	0	0	Benzonitrile, 2,4,6-trimethyl-
2581-34-2	1	0	0	Phenol, 3-methyl-4-nitro-
2586-89-2	1	0	0	3-Heptyne
2591-79-9	1	0	0	Formamide, *N*-pentyl-
2595-97-3	0	1	0	*D*-Allose
2597-03-7	0	1	0	Phosphorodithioic acid, *O*,*O*-dimethyl-S-(α-ethoxycarbonylbenzyl) ester {Fenthoate®, Phenthoate®}
2597-44-6	1	0	0	Formyl radical
2598-99-4	1	1	1	Hexadecanoic acid, octadecyl ester
2599-01-1	1	1	1	Tetradecanoic acid, hexadecyl ester
2610-95-9	0	1	0	2*H*-Pyran-2-one, tetrahydro-6,6-dimethyl-
2610-98-2	0	1	0	2(3*H*)-Furanone, dihydro-5-ethyl-3-methyl-
2617-98-3	1	0	0	Quinoline, 2-methyl-5,6,7,8-tetrahydro-
2623-50-9	1	0	0	Quinoline, 5,8-dimethyl-
2628-17-3	1	1	1	Phenol, 4-ethenyl-
2642-71-9	0	1	0	Phosphorodithioic acid, *O*,*O*-diethyl S-[(4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl] ester {Azinphos Ethyl®}
2642-80-0	1	1	1	Benzene, 1,1′-(2-chloroethylidene)bis[4-chloro- {DDMS}
2642-98-0	1	0	0	Chrysene, 6-amino- {6-chysenamine}
2645-22-4	0	1	0	Cholest-5-en-3-ol (3β)-, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {cholesteryl linolenate}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
2675-88-9	1	0	0	Propanamide, *N*,2-dimethyl-
2687-69-6	1	0	0	3-Cyclopentene-1,2-dione, 3,5-dimethyl-
2687-91-4	1	0	0	2-Pyrrolidinone, 1-ethyl-
2693-46-1	1	0	0	3-Fluoranthenamine
2717-42-2	1	1	1	Naphthalene, 1,2,4-trimethyl-
2717-44-4	1	0	0	Naphthalene, 1,2-dihydro-3-methyl-
2717-47-7	1	0	0	Naphthalene, 1,2-dihydro-6-methyl-
2718-25-4	0	1	0	Rheadan, 8-β-methoxy-6-methyl-2,3,10,11-[methylenebis(oxy)]- {rhoeadin}
2721-22-4	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-nonyl- {tetradecalactone}
2724-57-4	1	1	1	Tridecanoic acid, 12-methyl-
2724-58-5	1	1	1	Heptadecanoic acid, 16-methyl-
2724-59-6	0	1	0	Octadecanoic acid, 17-methyl-
2738-19-4	1	0	0	2-Hexene, 2-methyl-
2739-16-4	0	1	0	1(2*H*)-Quinolinecarboxaldehyde, 3,4-dihydro-
2743-90-0	0	1	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (±)-
2745-26-8	1	0	0	2-Furanacetic acid
2748-08-5	1	0	0	2-Cyclohexen-1-one, 3,6-dimethyl-2-hydroxy-
2748-09-6	1	0	0	2-Cyclohexen-1-one, 3,5-dimethyl-2-hydroxy-
2756-56-1	0	1	0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, propanoate, exo-
2758-18-1	1	1	1	2-Cyclopenten-1-one, 3-methyl-
2765-11-9	0	1	0	Pentadecanal
2765-18-6	1	0	0	Naphthalene, 1-propyl-
2778-96-3	1	1	1	Octadecanoic acid, octadecyl ester
2785-75-3	1	0	0	1,2-Benzenediol, 3,5-dimethyl-
2785-78-6	1	0	0	1,2-Benzenediol, 3,6-dimethyl-
2785-85-5	1	0	0	Phenol, 3,5-dimethyl-2-methoxy-
2785-87-7	1	1	1	Phenol, 2-methoxy-4-propyl-
2785-88-8	1	0	0	Phenol, 5-ethyl-2-methoxy-
2785-89-9	1	1	1	Phenol, 4-ethyl-2-methoxy- {ethylguaiacol}
2787-43-1	1	0	0	1,3-Pentadiene, 3-methyl-
2787-45-3	1	0	0	1,3-Pentadiene, 3-methyl- (isomer)
2792-39-4	1	0	0	2,6-Octadiene, 2,6-dimethyl-
2808-76-6	1	0	0	Cyclohexene, 1,3-dimethyl-
2809-64-5	1	1	1	Naphthalene, 5-methyl-1,2,3,4-tetrahydro-
2816-57-1	0	1	0	Cyclohexanone, 2,6-dimethyl-
2820-37-3	1	0	0	1*H*-Pyrazole, 3,4-dimethyl-
2820-51-1	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, hydrochloride, (S)-
2820-55-5	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, 1-oxide, (S)- {nicotine *N*-oxide}
2835-82-7	0	1	0	Butanoic acid, 3-amino-
2840-51-9	1	1	1	9*H*-Fluoren-9-one, 2-methyl-
2845-25-2	1	0	0	Benzenepropanol, γ-ethyl-, (S)-
2847-30-5	0	1	0	Pyrazine, 3-methoxy-2-methyl-
2865-82-9	0	1	0	2(3*H*)-Furanone, dihydro-5-ethyl-5-methyl-
2867-05-2	0	1	0	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)- {3-thujene}
2876-08-6	1	0	0	1*H*-Benzimidazole, 1,2-dimethyl-
2878-14-0	1	0	0	2-Propen-1-amine, 2-methyl-
2882-21-5	0	1	0	Pyrazine, 6-methoxy-2-methyl-
2882-22-6	0	1	0	Pyrazine, 5-methoxy-2-methyl-
2882-96-4	1	1	1	Pentadecane, 3-methyl-
2883-98-9	0	1	0	Benzene, 1,2,4-trimethoxy-5-(2-propenyl)-, (*Z*)-
2896-60-8	1	0	0	1,3-Benzenediol, 4-ethyl-
2896-63-1	1	0	0	1,2-Benzenediol, 3-propyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
2896-66-4	1	0	0	Phenol, 4,6-dimethyl-2-methoxy-
2896-67-5	1	0	0	Phenol, 2-methoxy-6-methyl-
2921-88-2	1	1	1	Phosphorothioic acid, *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester {Chlorpyrifos®, Chlorpyriphos®, Dursban®}
2931-10-4	1	0	0	2-Cyclopenten-1-one, 2-ethyl-
2935-44-6	1	1	1	2,5-Hexanediol
2944-05-0	1	0	0	Carbon sulfide
2947-61-7	1	0	0	Benzeneacetonitrile, 4-methyl-
2981-96-6	1	0	0	2(3*H*)-Furanone, dihydro-4,5,5-trimethyl-
2983-37-1	0	1	0	Hexanoic acid, 2-ethyl-, ethyl ester
2983-65-5	1	1	1	2-Propen-1-one, 1-(4-hydroxy-3-methoxyphenyl)-
2996-58-9	1	1	1	2-Pyrrolidinone, 4-methyl-
3000-74-6	1	1	1	3-Pyridinebutanamine, *N*-methyl- {dihydrometanicotine}
3000-75-7	1	0	0	3-Pyridinemethanamine, *N*-ethyl-
3000-81-5	1	1	1	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)- {*N*′-formylnornicotine} [2 CAS Nos.]
38840-03-8				
3002-23-1	0	1	0	2,4-Heptanedione, 6-methyl-
3004-93-1	0	1	0	Octanoic acid, 2-methyl-
3008-40-0	1	1	1	1,2-Cyclopentanedione
3008-43-3	0	1	0	1,2-Cyclohexanedione, 6-methyl-
3031-05-8	1	1	1	Naphthalene, 1,2,6-trimethyl-
3031-08-1	1	1	1	Naphthalene, 1,3,6-trimethyl-
3059-71-0	1	0	0	4(1*H*)-Pyrimidinone, 2,5-dimethyl- = 6-pyrimidinol, 2,5-dimethyl-
67383-34-0				
3060-89-7	1	1	1	Urea, *N*′-(4-bromophenyl)-*N*′-methoxy-*N*′-methyl- {Metobromuron®, Patoran®}
3068-00-6	0	1	0	1,2,4-Butanetriol
3073-66-3	1	0	0	Cyclohexane, 1,1,3-trimethyl-
3074-61-1	1	0	0	Cyclopentene, 1-propyl-
3102-33-8	0	1	0	3-Penten-2-one, (*E*)
3123-97-5	0	1	0	2(3*H*)-Furanone, dihydro-5,5-dimethyl-
3128-06-1	1	0	0	Hexanoic acid, 5-oxo-
3128-07-2	1	0	0	Heptanoic acid, 6-oxo-
3131-63-3	1	0	0	Benzofuran, 2-ethyl-
3133-01-5	1	1	1	1-Tricosanol
3142-72-1	1	1	1	2-Pentenoic acid, 2-methyl-
3147-18-0	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [3S-[3α(2*E*,7S*,11S*),4β,21β]]- {pheophytin B}
3149-28-8	0	1	0	Pyrazine, methoxy-
3155-42-8	0	1	0	Octadecanoic acid, 18-hydroxy-
3163-07-3	1	0	0	1,3-Benzenediol, 4-nitro-
3171-45-7	1	0	0	1,2-Benzenediamine, 4,5-dimethyl-
3174-67-2	1	0	0	1,3-Pentanediol
3177-92-2	1	1	1	Stigmast-5-en-3-ol, 9,12,15-octadecatrienoate, [3β(9*Z*,12*Z*,15*Z*)]- {β-sitosteryl linolenate}
3180-09-4	1	0	0	Phenol, 2-butyl-
3184-35-8	1	1	1	Hexanedioic acid, 2-oxo-
3188-00-9	1	1	1	3(2*H*)-Furanone, dihydro-2-methyl- {2-methyltetrahydrofuran-3-one}
3189-12-6	1	0	0	1*H*-Indole, 3,5-dimethyl-
3194-15-8	1	0	0	1-Propanone, 1-(2-furanyl)-
3208-16-0	1	1	1	Furan, 2-ethyl-
3208-40-0	0	1	0	Furan, tetrahydro-2-(3-phenylpropyl)-
3220-74-4	0	1	0	1*H*-Pyrrole-2-carboxylic acid, 2,5-dihydro-
3222-52-4	1	0	0	3-Pyridinecarbonitrile, 6-ethyl-
3225-29-4	1	0	0	*p*-Benzosemiquinone radical

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
3226-65-1	0	1	0	Butanoic acid, 2-amino-4-(methylsulfonyl)- [2 CAS Nos.] {methionine sulfone, methionine *S*-oxide}
1118-85-0				
3233-32-7	1	0	0	1,4-Benzenediol, monoacetate
3233-90-7	0	1	0	Hexadecanoic acid, 10,16-dihydroxy-
3234-28-4	1	0	0	Oxirane, dodecyl- {tetradecane, 1,2-epoxy}-
3234-81-9	1	1	1	Tetradecanoic acid, octadecyl ester
3234-85-3	1	1	1	Tetradecanoic acid, tetradecyl ester
3237-44-3	0	1	0	Butanedioic acid, 2-hydroxy-2-(1-methylethyl)-
3238-38-8	1	0	0	Phenol, 2,3,4,6-tetramethyl-
3238-55-9	1	0	0	1-Propanone, 1-(2-pyridinyl)-
3242-05-5	0	1	0	Naphthalene, decahydro-1,8a-dimethyl-7-(1-methylethyl)-, [1S-(1α,4aα,7α,8aα)]-
3243-36-5	0	1	0	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-methylene-, [1S-(1α,4aβ,8aα)]-
3249-68-1	1	0	0	Hexanoic acid, 3-oxo-, ethyl ester
3251-23-8	0	1	0	Nitric acid, copper (+2) salt
3268-49-3	1	1	1	Propanal, 3-(methylthio)- {methional}
3268-87-9	1	0	0	Dibenzo[*b,e*][1,4]dioxin, octachloro-
3274-29-1	0	1	0	Heptanoic acid, 2-ethyl-
3279-76-3	1	0	0	2(1*H*)-Pyridinone, 6-methyl- {2-pyridinol, 6-methyl-}
3284-51-3	1	0	0	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-, ethyl ester
3284-93-3	0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-propyl-
3285-47-0	1	0	0	2(3*H*)-Furanone, dihydro-4-hydroxy-3,3-dimethyl-
3293-47-8	0	1	0	2-Butanol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
3301-94-8	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-butyl- {δ-nonalactone}
3303-26-2	0	1	0	Pyrido[3,2-*d*]pyrimidin-4-ol, 2-methyl-
3311-23-7	1	0	0	4-Piperidinone, 2,2,6-trimethyl-, (R)-
3316-09-4	1	0	0	1,2-Benzenediol, 4-nitro-
3317-61-1	1	0	0	2*H*-Pyrrole, 3,4-dihydro-2,2-dimethyl-, 1-oxide
3332-08-9	1	0	0	2-Propanamine, *N*-(1-methylethylidene)-
3340-94-1	1	0	0	Benz[*c*]acridine, 7-methyl-
3344-18-1	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, magnesium salt
3347-62-4	0	1	0	1*H*-Pyrazole, 3-methyl-5-phenyl-
3350-86-5	1	1	1	Piperidine, 1-acetyl-2-(3-pyridinyl)-, (S)-
3351-28-8	1	0	0	Chrysene, 1-methyl-
3351-30-2	1	0	0	Chrysene, 4-methyl-
3351-31-3	1	0	0	Chrysene, 3-methyl-
3351-32-4	1	0	0	Chrysene, 2-methyl-
3352-57-6	1	0	0	Hydroxide radical
3353-12-6	1	0	0	Pyrene, 4-methyl-
3361-10-2	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15-tetramethylhexadecyl)-6-methyl-
3363-56-2	0	1	0	1*H*-Benzimidazole, 2,5,6-trimethyl-
3366-65-2	1	0	0	2-Phenanthrenamine
3376-24-7	1	0	0	2-Propanamine, 2-methyl-*N*-(phenylmethylene)-, *N*-oxide
3378-71-0	1	0	0	Pyrrolidine, 2,5-dimethyl-
3387-41-5	0	1	0	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- {sabinene}
3391-86-4	0	1	0	1-Octen-3-ol
3392-97-0	1	1	1	Benzaldehyde, 2,6-dimethoxy-
3393-45-1	0	1	0	2*H*-Pyran-2-one, 5,6-dihydro-
3400-45-1	0	1	0	Cyclopentanecarboxylic acid {cyclopentanoic acid}
3400-78-0	**1**	**0**	**0**	**2-Cyclohexen-1-one, 2-hydroxy-3-methyl-**
3404-61-3	**1**	**0**	**0**	**1-Hexene, 3-methyl-**
3404-62-4	1	0	0	2-Hexene, 5-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
3404-73-7	1	0	0	1-Pentene, 3,3-dimethyl-
3404-78-2	1	0	0	2-Hexene, 2,5-dimethyl-
3405-42-3	1	0	0	1-Propanamine, *N*-methyl-*N*-propyl-
3416-24-8	0	1	0	*D*-Glucose, 2-deoxy-, 2-amino- {glucosamine}
3420-02-8	1	0	0	1*H*-Indole, 6-methyl-
3420-59-5	0	1	0	Ethanone, 1-(3-hydroxy-2-furanyl)- {isomaltol}
3424-82-6	1	0	0	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethenyl]-
3430-10-2	1	0	0	3-Pyridinamine, 2-methyl-
3430-27-1	1	0	0	3-Pyridinamine, 4-methyl-
3435-51-6	1	0	0	Benzonitrile, 4-ethenyl-
3438-46-8	1	0	0	Pyrimidine, 4-methyl-
3442-78-2	1	0	0	Pyrene, 2-methyl-
3452-07-1	1	1	1	1-Eicosene
3452-09-3	1	0	0	1-Nonyne
3452-97-9	0	1	0	1-Hexanol, 3,5,5-trimethyl-
3458-28-4	1	1	1	*D*-Mannose {seminose}
3459-80-1	0	1	0	Benzene, [(1,1-dimethylethoxy)methyl]-
3471-05-4	0	1	0	2,3′-Bipyridine, 3,4,5,6-tetrahydro- {anabaseine}
3484-18-2	1	0	0	1*H*-Indole, 2-ethyl-
3511-27-1	1	0	0	1,5-Heptadien-3-yne
3511-31-7	1	1	1	3(2*H*)-Furanone
3520-52-3	1	0	0	Phenol, 2-methyl-6-propyl-
3524-73-0	1	0	0	1-Hexene, 5-methyl-
3548-78-5	0	1	0	3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (*E,E*)- {pseudoionone}
3552-33-8	1	1	1	2,5-Furandione, 3-ethyl-4-methyl-
3558-69-8	1	0	0	Pyridine, 2,6-diphenyl-
3577-13-7	1	1	1	Stigmast-5-en-3-ol, 9,12-octadecadienoate, [3β(*Z,Z*)]- {β-sitosteryl linoleate}
3581-87-1	1	0	0	Thiazole, 2-methyl-
3581-89-3	1	0	0	Thiazole, 5-methyl-
3581-91-7	1	0	0	Thiazole, 4,5-dimethyl-
3589-72-8	1	0	0	9*H*-Pyrido[3,4-*b*]indole,6-methoxy-1-methyl-
3589-73-9	1	0	0	3*H*-Pyrido[3,4-*b*]indole, 4,9-dihydro-6-methoxy-1-methyl-
3609-96-9	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, dipotassium salt
3612-68-8	0	1	0	1-Penten-3-one, 2,4-dimethyl-
3615-41-6	1	1	1	*L*-Mannose, 6-deoxy- {α-rhamnose}
3615-55-2	0	1	0	Ribose, 5-(dihydrogen phosphate)
3615-82-5	0	1	0	myo-Inositol, hexakis(dihydrogen phosphate), calcium magnesium salt {phytin}
3616-06-6	0	1	0	Uridine 5′-(trihydrogen diphosphate), *P*′-α-*D*-xylopyranosyl ester
3619-22-5	1	0	0	Benzoic acid, 4-methyl-, hydrazide
3625-52-3	1	0	0	Dotriacontanoic acid
3637-01-2	1	0	0	Ethanone, 1-(3,4-dimethylphenyl)-
3648-21-3	0	1	0	1,2-Benzenedicarboxylic acid, diheptyl {diheptyl phthalate}
3652-91-3	1	0	0	9*H*-Carbazole, 2-methyl-
3658-77-3	1	1	1	3(2*H*)-Furanone, 4-hydroxy-2,5-dimethyl- {furaneol}
3658-80-8	1	0	0	Trisulfide, dimethyl-
3674-66-6	1	0	0	Phenanthrene, 2,5-dimethyl-
3674-69-9	1	0	0	Phenanthrene, 4,5-dimethyl-
3675-21-6	0	1	0	2-Pentenoic acid, 3-methyl-
3681-71-8	0	1	0	3-Hexen-1-ol, acetate, (*Z*)-
3690-05-9	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)- {coumaryl alcohol}
3693-22-9	1	0	0	2-Dibenzofuranamine
3697-24-3	1	0	0	Chrysene, 5-methyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
3710-43-8	1	0	0	Furan, 2,4-dimethyl-
3712-16-1	1	1	1	Stigmast-5-en-3-ol, 9-octadecenoate, [3β(*Z*)]- {β-sitosteryl oleate}
3714-73-6	1	0	0	Benzenepropanoic acid, 2,3-dihydroxy-
3718-67-0	1	0	0	2(1*H*)-Pyridinone, 3,5-dimethyl-
3724-65-0	1	1	1	2-Butenoic acid {crotonic acid}
3727-35-3	1	1	1	2-Cyclopenten-1-one, 3-methyl-2-(2-oxopropyl)-
3731-52-0	1	1	1	Pyridine, 3-(aminomethyl)-
3736-81-0	1	0	0	2-Furancarboxylic acid, 4-[(2,2-dichloroacetyl)-methylamino]phenyl ester
3738-00-9	0	1	0	Naphthalene, decahydro-1-ethoxido-2,5,5,8a-tetramethyl- {ambroxan}
3739-30-8	0	1	0	Butanoic acid, 2-hydroxy-2-methyl-
3743-22-4	1	0	0	Phenol, 2-(dimethylamino)-
3757-53-7	1	0	0	1*H*-Pyrrole-2-carboxylic acid, 5-methyl-
3760-11-0	1	1	1	2-Nonenoic acid
3760-54-1	1	1	1	1-Pyrrolidinecarboxaldehyde
3769-23-1	1	0	0	1-Hexene, 4-methyl-
3770-48-7	1	0	0	9*H*-Carbazole, 4-methyl-
3777-69-3	0	1	0	Furan, 2-pentyl-
3778-29-8	0	1	0	2-Quinolinecarboxylic acid, 4,6-dihydroxy- {6-hydroxykynurenic acid}
3779-61-1	0	1	0	1,3,6-Octatriene, 3,7-dimethyl-, (*E*)-
3779-64-4	1	0	0	2-Cyclopenten-1-one, 2,3-dimethyl-4-(1-methylethyl)-
3780-58-3	0	1	0	Hexanoic acid, 3-methyl-
3782-00-1	1	0	0	Benzofuran, 2,3-dimethyl-
3790-71-4	1	1	1	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- [2 CAS Nos.] {sinensol, farnesol}
4602-84-0				
3794-96-5	0	1	0	Benzene, 2-methoxy-1-methyl-4-(1-methylethenyl)-
3796-70-1	1	1	1	5,9-Undecadien-2-one, 6,10-dimethyl-, (*E*)- {geranylacetone}
3810-26-2	1	0	0	2-Cyclopenten-1-one, 3-phenyl-
3811-49-2	0	1	0	4*H*-1,3,2-Benzodioxaphosphorin-2-sulfide, 2-methoxy- {Salithion®}
3819-09-8	0	1	0	Plastoquinol
3848-24-6	1	0	0	2,3-Hexanedione
3855-26-3	1	0	0	Phenol, 2-ethyl-4-methyl-
3857-25-8	1	1	1	2-Furanmethanol, 5-methyl-
3859-41-4	1	1	1	1,3-Cyclopentanedione
3877-15-4	1	0	0	Propane, 1-(methylthio)-
3877-19-8	1	1	1	Naphthalene, 2-methyl-1,2,3,4-tetrahydro-
3878-55-5	1	1	1	Butanedioic acid, monomethyl ester
3879-26-3	1	1	1	5,9-Undecadien-2-one, 6,10-dimethyl-, (*Z*)- {nerylacetone}
3883-39-4	1	0	0	Pyridine, 2-ethenyl-5-methyl-
3885-29-8	1	0	0	2-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester
3891-98-3	1	1	1	Dodecane, 2,6,10-trimethyl- (farnesane)
3892-00-0	1	0	0	Pentadecane, 2,6,10-trimethyl-
3899-18-1	1	0	0	2,6,10-Dodecatriene, 2,6,10-trimethyl-, (*E,E*)-
3913-50-6	0	1	0	Propanoic acid, 2-oxo-3-(phosphonooxy)-
3913-71-1	0	1	0	2-Decenal, (*E*)-
3917-48-4	0	1	0	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-, (1R)-
3929-61-1	0	1	0	*L*-Glutamic acid, *N*-*L*-α-glutamyl-
3929-89-3	1	0	0	Benzoic acid, 2,3-dihydroxy-4-methyl-
3934-81-4	1	0	0	Benzoic acid, 2,3-dihydroxy-4-methoxy-
3937-56-2	0	1	0	1,9-Nonanediol
3943-74-6	1	1	1	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester
3973-43-1	1	0	0	4-Pentenal, 4-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
3978-81-2	1	1	1	Pyridine, 4-(1,1-dimethylethyl)- {4-*tert*-butylpyridine}
3999-78-8	1	0	0	Pyridine, 3-ethyl-5-methyl-
4026-18-0	1	1	1	Butanoic acid, 2-hydroxy-3-methyl-
4028-66-4	1	0	0	Benzene, 2-methoxy-1,3,5-trimethyl-
4030-18-6	1	1	1	Pyrrolidine, 1-acetyl-
4030-22-2	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4-dimethyl-
4030-23-3	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,4,5-trimethyl-
4030-24-4	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-4-ethyl-
4031-15-6	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-
4041-09-2	1	0	0	Cyclopentanone, 2,5-dimethyl-
4041-11-6	1	0	0	2-Cyclopenten-1-one, 2,5-dimethyl-
4045-53-8	1	0	0	1,3-Cyclopentadiene, 1,3-dimethyl-
4050-45-7	1	0	0	2-Hexene, (*E*)-
4074-46-8	1	0	0	Phenol, 4-methyl-2-propyl-
4096-34-8	1	0	0	3-Cyclohexen-1-one
4100-80-5	1	0	0	2,5-Furandione, dihydro-3-methyl-
4104-44-3	0	1	0	1-Butanamine, *N*,3-dimethyl-
4106-66-5	1	0	0	3-Dibenzofuranamine
4110-50-3	1	0	0	Propane, 1-(ethylthio)-
4124-88-3	0	1	0	3-Nonenoic acid
4128-31-8	1	0	0	2-Octanol
123-96-6				
4130-42-1	1	1	1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-
4151-33-1	0	1	0	Propanoic acid, 2-oxo-, potassium salt
4160-77-4	1	0	0	2,4(1*H*,3*H*)-Pyrimidinedione, 3,5-dimethyl-
4161-60-8	1	1	1	2-Pentanone, 4-hydroxy-
4167-75-3	1	0	0	Phenol, 2-(2-methylpropyl)-
4170-30-3	1	1	1	2-Butenal {crotonaldehyde}
4172-43-4	1	0	0	Pentanoic acid, 2,3,4,5-tetrahydroxy- [4 CAS Nos.]
4172-44-5 L				
17828-56-7 DL				
526-91-0 D				
4172-44-5 L	1	0	0	Pentanoic acid, 2,3,4,5-tetrahydroxy- [4 CAS Nos.]
526-91-0 D				
17828-56-7 DL				
4172-43-4				
4175-66-0	1	0	0	Thiazole, 2,5-dimethyl-
4176-17-4	0	1	0	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-, (R)-
4176-53-8	1	0	0	1-Phenanthrenamine
4177-16-6	1	1	1	Pyrazine, 2-ethenyl-
4181-95-7	1	0	0	Tetracontane
4182-41-6	0	1	0	2(5*H*)-Furanone, 4,5,5-trimethyl-
4192-31-8	0	1	0	3-Pyridinebutanoic acid, γ-oxo-
4219-24-3	1	1	1	3-Hexenoic acid {hydrosorbic acid}
4221-98-1	1	1	1	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)-, (R)- {α-phellandrene}
4250-38-8	1	1	1	Nonacosanoic acid
4250-90-2	0	1	0	Benzo[*g*]pteridine-10(2*H*)-acetaldehyde, 3,4-dihydro-7,8-dimethyl-2,4-dioxo-
4254-13-1	1	1	1	1,2,3-Propanetriol, labeled with ^{14}C {glycerol-^{14}C}
4265-16-1	1	0	0	2-Benzofurancarboxaldehyde
4265-25-2	1	0	0	Benzofuran, 2-methyl-
4269-05-0	1	0	0	9*H*-Fluoren-9-one, 4-methyl-
4272-12-2	1	0	0	Propanoic acid, 3-(acetyloxy)-
4293-57-6	1	0	0	Acetamide *N*-(2-hydroxypropyl)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
4294-16-0	0	1	0	Adenosine, *N*-(phenylmethyl)-
4299-57-4	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2,3-dimethyl-5-(3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22, 26,30,34-hexatriacontanonaenyl)-, (all-*E*)- {plastoquinone 9}
4313-03-5	0	1	0	2,4-Heptadienal [2 CAS Nos.]
5910-85-0				
4313-57-9	1	0	0	1,4-Cyclohexadiene, 1-methyl-
4314-66-3	1	0	0	3-Pyridinecarboxamide, *N*-ethyl-
4325-74-0	1	0	0	1,2′-Binaphthalene
4325-82-0	1	0	0	3-Penten-2-ol, 4-methyl-
4329-12-8	1	1	1	Benzene, 1-chloro-3-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- {*m,p′*-DDD}
4340-76-5	1	0	0	2-Eicosanol
4360-47-8	1	0	0	2-Propenenitrile, 3-phenyl- {cinnamonitrile}
4361-87-9	1	1	1	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, (*Z*)- {*cis*-caffeic acid}
4363-93-3	0	1	0	4-Quinolinecarboxaldehyde
4373-13-1	1	0	0	Naphthalene, 1,2-dihydro-4-methyl-
4382-17-6	0	1	0	4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-methoxy-
4385-67-5	1	0	0	Pyridine, 3-(3-methylphenyl)-
4390-05-0	0	1	0	Butanal, 4-amino-
4393-06-0	0	1	0	Benzenemethanol, α-ethenyl-
4407-36-7	0	1	0	2-Propen-1-ol, 3-phenyl-, (*E*)-
4411-89-6	1	1	1	Benzeneacetaldehyde, α-ethylidene- {2-phenyl-2-butenal}
4412-10-6	0	1	0	Benzeneacetic acid, α-ethylidene-
4412-16-2	0	1	0	2-Dodecenoic acid
4412-91-3	1	0	0	3-Furanmethanol
4412-96-8	1	0	0	3-Furancarboxylic acid, 3-methyl-
4417-81-6	1	0	0	Butanal, 2-oxo- {ethylglyoxal}
4425-82-5	1	0	0	9*H*-Fluorene, 9-methylene-
4427-56-9	1	0	0	Phenol, 4-methyl-2-(1-methylethyl)-
4429-05-4	0	1	0	Glycine, *N*-(1-deoxy-*D*-fructos-1-yl)-
4430-31-3	0	1	0	2*H*-1-Benzopyran-2-one, octahydro-
4435-50-1	1	0	0	1,2,3-Butanetriol {1-methylglycerol}
4436-75-3	0	1	0	3-Hexene-2,5-dione
4437-50-7	1	0	0	2,5-Hexanedione, 3-methyl-
4437-51-8	1	0	0	3,4-Hexanedione
4451-30-3	1	1	1	β-*D*-Glucofuranose, 1,5:3,6-dianhydro-
4461-48-7	1	0	0	2-Pentene, 4-methyl-
4464-20-4	1	0	0	Propanedial, dihydroxy-
4466-14-2	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester {Pyrethrin (natural), Jasmolin 1®}
4466-24-4	1	1	1	Furan, 2-butyl-
4471-47-0	1	0	0	Acetonitrile, oxo-
4476-02-2	1	0	0	Butanenitrile, 2-hydroxy-
4478-63-1	0	1	0	Ethanone, 1-(3,3-dimethyloxiranyl)- {mesityl oxide epoxide}
4482-75-1	0	1	0	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin, α-maltose}
4497-92-1	0	1	0	Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-, (1R, 6R)- {(+)-2-carene}
4501-31-9	1	1	1	2-Propenoic acid, 3-(4-hydroxyphenyl)-, (*Z*)- {*cis*-coumaric acid}
4506-36-9	1	1	1	Naphthalene, 1,2-dihydro-1,5,8-trimethyl-
4513-94-4	1	0	0	1*H*-Pyrrole-2-carbonitrile
4515-18-8	1	1	1	2-Piperidinecarboxylic acid, 1-nitroso- {*N*-nitrosopipecolic acid (NPIC)}
30310-81-7				
4526-77-6	1	0	0	2,5-Piperazinedione, 3-methyl-, (S)-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
4536-23-6	1	1	1	Hexanoic acid, 2-methyl- {2-methylhexanoic acid}
4536-26-9	1	1	1	Hexadecanoic acid, tetradecyl ester
4539-51-9	1	0	0	9*H*-Carbazole, 2-amino-
4541-89-3	1	0	0	Benzene, 1,1′-(chloroethenylidene)bis-
4542-64-7	1	0	0	1,2-Cyclopentanedione, 4-phenyl-
4546-59-2	0	1	0	9,12-Octadecadienoic acid, 18-hydroxy-, (*Z,Z*)-
4549-74-0	1	0	0	1,3-Pentadiene, 3-methyl- (*E*)- or (*Z*)-
4551-72-8	1	0	0	1*H*-Pyrrole-2-carboxamide
4569-45-3	1	0	0	9*H*-Fluorene, 9,9-dimethyl-
4586-22-5	0	1	0	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, stereoisomer
4588-18-5	1	0	0	1-Octene, 2-methyl-
4593-38-8	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-5-methyl-
4593-90-2	1	0	0	Benzenepropanoic acid, β-methyl-
4602-84-0	1	1	1	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- [2 CAS Nos.] {sinensol, farnesol}
3790-71-4				
4607-33-4	1	0	0	Dibenzo[*b,h*][1]benzopyrano[2,3,4-*de*][1,6]naphthyridine
4609-89-6	1	0	0	Pentane, 2-nitro-
4612-63-9	1	1	1	9*H*-Fluorene, 2,3-dimethyl-
4613-38-1	0	1	0	2,6-Octadienoic acid, 3,7-dimethyl-, (*Z*)-
4616-73-3	1	0	0	Eicosanenitrile
4630-07-3	0	1	0	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7β,8aα] {valencene}
4630-08-4	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-2-hydroxy-α,2,5,5,8a-pentamethyl-, [1R-[1α(S*),2β,4aβ,8aα]]- {episclareol}
4630-20-0	1	0	0	9*H*-Carbazole, 3-methyl-
4634-87-1	1	0	0	2,4-Heptadiene, 2,6-dimethyl-
4657-58-3	0	1	0	9,19-Cyclolanostan-3-ol, (3β)-
4669-02-7	1	1	1	Pentadecanoic acid, 14-methyl-
4670-09-1	1	0	0	Benzeneacetic acid, 3,5-dihydroxy-
4673-31-8	1	0	0	Pyridine, 3-propyl-
4674-50-4	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4α,4aα,6β)]-{bicyclo[4.4.0]dec-1-en-3-one, 5,6-dimethyl-8-isopropenyl-} {nootkatone}
4675-87-0	0	1	0	2-Buten-1-ol, 2-methyl-
4693-31-6	1	0	0	1,4-Benzenediol, 2-propyl-
4694-67-1	1	0	0	3-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester
5204-91-1				
4695-13-0	0	1	0	Benzeneacetamide, α-phenyl-
4695-62-9	0	1	0	Bicyclo[2,2,1]heptan-2-one, 1,3,3-trimethyl- {*d*-fenchone}
4698-08-2	0	1	0	2,6-Octadienoic acid, 3,7-dimethyl-, (*E*)-
4730-22-7	0	1	0	2-Heptanol, 6-methyl-
4730-63-6	1	1	1	Tricosanoic acid, 22-methyl-
4736-56-5	0	1	0	Stigmast-22-en-3-ol (3β,5α,22Z,24S)-
4740-12-9	1	0	0	Acridine, 3-methyl-
4747-21-1	1	1	1	2-Propanamine, *N*-methyl-
4748-78-1	0	1	0	Benzaldehyde, 4-ethyl-
4754-27-2	1	0	0	Pyridine, 3-(1-hydroxyethyl)-
4760-34-3	1	0	0	1,2-Benzenediamine, *N*-methyl-
4775-98-8	1	0	0	2-Piperidinone, 6-methyl-
4784-86-5	1	0	0	1,3-Cyclopentadiene, 1,2-dimethyl-
4786-19-0	1	0	0	3-Butenenitrile, 3-methyl-
4786-20-3	1	0	0	2-Butenenitrile {crotononitrile}
4786-24-7	1	0	0	2-Butenenitrile, 3-methyl-
4835-90-9	0	1	0	Propanoic acid, 3-hydroxy-,2,2-dimethyl- {hydroxypivalic acid}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
4868-20-6	1	0	0	Furan, 2-(3-hexenyl)-5-methyl-, (*Z*)-
4889-83-2	0	1	0	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-
4915-21-3	1	0	0	2-Furanacetic acid, ethyl ester
4920-77-8	1	0	0	Phenol, 3-methyl-2-nitro-
4925-88-6	1	0	0	Benzaldehyde, 2,5-dimethoxy-4-methyl-
4940-11-8	1	1	1	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy- {ethylmaltol}
4940-16-3	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-propyl-
4940-17-4	1	0	0	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-
4940-18-5	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylpropyl)-
4945-28-2	1	0	0	Quinoline, 2,3,8-trimethyl-
4949-20-6	1	0	0	2,4-Pentadien-1-ol
4964-76-5	1	0	0	Quinoline, 7-methoxy-
4965-09-7	1	0	0	Isoquinoline, 1-methyl-1,2,3,4- tetrahydro-
4971-18-0	1	0	0	Cyclopentanone, 2-ethyl-
4981-99-1	1	1	1	Hentriacontane, 3-methyl-
5006-66-6	0	1	0	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
5026-62-0	0	1	0	Benzoic acid, 4-hydroxy-, methyl ester, sodium salt
5031-83-4	0	1	0	Benzeneacetaldehyde, α-(2-phenylethylidene)-
5037-60-5	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-4,7-dimethyl-
5040-23-3	1	0	0	Benzeneethanol, α,4-dimethyl-
5058-01-5	1	0	0	2*H*-Pyran-2-one, tetrahydro-3-hydroxy-
5058-19-5	1	0	0	Pyridine, 2-butyl-
5075-92-3	1	0	0	2-Pyrrolidinone, 1,5-dimethyl-
5076-72-2	1	0	0	Benzene, 1-ethoxy-4-methoxy
5076-82-4	1	0	0	2,5-Piperazinedione, *N,N*-dimethyl-
5077-67-8	1	1	1	2-Butanone, 1-hydroxy-
5103-71-9	0	1	0	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- {α-Chlordane®}
5121-74-4	1	1	1	Benzene, 1,1′-(1,2-ethenediyl)bis[4-chloro- {DCS = dichlorostilbene}
5129-58-8	0	1	0	Tridecanoic acid, 12-methyl-, methyl ester
5129-61-3	0	1	0	Heptadecanoic acid, 16-methyl-, methyl ester
5129-72-6	1	0	0	Propanamide, *N*-ethyl-
5145-01-7	1	1	1	2(3*H*)-Furanone, dihydro-3,5-dimethyl-
5145-64-2	1	0	0	1*H*-Pyrrole, 1-propyl-
5147-00-2	0	1	0	*L*-Serine, acetate (ester)
5150-42-5	1	1	1	Phenol, 2,3-dimethoxy-
5153-92-4	1	1	1	1*H*-Naphtho[2,1-*b*]pyran, 4a,5,6,6a,7,8,9,10,10a,10b-decahydro-3,4a,7,7,10a-pentamethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]-
5154-01-8	0	1	0	2(1*H*)-Pyridinone, 5-hydroxy- {2,5-pyridinediol}
5157-09-5	0	1	0	Norleucine {2-aminohexanoic acid}
327-57-1				
5162-03-8	0	1	0	Methanone, (2-chlorophenyl)phenyl-
5164-76-1	0	1	0	2-Pentenedioic acid, dimethyl ester
5164-78-3	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*E,E*)- {megastigmatrienone} {*trans*-, *trans*-K_{1a}}
5164-79-4	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,Z*)- {*cis*-, *cis*-K_{2b}}
5166-53-0	1	1	1	3-Hexen-2-one, 5-methyl-
5185-97-7	1	1	1	2-Pentanone, 5-(acetyloxy)-
5187-71-3	1	0	0	4-Pentenal, 2-methyl-
5192-03-0	1	0	0	1*H*-Indole, 5-amino-
5204-91-1	1	0	0	3-Furancarboxylic acid, tetrahydro-5-oxo-, methyl ester
4694-67-1				
5211-62-1	1	0	0	2-Propanone, 1-(2-methoxyphenyl)-
5220-49-5	1	0	0	2-Cyclohexen-1-one, 3-amino-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
5221-53-4	0	1	0	Pyrimidine, 5-butyl-2-dimethylamino-4-hydroxy-6-methyl- {Dimetherimol®}
5241-22-5	0	1	0	Cholest-8-en-3-ol, 4-methyl-, (3β,4α,5α)-
5241-24-7	0	1	0	Cholest-8-en-3-ol, 4,4-dimethyl-, (3β,5α)-
5256-65-5	1	0	0	Cyclohexene, 3-methyl-6-(1-methylethyl)-
5259-88-1	0	1	0	1,4-Oxathiin-3-carboxamide 4,4-dioxide, 5,6-dihydro-2-methyl-*N*-phenyl- {Oxycarboxin®}
5263-87-6	1	0	0	Quinoline, 6-methoxy-
5264-15-3	1	0	0	4-Pyridinebutanol
5266-85-3	0	1	0	Benzenamine, 2-methyl-6-(1-methylethyl)-
5273-86-9	0	1	0	Benzene, 1,2,4-trimethoxy-5-(2-propenyl)-, (*E*)-
5293-97-0	1	1	1	Methanone, bis(2-chlorophenyl)-
5298-13-5	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*E,Z*)- {*trans*-, *cis*-K_{2a}}
5303-25-3	1	1	1	Octadecanoic acid, dodecyl ester
5309-52-4	0	1	0	2-Hexenoic acid, 2-ethyl-
5328-37-0	1	1	1	*L*-Arabinose
87-72-9				
5328-43-8	0	1	0	Rhamnitol
5331-48-6	1	0	0	Acetamide, *N*-propyl-
5335-75-1	1	0	0	Pyridine, 4-butyl-
5337-93-9	1	0	0	1-Propanone, 1-(4-methylphenyl)-
5341-95-7	1	0	0	2,3-Butanediol, (R*,S*)-
5349-62-2	0	1	0	2-Pentanone, 4-methyl-1-phenyl-
5362-56-1	1	1	1	2-Pentenal, 4-methyl-
5263-87-6	1	0	0	Quinoline, 6-methoxy-
5347-68-2	1	0	0	Piperidine, 2,3-dimethyl-
5349-60-0	0	1	0	1-Propanol, 1-(4-methoxyphenyl)-
5371-49-3	1	0	0	Acetaldehyde, (acetyloxy)-
5385-22-8	1	0	0	Naphth[1,2-*e*]acephenanthrylene {dibenzo[*b,j*]fluoranthene}
5385-75-1	1	0	0	Dibenz[*a,e*]aceanthrylene {dibenzo[*a,e*]fluoranthene}
5392-40-5	1	1	1	2,6-Octadienal, 3,7-dimethyl- {citral}
141-27-5				
5421-17-0	0	1	0	Benzeneacetic acid, hexyl ester
5444-01-9	1	0	0	3-Pyridinecarbonitrile, 4-methyl-
5451-83-2	1	0	0	Phenol, 3-methoxy-, acetate
5460-63-9	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, methyl ester
5464-28-8	1	0	0	1,3-Dioxolane-4-methanol
5469-16-9	1	1	1	2(3*H*)-Furanone, dihydro-4-hydroxy-
5471-51-2	1	1	1	2-Butanone, 4-(4-hydroxyphenyl)- {4-(*p*-hydroxyphenyl)-2-butanone}
5492-79-5	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, (*Z,E*)- {*cis*-, *trans*-K_{1b}}
5501-37-1	1	0	0	9*H*-Fluoren-9-one, 1-methyl-
5502-88-5	1	1	1	Cyclohexene, 1-methyl-4-(1-methylethyl)-
5502-94-3	1	1	1	Tetradecanoic acid, 12-methyl-
5746-58-7				
5519-42-6	1	0	0	1*H*-Pyrazole, 3,4,5-trimethyl-
5522-43-0	1	0	0	Pyrene, 1-nitro-
5541-68-4	1	0	0	8-Quinolinol, 7-methyl-
5548-09-4	0	1	0	1*H*-Indole-3-propanoic acid, methyl ester
5584-69-0	1	1	1	2(5*H*)-Furanone, 3,5-dimethyl-
5597-50-2	1	0	0	Benzenepropanoic acid, 4-hydroxy-, methyl ester
5601-60-5	0	1	0	Decanoic acid, 8-methyl-
5604-55-7	0	1	0	3-Pentenal
5615-90-7	1	1	1	2,5-Pyrrolidinedione, 3-methyl-
5621-14-7	1	0	0	1*H*-Indole, 3,7-dimethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
5621-15-8	1	0	0	1*H*-Indole, 1,6-dimethyl-
5621-16-9	1	0	0	1*H*-Indole, 1,7-dimethyl-
5625-46-7	1	0	0	2,5-Piperazinedione, 3,6-dimethyl-
5625-53-6	1	0	0	2,5-Piperazinedione, 3-methyl-
5631-68-5	1	0	0	Benzenepropanoic acid, 2,4-dihydroxy-
5636-65-7	0	1	0	4-Hexenoic acid, 5-methyl-
5650-10-2	1	0	0	Benzenamine, 4-(1-methylethyl)-*N*-phenyl-
5654-86-4	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-
5663-62-7	1	0	0	Acetamide, *N*-(2-furanylmethyl)-
5667-11-8	1	0	0	9*H*-Pyrido[3,4-*b*]indole, methyl- {?-methylnorharman}
5676-58-4	1	0	0	Benzoxazole, 2,5-dimethyl-
5682-69-9	1	0	0	2-Cyclopenten-1-one, 3-ethyl-
5682-72-4	1	0	0	2-Cyclopenten-1-one, 2-ethyl-3-methyl-
5692-15-9	0	1	0	*L*-Serine, labeled with ^{14}C
5715-25-3	0	1	0	2-Cyclohexen-1-one, 4,5-dimethyl-
5716-15-4	0	1	0	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt
21422-41-3				
5724-56-1	1	0	0	Benzonitrile, 2,3-dimethyl-
5724-81-2	1	0	0	1*H*-Pyrrole, 3,4-dihydro-
5743-26-0	0	1	0	Acetic acid, calcium salt, monohydrate
5746-58-7	1	1	1	Tetradecanoic acid, 12-methyl-
5502-94-3				
5746-86-1	1	0	0	Pyridine, 3-(2-pyrrolidinyl)-
5760-58-7	1	0	0	2-Cyclopenten-1-one, 2-methyl-3-propyl-
5765-44-6	1	0	0	Isoxazole, 5-methyl-
5768-79-6	1	0	0	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione, tetrahydro-
5779-94-2	1	1	1	Benzaldehyde, 2,5-dimethyl-
5780-66-5	1	0	0	Pyrazinecarboxaldehyde
5794-13-8	0	1	0	*L*-Asparagine monohydrate
5803-57-6	1	0	0	Pentonic acid, 5-deoxy-, γ-lactone
5813-64-9	1	0	0	1-Propanamine, 2,2-dimethyl-
5834-16-2	1	1	1	2-Thiophenecarboxaldehyde, 3-methyl-
5835-18-7	1	1	1	7*H*-1-Benzopyran-7-one, octahydro-2,5,5,8a-tetramethyl- {7-chromanone, hexahydro-2,5,5,8a-tetramethyl-}
5835-19-8	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6-tetrahydro-4,4,7-trimethyl-
5851-44-5	1	0	0	1*H*-Benzimidazole, 2-butyl-
5851-46-7	1	0	0	1*H*-Benzimidazole, 2-pentyl-
5870-63-3	0	1	0	2-Cyclopenten-1-one, 3-hydroxy-2-methyl-
5870-68-8	1	1	1	Pentanoic acid, 3-methyl-, ethyl ester
5894-59-7	0	1	0	Digalacturonic acid
5896-02-6	1	1	1	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-trimethyl-
5905-46-4	1	0	0	Disulfide, 1-propenyl propyl
5905-47-5	1	0	0	Disulfide, methyl 1-propenyl
5908-87-2	1	0	0	Docosanoic acid, ethyl ester
5910-85-0	0	1	0	2,4-Heptadienal [2 CAS Nos.]
4313-03-5				
5910-87-2	1	1	1	2,4-Nonadienal, (*E*,*E*)-
6750-03-4				
5910-89-4	1	1	1	Pyrazine, 2,3-dimethyl-
5912-86-7	1	1	1	Phenol, 2-methoxy-4-(1-propenyl)-, (*Z*)- {*cis*-isoeugenol}
5918-29-6	1	1	1	Hexadecanoic acid, 14-methyl-
5932-68-3	1	1	1	Phenol, 2-methoxy-4-(1-propenyl)-, (*E*)- {*trans*-isoeugenol}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
5948-04-9	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, *trans*-
5953-51-5	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-methyl-, (S)-
5979-92-0	1	1	1	Pyridine, 3-(1-ethyl-2-pyrrolidinyl)-, (S)-
5979-94-2	1	1	1	Pyrrolidine, 1-acetyl-2-(3-pyridinyl)-, (S)- {*N*′-acetylnornicotine}
5980-06-3	1	1	1	2-Pyrrolidinone, 5-(3-pyridinyl)-, (S)- {norcotinine}
5980-21-2	0	1	0	Pentanoic acid, 3-hydroxy-4-methyl-
5986-36-7	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,8-tetramethyl-, (R)-
5989-02-6	1	1	1	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-
5989-24-2	1	1	1	Spiro[furan-2(3*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5(4*H*)-one, decahydro-3,3′a,6′,6′,9′a-pentamethyl- {α-levantenolide}
30987-48-5				
5989-27-5	1	0	0	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- {*d*-limonene}
5989-33-3	0	1	0	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*Z*)- {*cis*-linalool oxide}
5989-54-8	1	0	0	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)- {*l*-limonene}
5997-61-5	1	0	0	1*H*-Pyrrole-2,5-dione, 3-ethyl-
6000-40-4	0	1	0	Propanoic acid, 2,3-dihydroxy-, (R)-
6004-60-0	1	0	0	Ethanone, 1-cyclopentyl-
6018-94-6	0	1	0	Ethanedioic acid, nickel salt
6021-23-4	0	1	0	3-Pyridinebutanamine
6025-53-2	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*E*)-
6027-71-0	1	1	1	Hexadecanoic acid, triacontyl ester
6032-29-7	0	1	0	2-Pentanol
6036-58-4	0	1	0	Cholest-7-en-3-ol, (3β)-
6051-03-2	1	0	0	2(3*H*)-Benzofuranone, hexahydro-
24871-12-3				
6052-73-9	1	1	1	2(1*H*)-Pyridinone, 5,6-dihydro- {2-piperidone, 3,4-dehydro-}
6053-02-7	1	1	1	1,2-Benzenediol, 4-ethenyl-
6061-10-5	0	1	0	Octanoic acid, 3-methyl-
6062-47-1	0	1	0	Cholest-8-en-3-ol, 14-methyl-, (3β,5α)-
6064-52-4	0	1	0	Nonanoic acid, 4-oxo-
6064-63-7	0	1	0	Hexanoic acid, 2-hydroxy-
6066-62-2	1	0	0	2(5*H*)-Furanone, 5-ethylidene-3,4-dimethyl-
6067-11-4	0	1	0	2(5*H*)-Furanone, 3,4-dimethyl-5-hydroxy-5-pentyl-
6072-57-7	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-3-methyl-
6082-44-6	0	1	0	1-Cyclohexene-1-carboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-4,5-dihydroxy-, (3α,4α,5β)-
6091-76-5	1	0	0	1*H*-Isoindol-1-one, 2,3-dihydro-3-methyl-
6094-02-6	1	0	0	1-Hexene, 2-methyl-
6100-05-6	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripotassium salt, monohydrate
6100-74-9	1	0	0	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-
6118-79-2	0	1	0	2-*O*-α-*D*-Galactopyranuronosyl-*L*-mannose, 6-deoxy-
6124-79-4	1	1	1	2(5*H*)-Furanone, 4-methyl-
6136-68-1	1	0	0	Benzonitrile, 3-acetyl-
6138-85-8	0	1	0	2-Butanone, 4-(2,2,6-trimethylcyclohexyl)- {tetrahydroionone}
6159-55-3	0	1	0	Pyrrolo[2,1-*b*]quinazolin-3-ol, 1,2,3,9-tetrahydro- {*l*-peganin, *l*-vasicin}
6161-62-2	1	0	0	Phenol, 2-ethyl-3-methyl-
6161-67-7	1	0	0	Phenol, 3-ethyl-4-methyl-
6175-49-1	0	1	0	2-Dodecanone
6214-01-3	1	1	1	1,2-Propanediol, 2-acetate
6232-48-0	1	0	0	Acephenanthrylene, 4,5-dihydro-
6238-69-3	0	1	0	4-Piperidinecarboxylic acid, 1-nitroso-
6250-72-2	1	1	1	Nonadecanoic acid, 18-methyl-
6252-26-2	0	1	0	1*H*-Naphtho[2,1-*b*]pyran, dodecahydro-3,4a,7,7,10a-pentamethyl-
6259-76-3	0	1	0	Benzoic acid, 2-hydroxy-, hexyl ester
6267-02-3	1	0	0	Acridine, 9,10-dihydro-9,9-dimethyl- {9,9-dimethylacridan}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
6270-63-9	1	0	0	Pyrazine, 2-hydroxy- = 2(*H*)-pyrazinone
6276-03-5	1	1	1	9*H*-Fluorene-1-carboxylic acid
6279-07-8	1	1	1	9*H*-Xanthene, 2-methyl-
6282-37-7	1	0	0	Benzenemethanol, 4-methyl-α-propyl-
6287-19-0	1	1	1	Piperidine, 2,4-dimethyl-
6290-37-5	0	1	0	Hexanoic acid, 2-phenylethyl ester
6291-17-4	1	0	0	2-Butanol, 3-amino-2-methyl-
6294-65-1	1	0	0	Quinoline, 2-(3-pyridinyl)-
6296-84-0	0	1	0	1,2-Cyclohexanediol, 1-methyl-
6302-03-0	1	1	1	2-Propanone, 1-(3-pyridinyl)-
6303-75-9	1	0	0	Pyrazine, pentyl-
6304-16-1	1	0	0	2-Propanone, 1-(4-pyridinyl)-
6304-24-1	1	0	0	Pyridine, 2-(2-methylpropyl)-
6312-09-0	1	0	0	Pyridine, 3-(2-phenylethyl)-
6338-41-6	1	0	0	2-Furancarboxylic acid, 5-(hydroxymethyl)-
6338-45-0	1	0	0	1*H*-Imidazole, 1,4-dimethyl-
6339-13-5	1	0	0	Pentanenitrile, 2-methyl-
6343-54-0	1	0	0	Formamide, *N*-(phenylmethyl)-
6343-58-4	1	0	0	Pyridine, 5-methyl-2-(1-methylethyl)-
6344-63-4	1	0	0	9*H*-Fluoren-1-amine
6376-59-6	1	0	0	Pentanoic acid, 2-oxo-, methyl ester
6379-73-3	0	1	0	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-
6380-21-8	1	0	0	Phenol, 2-(1-propenyl)-
6380-23-0	1	1	1	Benzene, 4-ethenyl-1,2-dimethoxy-
6380-97-8	1	1	1	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-2-(hydroxymethyl)-
6387-89-9	0	1	0	Oxiranemethanol, acetate {glycidyl acetate}
6400-69-4	1	0	0	2*H*-Pyran-2-one, 5,6-dihydro-6-propyl-
6416-57-5	0	1	0	Resinol: resinol, brown
6418-41-3	0	1	0	Tridecane, 3-methyl-
6418-43-5	0	1	0	Hexadecane, 3-methyl-
6418-44-6	0	1	0	Heptadecane, 3-methyl-
6418-46-8	0	1	0	Eicosane, 3-methyl-
6418-47-9	1	0	0	Heneicosane, 3-methyl-
6456-92-4	1	0	0	2(1*H*)-Pyridinone, 1,3-dimethyl-
6484-52-2	0	1	0	Nitric acid, ammonium salt
6485-40-1 99-49-0	1	1	1	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)- {*l*-carvone}
6505-86-8	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-, sulfate
6510-65-2	1	0	0	9*H*-Carbazole, 1-methyl-
6531-35-7	1	0	0	9,10-Anthracenedione, 2,3-dimethyl-
6542-88-7	1	0	0	Acetaldehyde, amino-
6556-12-3	1	1	1	*D*-Glucuronic acid
6561-44-0	0	1	0	Octadecane, 3-methyl-
6570-87-2	0	1	0	1-Pentanol, 3,4-dimethyl-
6575-13-9	1	0	0	Benzonitrile, 2,6-dimethyl-
6596-86-7	1	0	0	2*H*-Indene, 2-methylene- {benzofulvene}
6600-40-4	0	1	0	Pentanoic acid, 2-amino-
6622-92-0	1	0	0	4(1*H*)-Pyrimidinone, 2,6-dimethyl- = 6-pyrimidinol, 2,4-dimethyl-
6624-76-6	0	1	0	1-Nonacosanol
6627-88-9	1	1	1	Phenol, 2,6-dimethoxy-4-(2-propenyl)-
6628-79-1	1	0	0	Pentanoic acid, 3-methyl-4-oxo-
6638-05-7	1	1	1	Phenol, 2,6-dimethoxy-4-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
6641-83-4	1	0	0	Pentanoic acid, 2-methyl-4-oxo-
6665-95-8	1	0	0	Phenol, 2,3-dimethyl-6-nitro- {phenol, 5,6-dimethyl-2-nitro-}
6665-98-1	1	0	0	1,2-Benzenediol, 3-nitro-
6704-01-4	1	1	1	Heneicosanoic acid, 20-methyl-
6704-02-5	1	0	0	5,9,13,17,21,25,29-Hentriacontaheptaen-2-one, 6,10,14,18,22,26,30-heptamethyl-
6705-31-3	1	1	1	Pyrazineethanol
6705-33-5	1	0	0	Pyrazinemethanol
6708-06-1	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, octahydro-
36588-48-4				
6728-26-3	1	1	1	2-Hexenal, (*E*)-
6728-31-0	0	1	0	4-Heptenal
6750-03-4	1	1	1	2,4-Nonadienal, (*E,E*)-
5910-87-2				
6750-34-1	0	1	0	1-Dodecanol, 3,7,11-trimethyl- {hexahydrofarnesol}
6753-98-6	0	1	0	1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (*E,E,E*)-
6760-12-9	1	0	0	Pyridine, 3-butyl-2,6-dimethyl-
6765-39-5	1	0	0	1-Heptadecene
6789-88-4	0	1	0	Benzoic acid, hexyl ester
6790-58-5	0	1	0	Naphtho[2,1-*b*]furan, dodecahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {ambroxide, ambroxyl}
65588-69-4				
6809-52-5	1	1	1	5,9,13,17-Nonadecatetraen-2-one, 6,10,14,18-tetramethyl-
6811-73-0	0	1	0	β,β-Carotene, 13-*cis*-
6812-78-8	0	1	0	7-Octen-1-ol, 3,7-dimethyl- [2 CAS Nos.] {rhodinol}
141-25-3				
6816-17-7	0	1	0	2-Decene
6818-07-1	1	0	0	Hexanoic acid, 4-methyl-5-oxo-
6869-99-4	0	1	0	Stigmast-7-en-3-ol, (3β)-
6872-06-6	0	1	0	1*H*-Indole, 2,3-dihydro-2-methyl-
6890-88-6	0	1	0	Lanost-8-en-3-ol, 24-methylene-, (3β)-
6898-94-8	1	1	1	Alanine
6898-95-9	1	1	1	Serine
6899-03-2	1	1	1	Aspartic acid
6899-04-3	0	1	0	Glutamine
6899-05-4	1	1	1	Glutamic acid
6899-06-5	0	1	0	Lysine
6901-97-9	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- {α-ionone}
127-41-3				
8013-90-9				
6902-54-1	1	1	1	Pentacosane, 3-methyl-
6909-25-7	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, (2S-*cis*)-
6912-85-2	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolinyl)- {2,3-dehydronicotine}
6912-86-3	0	1	0	Tryptophan
6915-15-7	1	1	1	Butanedioic acid, hydroxy- {malic acid}
6915-18-0	0	1	0	2-Butenedioic acid
6917-35-7	1	1	1	Inositol
6921-64-8	0	1	0	Ethanone, 1-(2-hydroxy-4-methylphenyl)-
6923-22-4	0	1	0	2-Butenamide, 3-hydroxy-*N*-methyl-, dimethylphosphate, (*Z*)- {Monocrotophos®}
6929-04-0	0	1	0	Hexadecanoic acid, 15-methyl-, methyl ester
6931-16-4	1	0	0	Quinoline, 2-methoxy-
6931-17-5	1	0	0	Quinoline, 3-methoxy-
6938-45-0	0	1	0	Hexanoic acid, phenylmethyl ester
6940-57-4	1	0	0	Ethanone, 1-(6-methyl-2-pyridinyl)-
6946-90-3	0	1	0	Hexanoic acid, 2-hydroxy-, ethyl ester

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
6947-94-0	1	0	0	3-Furancarboxylic acid, 2-methyl-
6960-22-1	1	0	0	3-Pyridinecarboxamide, 6-methyl-
6969-43-3	0	1	0	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4,5-trimethyl-
6971-63-7	1	1	1	2(3*H*)-Furanone, dihydro-4,5-dimethyl-
6972-40-3	1	0	0	Pyridine, 1-ethyl-1,2,3,6-tetrahydro-
6973-66-6	1	0	0	Pyridine, 2-(3-methylbutyl)-
6975-60-6	1	1	1	2-Propanone, 1-(2-furanyl)-
6975-98-0	0	1	0	Decane, 2-methyl-
6982-25-8	1	0	0	*DL*-2,3-Butanediol
6982-72-5	1	1	1	Ethanone, 1-(5-methyl-1*H*-pyrrol-2-yl)- {2-acetyl-5-methylpyrrole}
7004-03-7	1	1	1	Valine
7004-04-8	1	1	1	Butanoic acid, 2-amino-3-hydroxy-
7004-09-3	0	1	0	Isoleucine
7004-12-8	0	1	0	Arginine
7005-03-0	1	1	1	Leucine
7005-18-7	0	1	0	Methionine
7006-33-9	1	1	1	Ornithine {2,3-diaminopentanoic acid}
7006-34-0	1	1	1	Asparagine
7006-35-1	0	1	0	Histidine
7035-68-9	1	0	0	1*H*-Benzimidazole, 1-ethyl-
7045-71-8	1	1	1	Undecane, 2-methyl-
7057-97-8	1	0	0	1*H*-Pyrrole, 1-(1-methylethyl)-
7068-83-9	1	0	0	1-Butanamine, *N*-methyl-*N*-nitroso-
7070-24-8	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-4-(3-oxo-1-butenyl)-3,5,5-trimethyl-
7073-61-2	1	1	1	β-*D*-Glucopyranoside, (3β)-cholest-5-en-3-yl- {cholesteryl glucoside}
7076-23-5	1	1	1	Pyridine, 3-(2-pyrrolidinyl)-, (R)- {*d*-nornicotine}
7083-63-8	1	0	0	9*H*-Fluoren-4-amine
7098-07-9	1	0	0	1*H*-Imidazole, 1-ethyl-
7099-42-5	1	0	0	9*H*-Benzo[*a*]cyclopent[*i*]anthracene, 10,11-dihydro- {6,7-cyclopentano-1,2-benzanthracene, 9,10-dihydro-}
7099-43-6	1	0	0	1*H*-Benzo[*a*]cyclopent[*h*]anthracene, 2,3-dihydro- {5,6-cyclopentano-1,2-benzanthracene, 2,3-dihydro-}
7126-38-7	1	0	0	1*H*-Pyrrole-3-carbonitrile
7130-15-6	1	0	0	3*H*-Benzo[*cd*]pyrene, 4,5-dihydro-
7132-64-1	1	1	1	Pentadecanoic acid, methyl ester
7138-40-1	1	0	0	Heptacosanoic acid
7194-84-5	1	1	1	Heptatriacontane
7194-85-6	1	1	1	Octatriacontane
7194-86-7	1	1	1	Nonatriacontane
7194-87-8	1	0	0	Hentetracontane
7196-71-6	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-methoxyphenyl]- {1-*O*-feruloylglucose}
14364-12-6				
7200-26-2	1	0	0	Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-, (all-*E*)-
7206-18-0	1	0	0	2-Octadecene, (*E*)-
7208-05-1	1	0	0	Oxazole, 2,4-dimethyl-
7212-44-4	1	1	1	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- {nerolidol}
7212-91-1	0	1	0	Stigmasta-7,24(28)-dien-3-ol, (3β,5α)-
7215-44-3	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-O-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-
20188-84-5				{quercetin 3, 3′-diglucoside}
7220-78-2	1	1	1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-
7220-81-7	0	1	0	Cyclopenta[*c*]furo[3′,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 2,3,6a,8,9,9a-hexahydro-4-methoxy-, (6aR-*cis*)-
				{aflatoxin B_2}
7226-86-0	1	0	0	2,6-Dodecadien-1-ol, 3,7,11-trimethyl-
7230-71-9	1	0	0	Benz[*c*]acridine, 10-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
7235-40-7	1	1	1	β,β-Carotene {β-carotene, all-*trans*}
7239-24-9	0	1	0	1-Propanamine, *N,N*,2-trimethyl-
7251-61-8	1	0	0	Quinoxaline, 2-methyl-
7251-82-3	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4-methyl-
7295-76-3	1	1	1	Pyridine, 3-methoxy-
7298-93-3	0	1	0	Adenosine 5′-(trihydrogen diphosphate), 5′ → 5′-ester with 3-(aminocarbonyl)-1-α-*D*- ribofuranosylpyridinium hydroxide, inner salt
7299-89-0	1	0	0	1,2-Benzenedicarboxylic acid, bis(2-ethylbutyl) ester
7300-28-9	1	0	0	Pyridine, 3-(2-propenyl)-
7307-02-0	1	0	0	2,4-Heptanedione
7311-34-4	1	1	1	Benzaldehyde, 3,5-dimethoxy-
7319-38-2	1	0	0	3-Butenal
7320-50-5	1	0	0	Dibenzofuran, 1-methyl-
7320-51-6	1	0	0	Dibenzofuran, 2-methyl-
7320-52-7	1	0	0	Dibenzofuran, 3-methyl-
7320-53-8	1	0	0	Dibenzofuran, 4-methyl-
7324-05-2	0	1	0	Propanamide, 2-amino-, (S)-
7326-19-4	0	1	0	Benzenepropanoic acid, α-hydroxy-, (R)-
7332-93-6	1	0	0	Pentanal, 2-oxo-
7335-06-0	1	0	0	Pyrrolidine, 1-ethyl-
7335-07-1	1	0	0	Pyrrolidine, 1-propyl-
7361-80-0	1	1	1	9,12,15-Octadecatrienoic acid, methyl ester {methyl linolenate}
7361-90-2	1	1	1	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*Z*)- {*cis*-sinapic acid}
7362-37-0	1	1	1	2-Propenoic acid, 3-(3,5-dimethoxy-4-hydroxyphenyl)-, (*E*)- {*trans*-sinapic acid}
7372-86-3	1	1	1	Naphthalene, 2-ethyl-6-methyl-
7372-87-4	1	0	0	Phenanthrene, 1,8-dimethyl-
7383-90-6	0	1	0	1,1′-Biphenyl, 3,4′-dimethyl-
7399-50-0	1	0	0	Pyridine, 2-(1-ethylpropyl)-
7400-08-0	1	1	1	2-Propenoic acid, 3-(4-hydroxyphenyl)- {coumaric acid}
7400-67-1	1	0	0	2(3*H*)-Furanone, 4-acetyldihydro-
7416-57-1	0	1	0	Dodecanoic acid, 10-methyl-
7425-74-3	1	1	1	β-*D*-Glucofuranose, 1,6-anhydro-
7429-90-5	1	1	1	Aluminum
7429-91-6	1	1	1	Dysprosium
7431-92-7	1	0	0	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl-, (all-*E*)-
7439-88-5	1	1	1	Iridium
7439-89-6	1	1	1	Iron
7439-91-0	1	1	1	Lanthanum
7439-92-1	1	1	1	Lead
7439-93-2	1	1	1	Lithium
7439-94-3	1	1	1	Lutecium
7439-95-4	1	1	1	Magnesium
7439-96-5	1	1	1	Manganese
7439-97-6	1	1	1	Mercury
7439-98-7	1	1	1	Molybdenum
7440-00-8	1	1	1	Neodymium
7440-02-0	1	1	1	Nickel
7440-03-1	1	0	0	Niobium
7440-04-2	1	1	1	Osmium
7440-05-3	1	1	1	Palladium
7440-06-4	0	1	0	Platinum
7440-08-6	1	1	1	Polonium
7440-09-7	1	1	1	Potassium

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
7440-10-0	1	1	1	Praseodymium
7440-14-4	1	1	1	Radium, isotope of mass 226 [2 CAS Nos.]
13982-63-3				
7440-15-5	1	1	1	Rhenium
7440-16-6	1	1	1	Rhodium
7440-17-7	1	1	1	Rubidium
7440-18-8	1	1	1	Ruthenium
7440-19-9	1	1	1	Samarium
7440-20-2	1	1	1	Scandium
7440-21-3	1	1	1	Silicon
7440-22-4	1	1	1	Silver
7440-23-5	1	1	1	Sodium
7440-24-6	1	1	1	Strontium
7440-25-7	1	1	1	Tantalum
7440-27-9	0	1	0	Terbium
7440-28-0	1	1	1	Thallium
7440-29-1	1	1	1	Thorium, isotope of mass 232
7440-30-4	1	1	1	Thulium
7440-31-5	1	1	1	Tin
7740-31-5				
7440-32-6	1	1	1	Titanium
7440-33-7	1	1	1	Tungsten
7440-34-8	1	1	1	Actinium
7440-36-0	1	1	1	Antimony
7440-37-1	1	0	0	Argon
7440-38-2	1	1	1	Arsenic
7440-39-3	1	1	1	Barium
7440-41-7	1	1	1	Beryllium
7440-42-8	1	1	1	Boron
7440-43-9	1	1	1	Cadmium
7440-44-0	1	1	1	Carbon
7440-45-1	1	1	1	Cerium
7440-46-2	1	1	1	Cesium
7440-47-3	1	1	1	Chromium
7440-48-4	1	1	1	Cobalt
7440-50-8	1	1	1	Copper
7440-52-0	1	1	1	Erbium
7440-53-1	1	1	1	Europium
7440-54-2	1	1	1	Gadolinium
7440-55-3	1	1	1	Gallium
7440-56-4	1	1	1	Germanium
7440-57-5	1	1	1	Gold
7440-58-6	1	1	1	Hafnium
7440-60-0	1	1	1	Holmium
7440-61-1	1	1	1	Uranium, isotope of mass 238
7440-62-2	1	1	1	Vanadium
7440-64-4	1	1	1	Ytterbium
7440-65-5	1	1	1	Yttrium
7440-66-6	1	1	1	Zinc
7440-67-7	1	1	1	Zirconium
7440-69-9	1	1	1	Bismuth

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
7440-70-2	1	1	1	Calcium
7440-74-6	1	1	1	Indium
7446-09-5	1	0	0	Sulfur dioxide
7446-11-9	1	0	0	Sulfur trioxide
7447-39 4	0	1	0	Copper chloride (cupric chloride)
7447-40-7	1	1	1	Potassium chloride
7452-79-1	0	1	0	Butanoic acid, 2-methyl-, ethyl ester
7469-77-4	1	0	0	1-Naphthalenol, 2-methyl-
7475-92-5	1	1	1	2,5-Furandione, dihydro-3,4-dimethyl-
7481-01-8	0	1	0	2,6,10,14-Hexadecatetraene, 2,6,10,14-tetramethyl-, (*E*,*E*)-
7487-88-9	0	1	0	Sulfuric acid, magnesium salt
7488-54-2	0	1	0	Sulfuric acid, rubidium salt
7488-99-5	0	1	0	β,ε-Carotene, (6′R)- {α-carotene}
7492-70-8	0	1	0	Butanoic acid, 2-butoxy-1-methyl-2-oxoethyl ester {butyl butyryl lactate}
7493-58-5	1	0	0	2,3-Pentanedione, 4-methyl-
7496-02-8	1	0	0	Chrysene, 6-nitro-
7500-42-7	0	1	0	Cyclohexanone, 2-hydroxy-2,6,6-trimethyl-
7515-80-2	1	0	0	2-Propanamine, 2-methyl-*N*-(1-methylethyl)-
7519-36-0	1	1	1	*L*-Proline, 1-nitroso- {NPRO}
7535-00-4	0	1	0	*D*-Galactose, 2-amino-2-deoxy- {galactosamine}
7548-13-2	0	1	0	2,6,10-Dodecatrienoic acid, 3,7,11-trimethyl-
7549-33-9	0	1	0	Benzenemethanol, 4-methoxy-, propanoate
7553-56-2	1	1	1	Iodine
7554-65-6	1	0	0	1*H*-Pyrazole, 4-methyl-
7558-79-4	1	0	0	Phosphoric acid, disodium salt
7558-80-7	1	1	1	Phosphoric acid, monosodium salt
7559-04-8	0	1	0	2,5-Cyclohexadiene-1,4-dione, 2-(3-hydroxy-3,7,11,15-tetramethylhexadecyl)-3,5,6-trimethyl-, [3R- (3R*,7R*,11R*)]-
7563-63-5	1	0	0	Phenol, 4-phenylmethyl-
101-53-1				
7616-22-0	0	1	0	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-
7631-86-9	1	1	1	Silica
7631-99-4	0	1	0	Nitric acid, sodium salt
7634-74-4	1	0	0	Quinoline, 6-butyl-
7642-09-3	1	0	0	3-Hexene, (*Z*)-
7643-75-6	1	1	1	Arabitinol
7645-25-2	0	1	0	Arsenic acid, lead salt
7647-10-1	0	1	0	Platinum chloride
7647-14-5	0	1	0	Sodium chloride
7661-38-3	1	0	0	Isoquinoline, 1-butyl-
7661-47-4	1	0	0	Quinoline, 7-ethyl-
7661-53-2	1	0	0	Quinoline, 8-propyl-
7661-55-4	1	0	0	Quinoline, 5-methyl-
7664-38-2	0	1	0	Phosphoric acid
7664-41-7	1	1	1	Ammonia
7664-93-9	0	1	0	Sulfuric acid
7665-54-5	1	0	0	Carbon-^{14}C monoxide
7683-64-9	1	1	1	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-
7688-21-3	1	0	0	2-Hexene, (*Z*)-
7696-12-0	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, (1-cyclohexene-1,2-dicarboximido)methyl ester {Tetramethrin®}
7697-37-2	1	1	1	Nitric acid
7704-34-9	1	1	1	Sulfur

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
7705-08-0	0	1	0	Iron chloride (ferric chloride)
7712-46-1	0	1	0	2-Cyclohexen-1-one, 5-(1-hydroxy-1-methylethyl)-2-methyl-
7713-69-1	1	1	1	2-Butanamine, *N*-methyl-
7719-93-9	1	1	1	Heptacontane
7722-76-1	0	1	0	Phosphoric acid, monoammonium salt
7722-84-1	1	0	0	Hydrogen peroxide
7723-14-0	1	1	1	Phosphorus
7724-09-6	0	1	0	β-*D*-Glucopyranoside, (2-hydroxyphenyl)methyl-
7724-76-7	0	1	0	Adenosine, *N*-(3-methyl-2-butenyl)-
7726-95-6	1	1	1	Bromine
7727-37-9	1	1	1	Nitrogen
7729-27-3	0	1	0	Butanal, 4-(methylamino)-
7732-18-5	1	1	1	Water
7733-02-0	0	1	0	Sulfuric acid, zinc salt
7737-16-8	1	0	0	Acetamide, *N*-(2-oxopropyl)-
7740-31-5	1	1	1	Tin
7440-31-5				
7754-93-0	0	1	0	2(5*H*)-Furanone, 3-(1-methylethyl)-
7756-96-9	0	1	0	Benzoic acid, 2-amino-. butyl ester
7757-79-1	0	1	0	Nitric acid, potassium salt
7757-82-6	0	1	0	Sulfuric acid, disodium salt
7757-83-7	0	1	0	Sulfurous acid, disodium salt
7757-86-0	0	1	0	Phosphoric acid, magnesium salt
7757-93-9	0	1	0	Phosphoric acid, calcium salt (1:1)
7758-98-7	0	1	0	Sulfuric acid, copper salt
7761-88-8	0	1	0	Nitric acid, silver salt
7764-50-3	1	0	0	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-
7771-25-7	1	0	0	Phenol, 4,5-dimethyl-2-methoxy-
7772-98-7	0	1	0	*Thiosulfuric acid*, *disodium salt*
7773-03-7	0	1	0	Sulfurous acid, monopotassium salt
7774-82-5	0	1	0	2-Tridecenal
7778-18-9	0	1	0	Sulfuric acid, calcium salt
7778-44-1	0	1	0	Arsenic acid, calcium salt
7778-53-2	0	1	0	Phosphoric acid, tripotassium salt
7778-77-0	1	1	1	Phosphoric acid, monopotassium salt
7778-80-5	0	1	0	Sulfuric acid, dipotassium salt
7778-85-0	1	0	0	Propane, 1,2-dimethoxy-
7779-65-9	1	1	1	2-Propenoic acid, 3-phenyl-, 3-methylbutyl ester
7779-78-4	0	1	0	Benzeneethanol, α-(2-methylpropyl)-
7779-88-6	0	1	0	Nitric acid, zinc salt
7782-24-3	1	0	0	Benzeneacetic acid, α-methyl-, (S)-(+)-
7782-26-5	1	0	0	Benzeneacetic acid, α-methyl-, (R)-(−)-
7782-41-4	1	1	1	Fluorine
7782-44-7	1	1	1	Oxygen, oxygen diradical
7782-49-2	1	1	1	Selenium
7782-50-5	1	1	1	Chlorine
7782-77-6	1	0	0	Nitrous acid
7783-06-4	1	0	0	Hydrogen sulfide
7783-20-2	0	1	0	Sulfuric acid, ammonium salt
7783-28-0	0	1	0	Phosphoric acid, diammonium salt
7784-40-9	0	1	0	Arsenic acid, lead salt

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
7784-42-1	1	0	0	Arsine
7785-26-4	1	1	1	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- [2 CAS Nos.] {α-pinene}
80-56-8				
7786-34-7	0	1	0	2-Butenoic acid, 3[(dimethoxyphosphinyl)oxy]-, methyl ester {Mevinphos®, Phosdrin®}
7786-44-9	0	1	0	2,6-Nonadien-1-ol
7786-61-0	1	1	1	Phenol, 4-ethenyl-2-methoxy- {4-vinylguaiacol}
7787-47-5	0	1	0	Beryllium chloride
7791-18-6	0	1	0	Magnesium chloride
7803-49-8	0	1	0	Hydroxylamine
7803-51-2	1	1	1	Phosphine
7935-59-1	0	1	0	2(5*H*)-Furanone, 3,4-dimethyl-5-pentylidene-, dihydro derivative
8000-41-7	1	0	0	3-Cyclohexene-1-methanol, α,α,4-trimethyl- {terpineol}
8001-35-2	0	1	0	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated {Toxaphene®}
8001-50-1	0	1	0	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, polychlorinated + bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, polychlorinated {Strobane®, Dichloricide®}
8001-81-8	1	1	1	9*H*-Pyrido[3,4-*b*]indole {norharman = β-carboline = 2-azacarbazole}
244-63-3				
8002-43-5	0	1	0	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl-, phosphatidyl- {lecithin}
8002-65-1	0	1	0	Neem oil
8012-69-9	0	1	0	Copper oxychloride sulfate
8013-90-9	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (*E*)- {α-ionone}
6901-97-9				
127-41-3				
8018-01-7	0	1	0	Manganese, [[1,2-ethanediylbis[carbamodithioato]](2-)] + zinc, [[1,2-ethanediylbis-[carbamodithioato]](2-)] {Mancozeb®}
8047-67-4	1	0	0	Azaindene
8049-97-6	0	1	0	Melanin
8064-26-4	0	1	0	Holocellulose
8068-00-6	0	1	0	Lignin, milled wood
8068-04-0	0	1	0	Lignin, Klason
9000-11-7	0	1	0	Cellulose, carboxymethyl ether
9000-69-5	0	1	0	Pectin
9000-83-3	0	1	0	Phosphatase, adenosine tri-
9000-86-6	0	1	0	Aminotransferase, alanine
9000-90-2	0	1	0	Amylase, α- {diastase}
9000-91-3	0	1	0	Amylase, β-
9000-92-4	0	1	0	Amylase
9000-95-7	0	1	0	Apyrase
9000-97-9	0	1	0	Aminotransferase, aspartate
9001-03-0	0	1	0	Dehydratase, carbonate
9001-04-1	0	1	0	Decarboxylase, pyruvate
9001-05-2	0	1	0	Catalase
9001-06-3	0	1	0	Chitinase
9001-12-1	0	1	0	*Clostridium*
9001-16-5	0	1	0	Oxidase, cytochrome c {cytochrome oxidase}
9001-22-3	0	1	0	Glucosidase, β- {emulsin, amygdalase, synaptase}
9001-34-7	0	1	0	Galactosidase
9001-36-9	0	1	0	Kinase (phosphorylating), gluco-
9001-39-2	0	1	0	Phosphatase, glucose 6-
9001-40-5	0	1	0	Dehydrogenase, glucose 6-phosphate
9001-41-6	0	1	0	Isomerase, glucose phosphate
9001-42-7	0	1	0	Glucosidase, α- {maltase}
9001-45-0	0	1	0	Glucuronidase, β-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
9001-46-1	0	1	0	Dehydrogenase, glutamic acid
9001-48-3	0	1	0	Reductase, glutathione
9001-50-7	0	1	0	Dehydrogenase, glyceraldehyde phosphate
9001-51-8	0	1	0	Kinase (phosphorylating), hexo-
9001-52-9	0	1	0	Phosphatase, fructose di-
9001-53-0	0	1	0	Oxidase, diamine
9001-57-4	0	1	0	β-Fructofuranosidase {β-fructosidase, invertase}
9001-58-5	0	1	0	Dehydrogenase, isocitrate
9001-59-6	0	1	0	Kinase (phosphorylating), pyruvate
9001-61-0	0	1	0	Aminopeptidase, cytosol
9001-62-1	0	1	0	Lipase {lipase, triacylglycerol}
9001-64-3	0	1	0	Dehydrogenase, malate
9001-68-7	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide phosphate
9001-77-8	0	1	0	Phosphatase, acid
9001-78-9	0	1	0	Phosphatase, alkaline
9001-80-3	0	1	0	Kinase (phosphorylating), phosphofructo-
9001-81-4	0	1	0	Phosphomutase, glucose
9001-82-5	0	1	0	Dehydrogenase, phosphogluconate
9001-92-7	0	1	0	Proteinase
9001-96-1	0	1	0	Oxidase, pyruvate
9001-97-2	0	1	0	Glycosyltransferase, α-glucan-branching
9001-99-4	0	1	0	Ribonuclease
9002-02-2	0	1	0	Dehydrogenase, succinate
9002-10-2	0	1	0	Polyphenoloxidase {oxygenase, monophenol mono-, tyrosinase}
9002-12-4	0	1	0	Oxidase, urate
9002-13-5	0	1	0	Urease
9002-17-9	0	1	0	Oxidase, xanthine
9002-91-9	0	1	0	Metaldehyde {acetaldehyde tetramer}
9003-28-5	1	0	0	1-Butene
106-98-9				
9003-98-9	0	1	0	Nuclease, deoxyribo-
9003-99-0	0	1	0	Peroxidase
9004-34-6	0	1	0	Cellulose
9004-53-9	0	1	0	Dextrin
9004-57-3	0	1	0	Cellulose, ethyl ether
9004-67-5	0	1	0	Cellulose, methyl ether
9005-25-8	1	1	1	Starch
9005-53-2	0	1	0	Lignin
9005-82-7	0	1	0	Amylose
9005-84-9	0	1	0	α-*D*-Glucopyranose, 4-*O*-α-*D*-glucopyranosyl- {amylodextrin, α-maltose}
9006-42-2	0	1	0	Carbamodithioic acid, 1,2-ethylene(bis-, polymer with ammonia complex of zinc ethylenebis-dithiocarbamate {Metiram®}
9006-50-2	0	1	0	Albumin
9007-49-2	0	1	0	Deoxyribonucleic acid
9007-57-2	0	1	0	Edestin
9007-83-4	0	1	0	Globulins, γ-
9012-25-3	0	1	0	Methyltransferase, catechol
9012-33-3	0	1	0	β-Acetylglucosaminidase
9012-39-9	0	1	0	Adenylyltransferase, sulfate
9012-40-2	0	1	0	Methyltransferase, homocysteine
9012-47-9	0	1	0	Glucosidase, amylo-1,6-
9012-49-1	0	1	0	Carbamoyltransferase, aspartate

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
9012-50-4	0	1	0	Kinase (phosphorylating), aspartate
9012-52-6	0	1	0	Adenosyltransferase, methionine
9012-54-8	0	1	0	Cellulase
9012-72-0	0	1	0	β-(1,3)-*D*-Glucan {glucan}
9012-90-2	0	1	0	Nucleotidyltransferase, deoxyribonucleate {polymerase, nucleic acid deoxyribo}
9013-02-9	0	1	0	Kinase (phosphorylating), adenylate
9013-03-0	0	1	0	Reductase, nitrate
9013-05-2	0	1	0	Phosphatase
9013-10-9	0	1	0	*Proteus* {isomerase, glucosamine phosphate}
9013-48-3	0	1	0	Synthase, malate
9013-66-5	0	1	0	Peroxidase, glutathione [2 CAS Nos.]
97089-70-8				
9013-79-0	0	1	0	Esterase
9014-08-8	0	1	0	Hydratase, phosphopyruvate
9014-12-4	0	1	0	Phosphorylase, polynucleotide {nucleotidyltransferase, polyribonucleotide}
9014-24-8	0	1	0	Nucleotidyltransferase, ribonucleate
9014-25-9	0	1	0	Ribonucleic acids, transfer
9014-35-1	0	1	0	Oxidase, succinate
9014-36-2	0	1	0	Synthetase, succinyl coenzyme A (guanosine diphosphate forming)
9014-48-6	0	1	0	Transketolase
9014-52-2	0	1	0	Synthase, tryptophan
9014-63-5	0	1	0	Xylan
9015-75-2	0	1	0	Lyase, pectate
9023-03-4	0	1	0	Reductase, cytochrome c (reduced nicotinamide adenine dinucleotide phosphate)
9023-35-2	0	1	0	Synthase, pseudouridylate
9023-47-6	0	1	0	Synthetase, valyl-transfer ribonucleate
9023-70-5	0	1	0	Synthetase, glutamine
9023-83-0	0	1	0	Isomerase, ribose phosphate
9024-05-9	0	1	0	*Megasphaera*
9024-08-2	0	1	0	*Bacillus pumilus* {racemase, glutamate}
9024-25-3	0	1	0	Hydratase, aconitate
9024-28-6	0	1	0	Ammonia-lyase, phenylalanine
9024-34-4	0	1	0	Dehydratase, threonine
9024-52-6	0	1	0	Aldolase, fructose diphosphate
9024-58-2	0	1	0	Decarboxylase, glutamate
9024-60-6	0	1	0	Decarboxylase, ornithine
9024-70-8	0	1	0	Decarboxylase, uroporphyrinogen
9024-77-5	0	1	0	Decarboxylase, arginine
9024-82-2	0	1	0	Pyrophosphatase, inorganic
9025-33-6	0	1	0	Dipeptidase, prolyl
9025-37-0	0	1	0	Glucanase, endo-1,3-β-
9025-42-7	0	1	0	Mannosidase, α-
9025-44-9	0	1	0	Nucleosidase
9025-53-0	0	1	0	β-Xylosidase
9025-57-4	0	1	0	Xylanase, endo-1,4-β-
9025-67-6	0	1	0	Inulase
9025-76-7	0	1	0	Phosphatase, phosphoglycolate
9025-82-5	0	1	0	Phosphodiesterase
9025-96-1	0	1	0	Chlorophyllase
9025-98-3	0	1	0	Esterase, pectin {pectase}
9026-22-6	0	1	0	Uridylyltransferase, glucose 1-phosphate
9026-28-2	0	1	0	Nucleotidyltransferase, ribonucleate, RNA dependent

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
9026-38-4	0	1	0	Dehydrogenase, glutathione (ascorbate)
9026-62-4	0	1	0	Kinase (phosphorylating), glucurono-
9026-67-9	0	1	0	Kinase (phosphorylating), choline
9026-81-7	0	1	0	Nuclease
9026-87-3	0	1	0	Dehydrogenase, shikimate
9026-94-2	0	1	0	Aldolase, phospho-2-keto-3-deoxyheptonate
9027-05-8	0	1	0	Hydrogenase
9027-19-4	0	1	0	Glucosyltransferase, uridine diphosphoglucose-1,4-β-glucan
9027-22-9	0	1	0	Decarboxylase
9027-23-0	0	1	0	Ribulose-1,5-bisphosphate carboxylase {Rubisco, Fraction 1 protein, F-1 protein, also known as carboxylase, ribulose diphosphate}
9027-40-1	0	1	0	Kinase (phosphorylating), pyruvate-phosphate di-
9027-41-2	0	1	0	Hydrolase
9027-45-6	0	1	0	Synthase, acetolactate
9027-69-4	0	1	0	Phosphatase, nucleoside di-
9027-77-4	0	1	0	Methyltransferase, methionine *S*-
9027-85-4	0	1	0	Oxidase, indoleacetate
9028-02-8	0	1	0	Synthetase, aminoacyl-transfer ribonucleate
9028-06-2	0	1	0	Oxygenase, protocollagen proline di-
9028-13-1	0	1	0	Dehydrogenase, homoserine
9028-28-8	0	1	0	Dehydrogenase, quinate
9028-31-3	0	1	0	Reductase, aldose
9028-32-4	0	1	0	Reductase, glyoxylate
9028-35-7	0	1	0	Reductase, hydroxymethylglutaryl coenzyme A (reduced nicotinamide adenine dinucleotide phosphate)
9028-47-1	0	1	0	Dehydrogenase, malate (oxalacetate-decarboxylating) (nicotinamide adenine dinucleotide phosphate)
9028-48-2	0	1	0	Dehydrogenase, isocitrate (nicotinamide adenine dinucleotide phosphate)
9028-67-5	0	1	0	Oxidase, choline
9028-71-1	0	1	0	Oxidase, glycolate
9029-12-3	0	1	0	Dehydrogenase, glutamate (nicotinamide adenine dinucleotide [phosphate])
9029-14-5	0	1	0	Dehydrogenase, methylenetetrahydrofolate
9029-17-8	0	1	0	Reductase, pyrroline-5-carboxylate
9029-27-0	0	1	0	Reductase, nitrate (reduced nicotinamide adenine dinucleotide [phosphate])
9029-29-2	0	1	0	Reductase, nitrite (reduced nicotinamide adenine dinucleotide [phosphate])
9029-44-1	0	1	0	Oxidase, ascorbate
9029-57-6	0	1	0	Oxygenase, 2,5-dihydroxypyridine 5,6-di-
9029-60-1	0	1	0	Lipoxygenase
9029-83-8	0	1	0	Hydroxymethyltransferase, serine
9030-05-1	0	1	0	Glucosyltransferase, uridine diphosphoglucose-fructose
9030-06-2	0	1	0	Glucosyltransferase, uridine diphosphoglucose-fructose phosphate
9030-26-6	0	1	0	Phosphoribosyltransferase, nicotinate
9030-28-8	0	1	0	Phosphorylase, guanosine
9030-42-6	0	1	0	Aminotransferase, ornithine-keto acid
9030-51-7	0	1	0	Kinase (phosphorylating), fructo-
9030-57-3	0	1	0	Kinase (phosphorylating), ribulo-
9030-77-7	0	1	0	Polyprenyltransferase, 4-hydroxybenzoate
9031-11-2	0	1	0	Lactase
9031-15-6	0	1	0	Synthetase, leucyl-transfer ribonucleate
9031-48-5	0	1	0	Glucosyltransferase
9031-51-0	0	1	0	Kinase (phosphorylating), shikimate
9031-55-4	0	1	0	Carboxylase
9031-56-5	0	1	0	Synthetase

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
9031-59-8	0	1	0	Synthase, anthranilate
9031-66-7	0	1	0	Aminotransferase
9031-72-5	0	1	0	Dehydrogenase, alcohol
9031-85-0	0	1	0	Aminoacyltransferase
9031-94-1	0	1	0	Aminopeptidase
9031-96-3	0	1	0	Peptidase
9031-98-5	0	1	0	Carboxypeptidase
9032-06-8	0	1	0	Reductase, hydroxylamine
9032-10-4	0	1	0	Phosphorylase a
9032-20-6	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide (phosphate) (quinone)
9032-21-7	0	1	0	Oxidase, reduced nicotinamide adenine dinucleotide
9032-22-8	0	1	0	Oxidase, reduced nicotinamide adenine dinucleotide phosphate
9032-64-8	0	1	0	Pyrophosphatase, nucleotide
9032-66-0	0	1	0	Kinase (phosphorylating), nicotinamide adenine dinucleotide
9032-75-1	0	1	0	Polygalacturonase
9032-88-6	0	1	0	Hydratase, fumarate
9032-96-6	0	1	0	Kinase (phosphorylating), phosphogluco-
9033-12-9	0	1	0	Mutase, ketone–aldehyde
9033-33-4	0	1	0	Nucleotidase
9033-44-7	0	1	0	Pyrophosphatase
9033-47-0	0	1	0	Fructosidase {polyfructosidase}
9034-32-6	0	1	0	Hemicellulose
9035-46-5	0	1	0	Cytochrome c6
9035-73-8	0	1	0	Oxidase
9035-74-9	0	1	0	Phosphorylase
9035-81-8	0	1	0	Trypsin inhibitor
9035-82-9	0	1	0	Dehydrogenase
9036-20-8	0	1	0	Decarboxylase, adenosylmethionine
9036-21-9	0	1	0	Phosphodiesterase, adenosine cyclic 3′,5′-phosphate
9036-37-7	0	1	0	Synthase, porphobilinogen
9036-66-2	1	1	1	*D*-Galacto-*L*-arabinan
9037-14-3	0	1	0	Synthetase, aminolevulinate {synthase, aminolevulinate}
9037-22-3	0	1	0	Amylopectin
9037-55-2	0	1	0	*D*-Galactan
9037-80-3	0	1	0	Reductase
9037-90-5	0	1	0	*D*-Fructan
9037-91-6	0	1	0	Glucan
9038-53-3	0	1	0	Pyrophosphatase, thiamin
9040-07-7	0	1	0	Acetyltransferase, chloramphenicol
9040-09-9	0	1	0	Ferredoxins
9040-27-1	0	1	0	Arabinoxylan
9040-29-3	0	1	0	*D*-Galacto-*D*-gluco-*D*-mannan
9044-61-5	0	1	0	Cytochrome b 559
9044-93-3	0	1	0	β-1,3-Glucanase
9045-78-7	0	1	0	Lyase, isocitrate
9046-27-9	0	1	0	Glutamyltransferase, γ-
9046-38-2	0	1	0	2-Pyrancarboxylic acid, 3,4,5,6-tetrahydroxytetrahydro- {oxane-2-carboxylic acid, 3,4,5,6-tetrahydroxy-, *D*-galacturonan}
9046-40-6	0	1	0	Pectic acid
9047-18-1	0	1	0	Pectinic acid
9047-56-7	0	1	0	Mutase
9048-46-8	0	1	0	Albumins, blood serum
9050-36-6	1	1	1	α-*D*-Glucose, labeled with ^{14}C {α-*D*-glucose-^{14}C}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
9050-70-8	0	1	0	Dehydrogenase, proline
9051-94-9	0	1	0	β-(1→4)-*D*-Galactan
9051-97-2	0	1	0	β-*D*-Glucan, (1→3)-
9054-63-1	0	1	0	Aminopeptidase, leucine
9054-84-6	0	1	0	Dehydrogenase, xanthine
9054-89-1	0	1	0	Dismutase, superoxide
9055-07-6	0	1	0	Methyltransferase, protein (arginine)
9055-11-2	0	1	0	Nuclease, endo-
9055-26-9	0	1	0	Permease, sulfate
9055-30-5	0	1	0	Phosphatase, phosphoglycerate
9055-40-7	0	1	0	Porphobilinogenase
9055-59-8	0	1	0	Synthase, dihydrodipicolinate
9055-95-2	0	1	0	Isomerase, pentose phosphate
9059-33-0	0	1	0	Phosphatase, sucrose
9061-41-0	0	1	0	Glutenin
9064-51-1	0	1	0	Callose [2 CAS Nos.] {1,3-β-*D*-glucan}
54724-00-4				
9067-16-7	0	1	0	Ribonucleic acid (*Bombyx mori* fibroin-specifying messenger)
9067-73-6	0	1	0	Amylase, iso-
9067-77-0	0	1	0	Carboxylase, phosphoenolpyruvate (phosphate)
9068-38-6	0	1	0	Nucleotidyltransferase, deoxyribonucleate, RNA dependent
9068-40-0	0	1	0	Oxygenase, *p*-coumarate 3-mono-
9068-73-9	0	1	0	Synthase, 5-enolpyruvoylshikimate 3-phosphate
9068-76-2	0	1	0	Synthetase, glutamyl-transfer ribonucleate
9073-95-4	0	1	0	Dehydrogenase, phosphogluconate (decarboxylating)
9075-39-2	0	1	0	Methyltransferase, putrescine
9075-51-8	0	1	0	Phosphatase, nucleoside tri-
9076-84-0	0	1	0	Oxidase, coproporphyrinogen
9077-14-9	0	1	0	Synthase, squalene
9077-75-2	0	1	0	Oxygenase, cinnamate 4-mono- {hydroxylase cinnamate}
9079-67-8	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide
9080-03-9	0	1	0	Reductase, nitrite
9473-19-9	1	1	1	*D*-erythro-Pentonic acid, 3-deoxy-, γ-lactone
10003-63-1	0	1	0	*D*-Fructose, 1-[(3-carboxypropyl)amino]-1-deoxy-
10008-73-8	1	0	0	2(3*H*)-Furanone, dihydro-5-methylene-
10024-97-2	1	1	1	Nitrogen oxide {nitrous oxide}
10028-15-6	0	1	0	Ozone
10030-73-6	1	1	1	9-Hexadecenoic acid, (*E*)- [2 CAS Nos.] {palmitelaidic acid}
2091-29-4				
10031-82-0	0	1	0	Benzaldehyde, 4-ethoxy-
10032-15-2	0	1	0	Butanoic acid, 2-methyl-, hexyl ester
10043-52-4	0	1	0	Calcium chloride
10043-92-2	1	0	0	Radon
10045-97-3	1	1	1	Cesium, isotope of mass 137
10083-24-6	0	1	0	Ethene, 1-(3,4-dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)- (*E*)- {*trans*-piceatannol}
10094-34-5	0	1	0	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester
10098-91-6	0	1	0	Yttrium, isotope of mass 90
10098-97-2	0	1	0	Strontium, isotope of mass 90
10099-74-8	0	1	0	Nitric acid, lead salt
10102-06-4	0	1	0	Nitric acid, uranium salt
10102-43-9	1	1	1	Nitrogen oxide {nitric oxide}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
10102-44-0	1	0	0	Nitrogen oxide {nitrogen dioxide}
10102-45-1	0	1	0	Nitric acid, thallium salt
10111-08-7	1	0	0	2-Imidazolecarboxaldehyde
10124-37-5	0	1	0	Nitric acid, calcium salt
10130-95-7	1	0	0	3-Cyclopentene-1,2-dione, 3-methyl-
10131-48-3	1	0	0	3-Pyridinecarboxamide, 2,6-dimethyl-
10139-18-1	0	1	0	α-*D*-Glucopyranose, 1,6-bis(dihydrogen phosphate)
10141-72-7	0	1	0	2*H*-Pyran, 2-methyltetrahydro-
10147-11-2	1	0	0	Benzene, 2-propynyl-
10150-87-5	1	0	0	2-Butanone, 4-(acetyloxy)-
10152-76-8	1	0	0	1-Propene, 3-(methylthio)-
10191-25-0	0	1	0	Pentanoic acid, 3-oxo-
10192-32-2	1	0	0	1-Tetracosene
10198-40-0	1	1	1	Cobalt, isotope of mass 60
10210-17-0	1	0	0	Benzenepropanol, 4-hydroxy-
10210-18-1	1	1	1	Hexacosanoic acid, hexacosyl ester
10210-68-1	1	0	0	Cobalt carbonyl
10219-75-7	0	1	0	Naphthalene, 1,8a-dimethyl-7-(1-methylethenyl)-1,2,3,5,6,7,8,8a-octahydro- [1R 1α,7 α,8a α] {eremophilene}
10235-63-9	0	1	0	Cyclohexanol, 1-methyl-4-(1-methylethylidene)-, acetate
10236-47-2	0	1	0	4*H*-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (S)- {naringin}
10247-46-8	0	1	0	*D*-Fructofuranose
10258-70-5	0	1	0	2-Propanone, 1-(formyloxy)-
10264-55-8	1	0	0	Cyclopentanone, 3-ethyl-
10265-92-6	0	1	0	Phosphoramidothioic acid, *O,*S-dimethyl ester {Methamidophos®}
10266-75-8	0	1	0	2-Butanone, 4-(decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl)-, [1S-(1α,4aβ,8aα)]-
10267-21-7	0	1	0	1-Naphthalenepentanol, decahydro-2-hydroxy-γ,2,5,5,8a-pentamethyl-, [1R-[1α(S*),2β,4aβ,8aα]]
10267-31-9	0	1	0	2-Naphthalenol, decahydro-1-(5-hydroxy-3-methyl-3-pentenyl)-2,5,5,8a-tetramethyl-, [1R-[1α(*E*),2β,4aβ,8aα]]-
10273-90-2	1	0	0	Pyridine, 3-methyl-2-phenyl-
10276-21-8	1	0	0	7-Oxabicyclo[4.1.0]heptan-2-one, 4,4,6-trimethyl-
10285-87-7	1	0	0	Formamide, *N*-(3-methylbutyl)-
10288-24-1	1	0	0	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-
10299-63-5	1	0	0	1*H*-Indole, 2,3,4-trimethyl-
10312-83-1	1	0	0	Acetaldehyde, methoxy-
10316-66-2	1	0	0	2-Cyclohexen-1-one, 2-hydroxy-
10321-71-8	0	1	0	2-Pentenoic acid, 4-methyl-
10340-23-5	0	1	0	3-Nonen-1-ol, (*Z*)-
10352-88-2	0	1	0	2-Heptenoic acid, (*E*)-
10361-29-2	1	0	0	Carbonic acid, ammonium salt
10361-39-4	0	1	0	Pentanoic acid, phenylmethyl ester
10361-82-7	0	1	0	Samarium chloride
10366-91-3	0	1	0	Benzoic acid, 2-(β-*D*-glucopyranosyloxy)-
10371-85-4	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 1-butyl-
10374-51-3	1	1	1	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-
10377-48-7	0	1	0	Sulfuric acid, dilithium salt
10377-60-3	0	1	0	Nitric acid, magnesium salt
10413-18-0	1	1	1	2*H*-Pyran-2-one, tetrahydro-5,6-dimethyl- [2 CAS Nos.]
24405-16-1				
10420-90-3	1	0	0	1,3-Hexadien-5-yne
10447-93-5	1	0	0	1*H*-Imidazole, 1,5-dimethyl-
10453-86-8	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, (5-phenylmethyl-3-furanyl)methyl ester {Resmethrin®}
10458-16-7	1	1	1	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
89-80-5				
14073-97-3				
10473-40-2	1	1	1	Stigmast-5-en-3-ol, tetradecanoate, (3β)- {β-sitosteryl myristate}
10477-94-8	1	0	0	Pyridine, 3-methyl-5-phenyl-
10478-42-9	1	1	1	β-Alanine, *N*-methyl-*N*-nitroso- = propanoic acid, 3-(methylnitrosoamino)- {NMPA}
10481-90-0	0	1	0	2(4*H*)-Benzofuranone, 6-hydroxy-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, *Z*-(±)- {loliolide}
10482-56-1	1	1	1	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, (S)-
10482-74-3	1	1	1	Pentacosanoic acid, pentacosyl ester
10486-19-8	0	1	0	Tridecanal
10493-98-8	1	0	0	2-Cyclopenten-1-one, 2-hydroxy
10500-57-9	1	0	0	Quinoline, 5,6,7,8-tetrahydro-
10504-04-8	1	0	0	Furan, 2,3,5-trmiethyl-
10504-06-0	0	1	0	Furan, 2,5-diethyl-
10504-11-7	1	0	0	Furan, 2-(2-methyl-1-propenyl)-
10504-13-9	1	0	0	Furan, 2-ethenyl-5-methyl- = furan, 5-ethenyl-2-methyl-
10516-09-3	0	1	0	2(1*H*)-Pyridinone, 5-(1-methyl-2-pyrrolidinyl)-, (S)-
10538-47-3	1	1	1	Benzenepropanoic acid, 2,5-dihydroxy-
10544-63-5	0	1	0	2-Butenoic acid (*E*)-, ethyl ester {ethyl crotonate}
10546-24-4	1	0	0	2-Naphthalenamine, 3-methyl-
10547-84-9	1	1	1	2(5*H*)-Furanone, 3,4-dimethyl-5-pentyl- {dihydrobovolide}
10547-85-0	1	1	1	2(5*H*)-Furanone, 4,5-dimethyl-
10547-88-3	0	1	0	2(3*H*)-Furanone, dihydro-4-(1-methylethyl)-
10547-89-4	1	1	1	2(5*H*)-Furanone, 4-(1-methylethyl)-
10551-58-3	0	1	0	2-Furancarboxaldehyde, 5-[(acetyloxy)methyl]-
10557-82-1	1	0	0	Isoxazole, trimethyl- = isoxazole, 3,4,5-trimethyl-
10567-95-0	1	0	0	Benz[*c*]acridine, 5,7-dimethyl-
10570-69-1	1	0	0	Phenol, 2,6-dimethyl-4-ethyl-
10580-24-2	0	1	0	Undecanoic acid, butyl ester
10595-95-6	1	1	1	Ethanamine, *N*-methyl-*N*-nitroso- {NEMA}
10602-14-9	0	1	0	1,2-Propanediol, 1-(dihydrogen phosphate)
10604-59-8	1	0	0	1*H*-Indole, 1-ethyl-
10605-21-7	0	1	0	1*H*-Benzimidazole-2-carbamic acid, methyl ester {Carbendazim®}
11005-16-6	0	1	0	Plastoquinone C
11006-34-1 15611-43-5	0	1	0	Magnesate(3-), [18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12, 17-tetramethyl-21*H*,23*H*-porphine-2-propanoato(5-)-*N*21,*N*22,*N*23,*N*24]-, trihydrogen, [*SP*-4-2-(2S-*trans*)]- [2 CAS Nos.] {chlorophyllin}
11017-44-0 71607-94-8	1	1	1	Hexadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester {solanesyl hexadecanoate, solanesyl palmitate}
11028-42-5	0	1	0	1*H*-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,7β,8aα)]- {cedrene}
469-61-4				
11030-10-7	1	0	0	1,6,10,14,18,23-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- {isosqualene}
11040-28-1	1	1	1	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,5α)-
11046-98-3	1	0	0	1,2,3-Propanetriol, propanoate
11057-45-7	1	0	0	Benzoperylene
11062-77-4	1	0	0	Superoxide (anion radical)
11078-27-6	0	1	0	Arabinan
11104-93-1	1	0	0	Nitrogen oxide
11105-12-7	0	1	0	Vanadium chloride
11126-30-0	0	1	0	Zirconium chloride
11141-17-6	0	1	0	1*H*,7*H*-Naphtho[1,8*a*,8-*bc*:4,4*a*-*c′*]difuran-3,7a-dicarboxylic acid, (3S,3aR,4S, 5S,5aR, 5a^{1}R 7aS,8R,10S,10aS)-8-acetoxy-3,3a,4,5a,5a^{1},7a,8,9,10-decahydro-3,5-dihydroxy-4-{(1S,3S,7S,8R,9S,11R)-7-hydroxy-9-methyl-2,4,10-trioxatetracyclo[6.3.1.0^{3,7}.0^{9,11}]dodeca-5-en-11-yl}-4-methyl-10[(*E*)-2-methylbut-2-enoyloxy]-, dimethyl ester {Azadirachtin® A and B, Neem®}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
12001-76-2	0	1	0	Vitamin B
12002-39-0	0	1	0	Stigmasta-7,24(28)-dien-3-ol, 4-methyl- {sitosterols}
12057-74-8	0	1	0	Phosphide, magnesium
12122-67-7	0	1	0	Zinc, [[1,2-ethanediylbis[carbamodithioato]](2-)]- {Zineb®}
12125-02-9	1	0	0	Ammonium chloride
12135-76-1	0	1	0	Ammonium sulfide
12136-45-7	0	1	0	Potassium oxide
12141-45-6	1	0	0	Sillimanite
12167-20-3	1	0	0	Phenol, methyl-nitro-
12427-38-2	0	1	0	Manganese, [[1,2-ethanediylbis[carbamodithioato]](2-)]- {Maneb®}
12612-55-4	1	0	0	Nickel carbonyl
13463-39-3				
12712-31-1	0	1	0	Phosphodoxin
12758-54-2	1	0	0	Furan, hexenyl methyl-
12778-15-3	0	1	0	Plastoquinone D
12789-03-6	0	1	0	4,7-Methano-1*H*-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- {γ-Chlordane®}
57-74-9				
13028-62-1	0	1	0	*L*-Cystine
56-89-3				
13054-97-2	1	0	0	Benzofuran, octahydro-
13066-19-8	1	1	1	Benzenamine, 2-(2-phenylethenyl)- {2-aminostilbene}
13067-27-1	1	1	1	Pyrazine, 2,6-diethyl-
13071-79-9	0	1	0	Phosphorodithioic acid, *O*,*O*-diethyl S-[(1,1-dimethylethyl)thio]methyl ester {Terbuphos®}
13078-04-1	1	0	0	Pyridine, 3-(2-piperidinyl)- {anabasine}
13092-55-2	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-
13092-66-5	0	1	0	Phosphoric acid, magnesium salt $Mg(H_2PO_4)_2$
13100-05-5	1	0	0	2-Propanone, 1-(2-hydroxyphenyl)-
13100-82-8	0	1	0	Alanine, 3-sulfo-
13101-54-7	0	1	0	Erlose (a trisaccharide)
13101-54-7	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1 → 4)-
13119-86-3	1	0	0	Coronene, methyl-
13121-99-8	1	0	0	4-Pyridineacetonitrile
13129-23-2	0	1	0	3-Furancarboxylic acid, methyl ester
13147-57-4	0	1	0	Acetic acid, (phosphonoxy)-
13151-34-3	1	0	0	Decane, 3-methyl-
13151-35-4	1	0	0	Decane, 5-methyl-
13171-21-6	0	1	0	Phosphoric acid, 2-chloro-3-(diethylamino-1-methyl-3-oxo-1-propenyl)-, dimethyl ester {Phosphamidon®}
13190-97-1	1	1	1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)- {solanesol}
13194-48-4	0	1	0	Phosphorodithioic acid, *O*-ethyl-S,S, dipropyl ester {Mocap®, Ethoprop®, Prophos®, Rovokil®, Ethoprophos®}
13200-35-6	1	0	0	4-Piperidinone, 2,6-dimethyl-, *cis*-
13201-46-2	1	1	1	2-Butenoic acid, 2-methyl-, (*Z*)- {angelic acid}
13207-66-4	0	1	0	8-Quinolinol, 5-amino-
13215-88-8	1	1	1	2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-
13215-89-9	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-
13215-90-2	0	1	0	2-Cyclohexen-1-ol, 4-(2-butenylidene)-3,5,5-trimethyl- {megastigmatrienol}
13238-84-1	1	1	1	Pyrazine, 2,5-diethyl-
13256-22-9	1	1	1	Glycine, *N*-methyl-*N*-nitroso- {NSAR}
13269-52-8	1	1	1	3-Hexene, (*E*)-
13277-77-5	0	1	0	1(3*H*)-Isobenzofuranone, 3,7-dihydroxy-3,4,5,6-tetramethyl-
13280-76-7	1	0	0	Arabinonic acid, γ-lactone
13287-12-2	1	0	0	2-Heptadecene, 2-methyl-
13287-23-5	1	0	0	Heptadecane, 8-methyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
13296-76-9	1	0	0	9,11,13-Octadecatrienoic acid
13314-90-4	1	0	0	Furan, 2,5-dihydro-2,5-bis(methylene)-
13341-72-5	0	1	0	Benzofuranone, dimethyltetrahydro-
13360-61-7	1	1	1	1-Pentadecene
13360-64-0	1	1	1	Pyrazine, 2-ethyl-5-methyl-
13360-65-1	1	1	1	Pyrazine, 2-ethyl-3,6-dimethyl- = pyrazine, 6-ethyl-2,5-dimethyl-
13368-65-5	1	0	0	Cyclohexanone, 3-methyl- (+)
13391-32-7	1	0	0	Phenol, 2-ethyl-4-methoxy-
13398-94-2	1	1	1	Benzeneethanol, 3-hydroxy-
13406-98-9	0	1	0	1-Piperidinecarboxylic acid
13410-45-2	0	1	0	Tricosane, 3-methyl-
13419-69-7	0	1	0	2-Hexenoic acid, (*E*)
13434-12-3	0	1	0	Acetamide, *N*-(3-methylbutyl)
13436-43-6	1	1	1	Furan, 2,5-dihydro-2-methoxy-
13446-35-0	0	1	0	Manganese chloride
13463-39-3	1	0	0	Nickel carbonyl
12612-55-4				
13463-40-6	1	0	0	Iron pentacarbonyl
13466-78-9	0	1	0	Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- {δ-3-carene}
498-15-7				
13484-66-7	0	1	0	5′-Adenylic acid, *N*-(phenylmethyl)-
13487-27-9	0	1	0	Cyclohexanemethanol, α-methyl-, acetate
13487-30-4	0	1	0	2,4-Cyclohexadien-1-one, 2,6,6-trimethyl-
13493-97-5	0	1	0	2-Furanmethanol, formate
13494-06-9	1	1	1	1,2-Cyclopentanedione, 3,4-dimethyl-
13494-07-0	1	1	1	1,2-Cyclopentanedione, 3,5-dimethyl-
13494-08-1	1	0	0	1,2-Cyclopentanedione, 3-ethyl-
13494-80-9	1	1	1	Tellurium
13505-34-5	1	1	1	2,6-Heptanedione
13509-17-6	1	0	0	2-Pyridinecarboxamide, 5-ethyl-
13532-18-8	0	1	0	Propanoic acid, 3-(methylthio)-, methyl ester
13545-04-5	0	1	0	Butanedioic acid, 2,3-dimethyl- {succinic acid, 2,3-dimethyl-}
13603-04-8	1	0	0	Pyrrolidine, 2,4-dimethyl-
13603-07-1	1	0	0	Piperidine, 3-methyl-1-nitroso-
13623-11-5	1	0	0	Thiazole, 2,4,5-trimethyl-
13651-14-4	1	0	0	Benzenemethanol, 2,3-dimethyl-
13678-51-8	1	0	0	Furan, 2-(2-furanylmethyl)-5-methyl-
13678-52-9	1	0	0	1*H*-Pyrrole, 1-[(5-methyl-2-furanyl)methyl]-
13678-73-4	0	1	0	Ethanone, 1-[1-(2-furanylmethyl)-1*H*-pyrrol-2-yl]-
13678-74-5	1	1	1	2-Propanone, 1-(5-methyl-2-furanyl)-
13678-79-0	0	1	0	1*H*-Pyrrole-2-carboxaldehyde, 1-(3-methylbutyl)-
13679-41-9	0	1	0	Furan, 3-phenyl-
13679-43-1	1	0	0	Furan, 2,2′-methylenebis[5-methyl]-
13679-56-6	1	1	1	2-Butanone, 4-(5-methyl-2-furanyl)-
13679-70-4	1	1	1	2-Thiophenecarboxaldehyde, 5-methyl-
13679-79-3	1	1	1	1*H*-Pyrrole, 1-(3-methylbutyl)-
13679-86-2	0	1	0	Furan, 2-ethenyltetrahydro-2-methyl-5-(1-methylethenyl)-
13708-12-8	0	1	0	Quinoxaline, 5-methyl-
13714-86-8	1	0	0	2-Furancarbonitrile, 5-methyl-
13717-00-5	0	1	0	Carbonic acid, magnesium salt
13730-09-1	1	0	0	Benzonitrile, 2,5-dimethyl-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
13752-83-5	0	1	0	Arabinonic acid
13788-32-4	0	1	0	1*H*-Pyrrole-2-carboxaldehyde, 1-(2-furanylmethyl)-
13828-33-6	0	1	0	Cyclohexene, 5-methyl-1-(1-methylethyl)- {*m*-menthene}
13828-34-7	1	0	0	Cyclohexane, 1-methyl-3-(1-methylethylidene)-
13831-30-6	1	1	1	Acetic acid, (acetyloxy)-
13835-30-8	0	1	0	3-Cyclohexene-1-ethanol, β,4-dimethyl-
13861-97-7	0	1	0	2(3*H*)-Furanone, dihydro-4,4-dimethyl-
13877-91-3	1	1	1	1,3,6-Octatriene, 3,7-dimethyl- {ocimene}
13891-87-7	1	0	0	4-Penten-2-one
13901-85-4	1	1	1	2,5-Heptanedione, 6-methyl-
13920-14-4	0	1	0	ψ,ψ-Carotene, 7,7′,8,8′,11,11′,12,12′-octahydro- {phytoene}
540-04-5				
13925-00-3	1	1	1	Pyrazine, ethyl- = pyrazine, 2-ethyl-
13925-03-6	1	1	1	Pyrazine, 2-ethyl-6-methyl- = pyrazine, 6-ethyl-2-methyl-
13925-05-8	1	0	0	Pyrazine, 2-methyl-5-(1-methylethyl)-
13925-06-9	1	0	0	Pyrazine, 2-methyl-3-(2-methylpropyl)-
13925-07-0	1	1	1	Pyrazine, 2-ethyl-3,5-dimethyl- = pyrazine, 3-ethyl-2,6-dimethyl-
13925-08-1	1	1	1	Pyrazine, 2-ethenyl-5-methyl-
13925-09-2	1	1	1	Pyrazine, 2-ethenyl-6-methyl-
13927-47-4	0	1	0	3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (*E,Z*)- {pseudoionone}
13939-91-8	1	0	0	1*H*-Pyrrolo[1,2-*c*]imidazole-1,3(2*H*)-dione
13950-21-5	0	1	0	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-
13952-84-6	1	1	1	2-Butanamine
13966-00-2	1	1	1	Potassium, isotope of mass 40
13966-29-5	0	1	0	Uranium, isotope of mass 234
13967-63-0	1	1	1	Scandium, isotope of mass 46
13967-70-9	1	1	1	Cesium, isotope of mass 134
13981-16-3	0	1	0	Plutonium, isotope of mass 238
13981-28-7	1	1	1	Lanthanum, isotope of mass 140
13981-52-7	1	1	1	Polonium, isotope of mass 210
13982-39-3	1	1	1	Zinc, isotope of mass 65
13982-63-3	1	1	1	Radium, isotope of mass 226 [2 CAS Nos.]
7440-14-4				
13982-78-0	0	1	0	Mercury, isotope of mass 203
13984-57-1	1	0	0	Hexanoic acid, 5-oxo-, ethyl ester
13989-82-7	1	0	0	Butanenitrile, 4-(dimethylamino)-
14059-92-8	1	1	1	Phenol, 2,6-dimethoxy-4-ethyl-
14064-37-0	1	0	0	Benzenamine, 3-(2-phenylethenyl)-, (*Z*)-
14066-20-7	0	1	0	Phosphate, dihydrogen
14072-82-3	1	0	0	Cyclohexene, 4-(1-methylethyl)-
14073-97-3	1	1	1	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, *trans*- {menthone}
89-80-5				
10458-16-7				
14119-33-6	1	1	1	Plutonium, isotope of mass 240
14127-61-8	0	1	0	Calcium, ion
14129-48-7	0	1	0	4-Octen-3-one
14156-12-8	1	0	0	2,5-Pyrrolidinedione, 3-ethylidene-
14158-27-1	0	1	0	Strontium, isotope of mass 89
14158-34-0	0	1	0	Chlorine, isotope of mass 38
14159-68-3	1	0	0	3-Pyridinol, 2-propyl-
14167-59-0	1	1	1	Tetratriacontane

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
14167-65-8	0	1	0	Tetratriacontane, 2-methyl-
14167-66-9	1	1	1	Heptacosane, 3-methyl-
14167-67-0	1	1	1	Nonacosane, 3-methyl-
14167-69-2	1	1	1	Tritriacontane, 3-methyl-
14171-85-8	1	0	0	9*H*-Carbazole, 1,9-dimethyl-
14189-85-6	1	0	0	2-Cyclopenten-1-one, 2-methoxy-3-methyl-
14191-95-8	1	0	0	Benzeneacetonitrile, 4-hydroxy-
14203-59-9	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-
14255-04-0	1	1	1	Lead, isotope of mass 210
14258-49-2	0	1	0	Ethanedioic acid, ammonium salt
14265-44-2	1	1	1	Phosphate
14265-45-3	1	1	1	Sulfite
14265-71-5	1	1	1	Selenium, isotope of mass 75
14269-63-7	1	1	1	Thorium, isotope of mass 230
14274-82-9	1	1	1	Thorium, isotope of mass 228
14287-61-7	0	1	0	Butanoic acid, 2,3-dimethyl-
14298-39-6	0	1	0	Phosphoric acid, holmium salt
14300-04-0	1	0	0	Piperidine, 2-ethyl-1-nitroso-
14300-74-4	1	0	0	2(5*H*)-Furanone, 3,4-dimethyl-5-methylene-
14307-02-9	0	1	0	*D*-Mannose, 2-amino-2-deoxy- {mannosamine}
14313-09-8	1	0	0	Ethanone, 1-(3-furanyl)-
14315-11-8	1	0	0	Benzo[*b*]thiophene, 4-methyl-
14319-90-5	1	0	0	Benz[*c*]acridine, 8-methyl-
14320-37-7	1	0	0	3-Cyclopenten-1-one
14331-54-5	1	0	0	Pyrimidine, 2,4-dimethyl-
14331-79-4	1	1	1	Bismuth, isotope of mass 210
14331-83-0	0	1	0	Actinium, isotope of mass 228
14331-88-5	0	1	0	Antimony, isotope of mass 129
14352-59-1	0	1	0	Octanoic acid, 3,3-dimethyl-
14360-50-0	1	0	0	1-Hexanone, 1-(2-furanyl)-
14364-05-7	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)phenyl]-
14364-12-6	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-methoxyphenyl]- {1-*O*-feruloylglucose}
7196-71-6				
14371-10-9	0	1	0	2-Propenal, 3-phenyl-, (*E*)- {*trans*-cinnamaldehyde}
14375-45-2	0	1	0	2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-, [S-(*Z*,*E*)]- [2 CAS Nos.]
21293-29-8				{abscisic acid}
14378-21-3	0	1	0	Potassium, isotope of mass 42
14391-76-5	1	1	1	Silver, isotope of mass 110
14391-97-0	0	1	0	Scandium, isotope of mass 49
14392-02-0	1	1	1	Chromium, isotope of mass 51
14398-34-6	0	1	0	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-
14398-35-7	0	1	0	3-Buten-2-one, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)-
14400-67-0	1	0	0	3(2*H*)-Furanone, 2,5-dimethyl-
14411-56-4	1	0	0	Benzene, 1-(1,1-dimethylethyl)-3-ethyl-
14428-12-7	0	1	0	Magnesate(1-), [9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoato(3-)-*N*23,*N*24,*N*25,*N*26]-, hydrogen, [*SP*-4-2-[3S-(3α,4β,21β)]]- {chlorophyllide b}
14458-76-5	1	0	0	1*H*-Benzo[*b*]fluorene
14475-60-6	0	1	0	1,4-Butanediamine, *N*-methyl-
14484-64-1	0	1	0	Iron, tris(dimethylcarbamodithioato-S,S′)-, (OC-6-11)- {Ferbam®}
14490-79-0	1	0	0	15-Tetracosenoic acid {nervonic acid}
14498-44-3	1	0	0	2-Pyrrolidinepropanol, 1-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
14506-65-1	0	1	0	2-Butanone, 4-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, (4aS-*trans*)-
14506-68-4	0	1	0	2(1*H*)-Naphthalenone, 1-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-5,5,8a-trimethyl-, [1R-[1α(R*),4aβ,8aα]]-
14529-53-4	1	0	0	Pyridine, 2-ethoxy-
14596-12-4	1	1	1	Iron, isotope of mass 59
14596-37-3	0	1	0	Phosphorus, isotope of mass 32
14660-91-4	0	1	0	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S,9′-*cis*)- {neoxanthin}
14667-55-1	1	1	1	Pyrazine, trimethyl-
14668-66-7	1	0	0	2(5*H*)-Furanone, 3-ethyl-5-methyl-
14668-67-8	1	0	0	2(5*H*)-Furanone, 3,5-diethyl-
14681-52-8	0	1	0	Manganese, isotope of mass 56
14683-10-4	1	1	1	Antimony, isotope of mass 124
14686-13-6	1	0	0	2-Heptene, (*E*)-
14686-69-2	1	1	1	Bromine, isotope of mass 82
14722-38-4	1	0	0	Cinnoline, 4-methyl-
14753-08-3	0	1	0	Benzene, 1,4-dimethoxy-2-methyl-5-(1-methylethyl)-
14755-02-3	0	1	0	2-Propenoic acid, 3-(3-hydroxyphenyl)-, (*E*)-
14757-43-8	1	0	0	1,6-Naphthyridine, 3-methyl-
14757-45-0	1	0	0	1,8-Naphthyridine, 2,6-dimethyl-
14759-22-9	1	0	0	1,8-Naphthyridine, 3-methyl-
14762-75-5	1	0	0	Carbon, isotope of mass 14
14762-78-8	0	1	0	Cerium, isotope of mass 144
14771-77-8	1	0	0	2,5-Piperazinedione, 3-(1-methylethyl)-
14779-25-0	1	0	0	2-Propenoic acid, 3-(5-methyl-2-furanyl)-
14797-55-8	1	1	1	Nitrate
14797-65-0	1	1	1	Nitrite
14798-03-9	1	1	1	Ammonium ion
14808-79-8	1	1	1	Sulfate ion
14812-03-4	0	1	0	2-Nonenoic acid, (*E*)-
14816-18-3	0	1	0	Phosphorothioic acid, *O*,*O*-diethyl *O*-(α-cyanobenzylideneamino)- {Phoxim®}
14833-49-9	0	1	0	Nickel, isotope of mass 65
14859-67-7	1	1	1	Radon, isotope of mass 222
14897-06-4	0	1	0	Magnesate(1-), [9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(3-)-*N*23,*N*24,*N*25,*N*26]-, hydrogen, [*SP*-4-2-[3*S*-(3α,4β,21β)]]- {chlorophyllide a}
14901-07-6	1	1	1	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- {β-ionone}
14905-56-7	0	1	0	Tetradecane, 2,6,10-trimethyl-
14920-89-9	1	0	0	Furan, 2,3-dimethyl-
14927-67-4	1	0	0	Pyrene, 1,2-dihydro-
14963-40-7	1	0	0	2-Cyclopenten-1-one, 5-methyl-
14982-50-4	1	1	1	Galacturonic acid
14984-34-0	0	1	0	*D*-Glucuronic acid, monosodium salt
14995-49-4	1	0	0	Dodecanamide, *N*-(1-methylethyl)-
15016-60-1	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*Z*),4α,5α]]-
15032-21-0	1	0	0	Pyridine, 2-methyl-4-phenyl-
15067-28-4	0	1	0	Lead, isotope of mass 214
15076-00-3	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1R-[1α,3β(*E*),4α,5α]]-
15092-94-1	0	1	0	Lead, isotope of mass 212
15104-03-7	1	0	0	Piperidine, 4-methyl-1-nitroso-
15117-48-3	1	1	1	Plutonium, isotope of mass 239
15117-96-1	0	1	0	Uranium, isotope of mass 235
15124-81-9	0	1	0	Calcium, isotope of mass 49
15174-69-3	1	0	0	Benzaldehyde, 4-hydroxy-3-methyl-
15189-14-7	0	1	0	Cyclohexanone, 2,2,5,5-tetramethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
15262-20-1	0	1	0	Radium, isotope of mass 228
15281-98-8	1	0	0	Iron carbonyl
15299-99-7	0	1	0	Propanamide, diethyl-2-(1-naphthyloxy)- {Devrinol®, Napropamide®}
15303-46-5	0	1	0	Hexanal, 2-(1-methylethyl)-5-oxo-
15306-27-1	1	0	0	1-Heptacosene
15310-01-7	0	1	0	Benzamide, 2-iodo-*N*-phenyl- {Benodanil®}
15344-34-0	1	0	0	Butanenitrile, 2-hydroxy-3-methyl-
15356-74-8	1	1	1	2(4*H*)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-
15356-75-9	0	1	0	3-Buten-2-one, 4-(1-hydroxy-2,2-dimethyl-6-methylenecyclohexyl)-
15356-76-0	0	1	0	3-Buten-2-one, 4-(1-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)-
15371-32-1	0	1	0	2,6,11,13-Tetradecatetraenal, 3,7,13-trimethyl-10-(1-methylethyl)-, [S-(*E,E,E*)]-
15376-62-2	1	1	1	Pyridine, 3-(1-propenyl)-
15379-45-0	1	0	0	2*H*-Indol-2-one, 1,3-dihydro-3-ethyl-
15401-34-0	0	1	0	3-Buten-2-one, 4-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-
15414-82-1	1	0	0	2,4-Imidazolidinedione, 5-ethyl-
15438-31-0	1	1	1	Iron, ion^{+2}
15457-05-3	0	1	0	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)- {Fluorodifen®}
15510-11-9	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*E*)-
15540-88-2	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4,7-dimethyl-
15542-96-8	1	0	0	2,5-Pyrrolidinedione, 1,3-dimethyl-
15542-97-9	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-1-methyl-
15542-99-1	1	0	0	2,5-Pyrrolidinedione, 1-methyl-3-(1-methylethyl)-
15569-85-4	1	0	0	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, 1-oxide {cotinine 1-oxide}
36508-80-2				
15575-20-9	0	1	0	Arsenic, isotope of mass 76
15594-90-8	1	1	1	1-Heneicosanol
15611-43-5	0	1	0	Magnesate(3-), [18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12, 17-tetramethyl-21*H*,23*H*-porphine-
11006-34-1				2-propanoato(5-)-*N*21,*N*22,*N*23,*N*24]-, trihydrogen, [*SP*-4-2-(2S-*trans*)]- [2 CAS Nos.] {chlorophyllin}
15657-58-6	0	1	0	1,4-Butanediamine, 2-methyl-
15664-29-6	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, [3S-(3α,4β,21β)]-
15679-09-1	1	0	0	Thiazole, 2-ethyl-
15679-10-4	1	0	0	Thiazole, 2-(1-methylethyl)-
15679-11-5	1	0	0	Thiazole, 2-methyl-4-(1,1-dimethylethyl)-
15679-12-6	1	0	0	Thiazole, 2-ethyl-4-methyl-
15679-13-7	1	0	0	Thiazole, 4-methyl-2-(1-methylethyl)-
15707-23-0	1	1	1	Pyrazine, 2-ethyl-3-methyl-
15707-24-1	1	1	1	Pyrazine, 2,3-diethyl-
15707-34-3	1	0	0	Pyrazine, 2,3-dimethyl-5-ethyl-
15764-16-6	1	0	0	Benzaldehyde, 2,4-dimethyl-
15769-88-7	1	1	1	2*H*-1,2-Oxazine, tetrahydro-2-methyl-6-(3-pyridinyl)-, (−)- {nicotone}
15825-89-5	1	0	0	Pyridine, 3-(1-methylethenyl)-
15827-72-2	0	1	0	Pyridine, 2,5-diphenyl-
15856-96-9	1	0	0	2-Pentenamide
15869-80-4	1	0	0	Heptane, 3-ethyl-
15873-27-5	1	1	1	3-Pyridinebutanoic acid, 1,6-dihydro-γ,6-dioxo-
15877-57-3	1	0	0	Pentanal, 3-methyl-
78-92-2	1	1	1	2-Butanol {*sec*-butyl alcohol}
15892-23-6				
15896-46-5	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-, (*Z*)-
15899-72-6	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-
15941-77-2	1	0	0	Thiocyanogen
505-14-6				

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
15972-60-8	0	1	0	Acetamide, 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)- {Alachlor®}
16039-53-5	0	1	0	Propanoic acid, 2-hydroxy-, zinc salt
16055-83-1	1	0	0	Chromium ion (3+)
16065-87-5	0	1	0	Molybdenum, ion
16096-32-5	1	0	0	1*H*-Indole, 4-methyl-
16115-08-5	1	0	0	2(1*H*)-Pyridinone, 4,6-dimethyl-
16124-24-6	0	1	0	*L*-Alanine, *N*-(1-deoxy-*D*-fructos-1-yl)-
25127-16-6				
16135-81-2	1	0	0	11*H*-Benzo[*cd*]fluoranthene [2 CAS Nos.]
42126-84-1				
16204-57-2	0	1	0	1*H*-Indene, 2,3-dihydro 1,1,4,5-tetramethyl-
16277-67-1	0	1	0	Benzene, (3-methoxy-1-propenyl)-
16279-34-8	1	0	0	1,4-Dioxane, 2-methyl-
16313-37-4	0	1	0	3-Pentenoic acid, 3-methyl-
16339-04-1	1	0	0	2-Propanamine, *N*-methyl-*N*-nitroso-
16356-11-9	1	0	0	1,3,5-Undecatriene
16386-93-9	0	1	0	4-Pentenoic acid, 2,2-dimethyl-
16395-79-2	1	1	1	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-
16397-91-4	0	1	0	Manganese, ion
16409-43-1	0	1	0	Pyran, tetrahydro-4-methyl-2-(2-methylpropen-1-yl)- {rose oxide}
16409-45-3	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate [2 CAS Nos.] {menthyl acetate}
89-48-5				
16409-46-4	0	1	0	Butanoic acid, 3-methyl-, 5-methyl-2-(1-methylethyl)-cyclohexanyl ester {menthyl isovalerate}
16411-13-5	0	1	0	Butanedinitrile, 2,3-dimethyl-
16426-50-9	0	1	0	Butanedioic acid, hydroxy-, calcium salt
16435-49-7	1	0	0	1-Dodecene, 2-methyl-
16449-30-2	0	1	0	*D*-Arabinohexose, 2-deoxy-4-*O*-β-*D*-glucopyranosyl-
16493-20-2	1	0	0	2,5-Furandione, 3-methyl-4-propyl-
16493-80-4	0	1	0	Octanoic acid, 4-ethyl-
16496-51-8	1	1	1	2(3*H*)-Furanone, dihydro-4-ethyl-
16499-18-6	1	0	0	Propoxyl radical
16543-55-8	1	1	1	Pyridine, 3-(1-nitroso-2-pyrrolidinyl)-, (S)- {NNN}
16586-18-8	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, labeled with ^{14}C, (S)-
16595-31-6	0	1	0	Propanoic acid, 2-hydroxy-, sodium salt {sodium lactate}
72-17-3				
16635-54-4	1	1	1	2-Hexenal, (*Z*)-
16655-82-6	1	1	1	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate) {3-Hydroxycarbofuran®}
16672-87-0	0	1	0	Phosphonic acid, 2-chloroethyl- {Ethephon®, Ethrel®}
16695-72-0	1	1	1	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (*E*)-
16695-73-1	1	1	1	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (*Z*)-
16709-30-1	0	1	0	Methylcarbamic acid, 2,2-dimethyl-3(2*H*)-oxobenzofuran-7-yl ester
16727-91-6	1	1	1	Naphthalene, 1-(2-methylpropyl)-
16748-73-5	0	1	0	Butanediamide, 2-amino-, (S)- {asparagine amide}
16752-77-5	0	1	0	Acetamidic acid, thio-, *N*-[(methylcarbamoyl)oxy]-, methyl ester {Methomyl®}
16753-27-8	1	1	1	Dotriacontane-16,17-$^{14}C_2$, labeled with ^{14}C
16759-28-7	0	1	0	Sodium, isotope mass 24
16778-27-1	1	1	1	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl- {mariolide, dihydroactinidiolide}
16814-81-6	0	1	0	Pentanoic acid, 5-amino-2-hydroxy-, (S)-
16824-61-6	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-, (*Z*)-
16825-04-0	0	1	0	Acetaldehyde, (2,6,6-trimethyl-4-oxo-2-cyclohexen-1-ylidene)-
16825-16-4	0	1	0	2-Pentadecanone, 6,10,14-trimethyl-, [R-(R*,R*)]- {phytone}
16825-90-4	1	1	1	Hexanoic acid, 2-(1-methylethyl)-5-oxo-, (S)-
16858-16-5	1	0	0	4(1*H*)-Pyrimidinone, 6-methyl-2-propyl- = 6-pyrimidinol, 4-methyl-2-propyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
16887-00-6	1	1	1	Chloride ion
16910-32-0	0	1	0	Ergosta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3β,4α,5α)-
16910-33-1	0	1	0	Ergost-8-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-
16935-34-5	1	0	0	2,4-Imidazolidinedione, 5-(1-methylethyl)-
16980-85-1	1	0	0	1-Pentacosene
16982-00-6	0	1	0	Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)-
16984-48-8	1	0	0	Fluoride
17001-28-4	1	1	1	Octadecanoic acid, 16-methyl-
17003-99-5	1	0	0	2-Nonene, 3-methyl-
17013-01-3	1	0	0	2-Butenedioic acid (*E*)-, disodium salt
17024-44-1	1	0	0	6-Oxabicyclo[3.1.0]hexan-4-one, 1-methyl-
17057-82-8	1	0	0	1*H*-Indene, 2,3-dihydro-1,2-dimethyl-
17057-92-0	1	1	1	Naphthalene, 1-ethyl-5-methyl-
17057-94-2	1	1	1	Naphthalene, 1-ethyl-3-methyl-
17057-98-6	1	0	0	9*H*-Fluorene, 1,9-dimethyl-
17059-52-8	1	0	0	Benzofuran, 5-methyl-
17059-53-9	1	1	1	Naphthalene, 2-ethyl-5-methyl- {naphthalene, 6-ethyl-1-methyl-}
17059-55-1	1	1	1	Naphthalene, 2-ethyl-7-methyl-
17063-17-1	0	1	0	2(4*H*)-Benzofuranone, 5,7a-dihydro-4,4,7a-trimethyl-, (R)-
17081-85-5	0	1	0	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-1,4a-dimethyl-7-(1-methylethenyl)- (4aS-*cis*)- {1,2-dehydro-α-cyperone}
17092-92-1	1	1	1	2(4*H*)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-
17093-82-2	0	1	0	2-Propenoic acid, 3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]- {1-*O*-caffeoylglucose}
17100-62-8	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4,6-dimethyl-
17105-75-8	1	0	0	Ergost-7-en-3-ol, (3β,24ξ)-
17113-33-6	1	0	0	Furan, 2-phenyl-
17119-15-2	1	0	0	Benzeneacetic acid, α,3-dihydroxy-
17179-41-8	1	1	1	Naphthalene, 2-ethyl-4-methyl- {naphthalene, 3-ethyl-1-methyl-}
17190-74-8	0	1	0	2-Cyclopenten-1-one, 2-(2-butenyl)-4-hydroxy-3-methyl-
17219-23-7	0	1	0	Cyclopropanecarboxylic acid, 2,3-dimethyl-
17266-64-7	1	0	0	1*H*-Pyrrolizin-1-one, 2,3-dihydro-
17270-48-3	0	1	0	3-Pyridinebutanoic acid, γ-(methylamino)-, (±)-
17271-70-4	1	0	0	Benzene, 1-methyl-3-(1-propenyl)-
17276-85-6	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 2-methyl-
17278-28-3	0	1	0	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3α,9β,10α,16α,23*E*)-
17301-23-4	0	1	0	Undecane, 2,6-dimethyl-
17312-57-1	1	1	1	Dodecane, 3-methyl-
17318-45-5	1	1	1	Eicosanoic acid, hexacosyl ester
17325-90-5	0	1	0	4-Hexen-3-one, 4,5-dimethyl-
17334-55-3	0	1	0	1aH-Cyclopropa[a]naphthalene, 1,1,7,7a-tetramethyl-2,3,5,6,7,7b-hexahydro {1(10)-aristolene, (+)}
17341-24-1	0	1	0	Lithium, ion
17341-25-2	0	1	0	Sodium, ion
17347-61-4	1	1	1	2,5-Furandione, dihydro-3,3-dimethyl-
17351-34-7	0	1	0	14-Pentadecenoic acid
17369-60-7	0	1	0	2-Cyclohexen-1-one, 5-ethyl-2,3,4,5-tetramethyl-
17374-27-5	1	0	0	2,4-Imidazolidinedione, 1,5-dimethyl-
17374-79-7	1	0	0	Phenoxyl, methyl radical
17398-16-2	0	1	0	Pyrazine, 2-ethyl-3,5,6-trimethyl-
17401-48-8	1	0	0	Benz[*a*]acridine, 9,12-dimethyl-
17423-48-2	1	0	0	4-Phenanthrenamine
17480-26-1	0	1	0	Ethanedioic acid, tin salt {stannous oxalate}
17496-14-9	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-2-methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
17507-24-3	1	0	0	Quinoline, 2-(1-methylethyl)-
17507-25-4	1	0	0	Quinoline, 4-(1-methylethyl)-
17539-43-4	0	1	0	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-
17570-26-2	1	1	1	2-Propenoic acid, 3-(3-methoxyphenyl)-, (*E*)-
17573-23-8	1	0	0	Benzo[*a*]pyrene, 7,8-dihydro-
17603-42-8	0	1	0	1,2,3-Propanetriol, 1-(dihydrogen phosphate), sodium salt
17605-67-3	1	1	1	Stigmasta-5,24(28)-dien-3-ol, (3β,24*E*)-
17608-52-5	0	1	0	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy- {4-*O*-caffeoylquinic acid}
17609-32-4	0	1	0	3,5,7-Nonatrien-2-one
17618-94-9	1	0	0	Pyridine, 2-(1-propenyl)-
17618-95-0	1	0	0	Pyridine, 4-(1-propenyl)-
17619-39-5	1	1	1	1*H*-Pyrrole-3-carboxaldehyde, 2-methyl-
17622-35-4	0	1	0	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, acetate, stereoisomer
17626-73-2	1	0	0	Thiazole, 5-ethyl-
17626-75-4	1	0	0	Thiazole, 2-propyl-
17650-84-9	0	1	0	4*H*-1-Benzopyran-4-one,3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-
17661-50-6	1	1	1	Octadecanoic acid, tetradecyl ester
17671-27-1	1	1	1	Docosanoic acid, docosyl ester
17673-49-3	1	1	1	9-Octadecenoic acid (*Z*)-, octadecyl ester
17673-60-8	1	1	1	9,12,15-Octadecatrienoic acid, octadecyl ester, (*Z,Z,Z*)-
17675-99-9	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-, (*Z*)-
17678-19-2	1	1	1	Ethanone, 1-(2-furanyl)-2-hydroxy-
17678-20-5	1	0	0	3(2*H*)-Furanone, 4-hydroxy-2-(hydroxymethyl)-5-methyl-
17714-57-7	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-3,5-dimethyl-
17721-95-8	1	0	0	Piperidine, 2.6-dimethyl-1-nitroso-
17747-43-2	1	0	0	3-Pyridinol, acetate (ester)
17781-15-6	0	1	0	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-
17781-16-7	0	1	0	3(2*H*)-Benzofuranone, 7-hydroxy-2,2-dimethyl-
17787-48-3	0	1	0	Ethanedioic acid, calcium salt (1:1), hydrate (2:5)
17804-35-2	0	1	0	1*H*-Benzimidazole-2-carbamic acid, 1-(butylcarbamoyl)-, methyl ester {Benomyl®}
17825-86-4	1	1	1	1*H*-Pyrrole-2,5-dione, 3,4-dimethyl-
17828-56-7 DL 526-91-0 D 4172-43-4 4172-44-5 L	1	0	0	Pentanoic acid, 2,3,4,5-tetrahydroxy- [3 CAS Nos.]
17910-08-6	0	1	0	4a(2*H*)-Naphthalenol, 1,5,6,7,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1α,4aβ,7α,8aα)]-
17912-87-7	0	1	0	4*H*-Benzopyran-4-one, 3-[(6-deoxy-α-*L*-mannopyranosyl)oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)- {myricitrin}
17924-92-4	0	1	0	1*H*-2-Benzoxacyclotetradecin-1,7(8*H*)-dione, 3,4,5,6,9,10-hexahydro-14,16-dihydroxy-3-methyl-, [S-(*E*)]-
17945-79-8	1	0	0	2-Pyridinebutanol
17980-16-4	1	0	0	Phenanthrene, 2,6-dimethyl-
17990-15-7	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-[1α(*E*),2β,4aβ,8aα]]-
17990-16-8	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1R-[1α(Z),2β,4aβ,8aα]]-
18028-53-0	1	0	0	2*H*-Pyrrolium, 3,4-dihydro-1-methyl-, chloride
18094-01-4	1	0	0	1-Tridecene, 2-methyl-
18102-31-3	1	0	0	Phenol, 2-methoxy-3-methyl-
18113-81-0	1	0	0	Pyridine, 2-ethyl-5-methyl-
18132-98-4	1	0	0	2(3*H*)-Furanone, dihydro-3-(hydroxymethyl)-
18138-03-9	1	0	0	Pyrazine, 2-propyl-
18138-04-0	1	1	1	Pyrazine, 2,3-diethyl-5-methyl-
18138-05-1	1	0	0	Pyrazine, 3,5-diethyl-2-methyl- = pyrazine, 2,6-diethyl-3-methyl-
18172-67-3 127-91-3	1	1	1	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- [2 CAS Nos.] {β-pinene}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
18178-54-6	1	1	1	2,3-Naphthalenediol, 1,2,3,4,5,6,7,8-octahydro-1-methyl-7-(1-methylethenyl)-, [1S-(1α,2β,3α,7β)]- {rishitin}
18277-27-5	1	0	0	Thiazole, 2-(1-methylpropyl)-
18299-74-6	1	1	1	Tetradecanoic acid, pentadecyl ester
18299-77-9	1	1	1	Hexadecanoic acid, pentadecyl ester
18299-78-0	1	1	1	Tetradecanoic acid, heptadecyl ester
18299-80-4	1	1	1	Octadecanoic acid, pentadecyl ester
18299-82-6	1	1	1	Octadecanoic acid, heptadecyl ester
18309-73-4	0	1	0	2*H*-1-Benzopyran-2-one, 6-methoxy-7-[(6-*O*-β-*D*-xylopyranosyl-β-*D*-glucopyranosyl)oxy]-
18310-19-5	1	0	0	1,2-Cyclohexanedione, 4-methyl-
18339-16-7	0	1	0	5α-Androst-16-en-3-one {androstenone}
18349-16-1	1	0	0	Cyclohexane, 1,1-dimethoxy-3-methyl-
18349-20-7	1	0	0	Cyclohexane, 1,1-dimethoxy-4-methyl-
18364-47-1	1	0	0	3-Pyridinamine, *N*-methyl-
18366-19-3	1	0	0	2,5-Pyrrolidinedione, 3-hydroxy- (S)
18368-73-5	1	0	0	Pyridine, 3-methyl-2-nitro-
18378-66-0	0	1	0	1-Cyclohexene-1-carboxaldehyde, 3-oxo-2,6,6-trimethyl-
18383-59-0	0	1	0	Cyclopropanemethanol, 2,2-dimethyl-3-(2-methylpropenyl)- {chrysanthemyl alcohol}
18409-17-1	0	1	0	2-Octen-1-ol, (*E*)-
18435-22-8	0	1	0	Tetradecane, 3-methyl-
18435-45-5	1	1	1	1-Nonadecene
18435-53-5	1	0	0	1-Triacontene
18435-54-6	1	0	0	1-Hentriacontene
18435-55-7	1	0	0	1-Dotriacontene
18441-55-9	1	0	0	Phenol, 2,3-dimethyl-6-ethyl-
18444-66-1	0	1	0	19-Norlanosta-1,5,23-triene-3,11,22-trione, 25-(acetyloxy)-2,16,20-trihydroxy-9-methyl-, (9β,10α,16α,23*E*)-
18444-79-6	0	1	0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-3-hydroxy-2-(1-methylethylidene)-, (5R-*cis*)-
18465-71-9	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-, (3R-*Z*)-
18466-06-3	1	1	1	Hexadecanoic acid, heptadecyl ester
18472-36-1	1	1	1	Stigmasta-5,24(28)-dien-3-ol, (3β)-
18476-57-8	1	0	0	2,6-Octadiene, 4,5-dimethyl-
18496-25-8	1	1	1	Sulfide
18515-43-0	1	0	0	4-Cyclopentene-1,3-dione, 4,5-dimethyl-
18540-29-9	1	0	0	Chromium ion (6+)
18610-59-8	0	1	0	*L*-Proline, 1-hydroxy-
18640-62-5	1	0	0	Benzene, 1-ethyl-4-(2-propenyl)-
18640-74-9	1	0	0	Thiazole, 2-(2-methylpropyl)-
18653-39-9	1	1	1	Tetradecanoic acid, tetracosyl ester
18707-60-3	0	1	0	2-Butenoic acid, methyl ester
18719-24-9	0	1	0	7-Octenoic acid
18719-76-1	0	1	0	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-, chloride
18734-79-7	0	1	0	Butanedioic acid, 2-methyl-3-phenyl-
18787-63-8	1	1	1	2-Hexadecanone
18793-19-6	1	1	1	Piperidine, 2,4-di(3-pyridinyl)- {pyridine, 3,3′-(2,4-piperidinediyl)bis-, anatalline}
18794-84-8	1	0	0	1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (*E*)- {β-farnesene}
18826-61-4	1	0	0	2-Propanone, 1-(3-methylphenyl)-
18829-56-6	0	1	0	2-Nonenal, (*E*)-
18835-32-0	1	1	1	1-Tricosene
18835-33-1	1	0	0	1-Hexacosene
18835-34-2	1	0	0	1-Octacosene
18835-35-3	1	0	0	1-Nonacosene

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
18875-39-3	0	1	0	Glycine, labeled with ^{14}C {glycine-^{14}C}
18908-70-8	0	1	0	Benzene, 1-ethyl-2-(1-phenylethyl)-
18920-65-5	0	1	0	Zinc, bis(thiocarbamato)-
18936-17-9	1	0	0	Butanenitrile, 2-methyl- [2 CAS Nos.]
25570-03-0				
18937-17-9	1	0	0	Butanenitrile, 2-methyl-
18937-71-8	1	0	0	1,5-Naphthyridine, 3-methyl-
18938-03-9	1	0	0	3-Butenamide, 3-methyl-
18990-98-2	1	0	0	1,3,6-Hexanetriol
18996-35-5	0	1	0	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monosodium salt
18999-28-5	1	1	1	2-Heptenoic acid
19005-95-9	1	0	0	Ethanone, 1-(2,4,5-trimethyl-1*H*-pyrrol-3-yl)-
19006-81-6	1	1	1	2(1*H*)-Pyridinone, 4-phenyl-
19020-26-9	1	0	0	Quinoline, 4-ethyl-
19037-58-2	1	1	1	2-Propanone, 1-(3,5-dimethoxy-4-hydroxyphenyl)-
19044-88-3	0	1	0	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro- {Oryzalin®}
19059-14-4	1	0	0	Nitrite, peroxy-
19062-98-7	1	0	0	Butoxyl radical
19088-13-2	0	1	0	Silicic acid, aluminum salt
19141-85-6	1	0	0	1*H*-Imidazole, 4-ethyl-
19147-78-5	0	1	0	Gibbane-1,10-dicarboxylic acid, 2,3-epoxy-4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1α,2β,3β,4aα,4bβ,10β)-
19150-20-0	1	0	0	2-Tridecene, (*Z*)-
19179-12-5	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-
19246-18-5	0	1	0	Glycine, *N*-*L*-cysteinyl-
19250-17-0	0	1	0	Bicyclo[3.1.1]hept-2-ene-2-carboxylic acid, 6,6-dimethyl-
19253-25-9	0	1	0	Uridine 5′-(trihydrogen pyrophosphate), mono(6-deoxymannopyranosyl) ester
19254-69-4	0	1	0	Ergosta-4,6,8(14),22-tetraen-3-one, (22*E*)-
19345-91-6	1	0	0	Acenaphthylene, 5-methyl-
19345-94-9	1	0	0	Acenaphthylene, 3-methyl-
19345-97-2	1	0	0	Acenaphthylene, 4-methyl-
19345-99-4	1	0	0	Acenaphthylene, 1-methyl-
19346-00-0	1	0	0	Acenaphthylene, 1,3-dimethyl-
19346-02-2	1	0	0	Acenaphthylene, 1,5-dimethyl-
19352-29-5	1	1	1	Pyridine, 4-methyl-3-phenyl-
19355-58-9	0	1	0	2,6-Benzofurandione, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-
19377-59-4	0	1	0	1-Oxaspiro[4.5]dec-6-en-8-one, 2,6,10,10-tetramethyl-
19405-98-2	1	0	0	2(3*H*)-Furanone, 4-(acetyloxy)dihydro-
19405-99-3	1	0	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-
19408-74-3	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8,9-hexachloro-
19432-05-4	0	1	0	2(4*H*)-Benzofuranone, tetrahydro-4,4,7a-trimethyl-
38725-47-2				
19432-09-8	1	1	1	2(3*H*)-Benzofuranone, 3a,4,5,7a-tetrahydro-4,4,7a-trimethyl-, *cis*-
19432-10-1	0	1	0	2(3*H*)-Benzofuranone, octahydro-4,4,7a-trimethyl- {tetrahydroactinidiolide}
19438-10-9	1	0	0	Benzoic acid, 3-hydroxy-, methyl ester
19444-84-9	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-
19444-86-1	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-3-(hydroxymethyl)-
19484-74-3	0	1	0	2*H*-1-Benzopyran-3-carboxylic acid, 7,8-dihydroxy-2-oxo-
19549-83-8	1	0	0	3-Heptanone, 2,6-dimethyl-
19620-37-2	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-2,6,6-trimethyl-
19655-56-2	1	0	0	Quinoline, 8-ethyl-
19683-91-1	1	0	0	Piperidine, 2,4-dimethyl-, *cis*-
19701-89-4	1	0	0	*DL*-Alanine, *N,N*-dimethyl-
19716-26-8	1	1	1	β-*D*-Glucopyranoside, (3β,22*E*)-stigmasta-5,22-dien-3-yl- {stigmasteryl glucoside}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
19730-04-2	1	1	1	Pyridine, 3-(1-methyl-2-piperidinyl)-, (S)- [2 CAS Nos.] {*N*-methylanabasine}
24380-92-5				
19752-84-2	1	0	0	2*H*-Pyran-3-ol, tetrahydro-
19780-80-4	0	1	0	Tridecane, 7-methylene-
19784-98-6	1	0	0	Phenol, 2-methoxy-5-(1-propenyl)-, (*E*)-
19838-07-4	1	0	0	2(1*H*)-Pyrazinone, 3-methyl-
19859-79-1	1	0	0	Ethanone, 1-(2-furanyl)-2-(acetyloxy)-
19870-37-2	1	0	0	4-Nonanol, 2,6,8-trimethyl-
19870-75-8	0	1	0	1*H*-3a,7-Methanoazulen, 6-methoxy-octahydro-3,6,8,8-tetramethyl- {cedryl methyl ether}
19894-91-8	0	1	0	1-Cyclohexene-1,4-dimethanol, α4,α4-dimethyl-, (S)-
19895-95-5	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-
19937-59-8	0	1	0	Urea, *N′*-(3-chloro-4-methoxyphenyl)-*N,N*-dimethyl {Metoxuron®}
19943-28-3	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-methyl-, (3R-*trans*)-
36357-32-1				
19961-52-5	1	0	0	Thiazole, 5-ethyl-2-methyl-
19961-53-6	1	0	0	Thiazole, 2-ethyl-5-methyl-
19983-83-6	1	0	0	1*H*-Pyrrole, 1-ethyl-2-methyl-
19988-45-5	1	0	0	Benzeneacetic acid, 2,3-dihydroxy-
20013-73-4	0	1	0	2-Cyclohexen-1-one, 2,6,6-trimethyl-
20019-64-1	0	1	0	2(5*H*)-Furanone, 5,5-dimethyl-
20030-85-7	1	0	0	Cyclopentanone, 2,4-dimethyl- {isomer}
20127-61-1	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 1-ethyl-
20129-49-1	1	1	1	Dotriacontane, 3-methyl-
20173-36-8	1	0	0	3-Buten-1-amine, *N,N*-dimethyl-4-(3-pyridinyl)-
20185-22-2	1	0	0	1*H*-Imidazole, 1,4,5-trimethyl-
20188-84-5	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-[(2-O-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy- {quercetin 3,3′-diglucoside}
7215-44-3				
20189-42-8	1	1	1	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-methyl-
20193-20-8	1	1	1	1-Propanamine, *N*-ethyl-
20193-21-9	1	1	1	1-Butanamine, *N*-propyl-
20194-48-3	0	1	0	1-Pentadecanol, 14-methyl-
20194-67-6	1	1	1	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-2,5,5,8a-tetramethyl- {1,5,5,9-tetramethyl-10-oxabicyclo[4.4.0]dec-6-en-3-one}
20194-68-7	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-
20194-70-1	1	1	1	2-Propanone, 1-(tetrahydro-4-methyl-2*H*-pyran-2-yl)-
20194-71-2	1	1	1	Pyridine, 2-methyl-5-(1-methylethyl)-
20197-09-5	0	1	0	*L*-Ornithine, *N*2-(1-carboxyethyl)-, (R)-
20200-86-6	0	1	0	2*H*-Indol-2-one, 1,3-dihydro-1,3,3-trimethyl-
20225-24-5	0	1	0	Pentanoic acid, 2-ethyl-
20236-97-9	0	1	0	*D*-Methionine, *N*-(carboxyacetyl)-
20239-99-0	0	1	0	3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-, [3S-(3α,4β,21β)]-
20242-97-1	1	1	1	Stigmasta-5,22-dien-3-ol, dodecanoate, (3β,22*E*)- {stigmasteryl laurate}
20242-98-2	1	1	1	Stigmasta-5,22-dien-3-ol, tetradecanoate, (3β,22*E*)- {stigmasteryl myristate}
20261-96-5	1	1	1	Arabinohexonic acid, 3-deoxy-, γ-lactone
20268-93-3	0	1	0	5′-Adenylic acid, *N*-(3-methyl-2-butenyl)-
20281-85-0	0	1	0	1-Butanol, 2,3-dimethyl-
20291-72-9	1	0	0	Phenanthrene, 1,2-dimethyl-
20291-74-1	1	0	0	Phenanthrene, 1,6-dimethyl-
20298-86-6	0	1	0	21*H*-Biline-8,12-dipropanoic acid, 18-ethyl-3-ethylidene-1,2,3,19,22,24-hexahydro-2,7,13,17-tetramethyl-1,19-dioxo-, (2R,3*E*)-
20300-00-9	0	1	0	Phosphorothioic acid, *O,O*-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfinyl]ethyl] ester
20304-54-5	0	1	0	Ergost-4-en-3-ol, (24R)- {campest-7-en-3-β-ol}

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
20307-84-0	0	1	0	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)- {δ-elemene}
20333-39-5	1	0	0	Disulfide, ethyl methyl
20357-65-7	1	0	0	2*H*-Pyran-2-one, 6-chloro-
20379-10-6	0	1	0	Actinium, isotope of mass 226
20390-21-0	1	0	0	1,2-Propanediol, 3-(furfuryloxy)-
20410-87-1	0	1	0	2,3′-Bipyridine, 5-(1-methyl-2-piperidinyl)-, (+)- {anabasamine}
20431-48-5	1	1	1	β-*D*-Glucopyranoside, (3β)-stigmast-5-en-3-yl- {β-sitosteryl glucoside}
474-58-8				
20432-26-2	0	1	0	Benzeneacetic acid, α-ethylidene-, (*E*)-
20461-54-5	0	1	0	Iodide
20469-61-8	1	0	0	Benzene, 1-methoxy-2,3,5-trimethyl-
20483-36-7	0	1	0	2-Butanone, 4-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-
20485-57-8	1	0	0	Fluoranthene, 8-methyl-
20490-42-0	1	1	1	1,4-Naphthalenedione, 2,3,6-trimethyl-
20496-16-6	1	0	0	Fluoranthene, 3-ethyl-
20497-93-2	0	1	0	Cyclopentanecarboxaldehyde, 2-hydroxy-1-methyl- {two isomers}
20547-99-3	1	1	1	1,4-Cyclohexanedione, 2,2,6-trimethyl- {4-ketodihydroisophorone}
20548-00-9	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-methylene- {methyleneisophorone}
20548-02-1	1	1	1	Cyclohexanone, 4-hydroxy-2,2,6-trimethyl-
20548-03-2	1	1	1	Cyclohexanone, 4-hydroxy-3,3,5-trimethyl-
20578-97-6	1	1	1	Phenol, 2,3-dimethoxy-4-ethyl-
20583-33-9	0	1	0	Ethanone, 1-(1*H*-pyrazol-3-yl)-
20653-90-1	0	1	0	2,3-Octanediol
20654-94-8	1	0	0	Oxazole, 4,5-dimethyl- [2 CAS Nos.]
20662-83-3				
20661-60-3	0	1	0	Glycine, *N*-methyl-*N*-nitro-
20662-83-3	1	0	0	Oxazole, 4,5-dimethyl- [2 CAS Nos.]
20654-94-8				
20662-84-4	1	1	1	Oxazole, trimethyl- = 2,4,5-trimethyloxazole
20675-95-0	1	1	1	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*E*)-
20721-17-9	1	0	0	2(1*H*)-Pyrazinone, 5-methyl-
20721-18-0	1	0	0	2(1*H*)-Pyrazinone, 6-methyl-
20724-30-5	1	0	0	9,10-Anthracenedione, 1,2-diethyl-
20780-49-8	0	1	0	1-Octanol, 3,7-dimethyl-, acetate {tetrahydrogeranyl acetate}
20810-06-4	1	1	1	1-Butanamine, *N*-(2-methylpropyl)-
20825-71-2	1	1	1	2(3*H*)-Furanone {butenolide}
20851-90-5	1	0	0	Phenanthrene, 3,6-dichloro-
20859-73-8	0	1	0	Phosphide, aluminum
20884-13-3	1	1	1	1*H*-Pyrrole, 1-(2-methylpropyl)-
20928-82-9	1	0	0	Benzo[*a*]pyren-6-yloxy
20970-50-7	1	0	0	Ethanone, 1-(1-methyl-1*H*-imidazol-5-yl)-
20970-75-6	1	0	0	2-Pyridinecarbonitrile, 3-methyl-
20970-77-8	1	0	0	2-Pyridinecarboxamide, 5-methyl-
20971-79-3	1	0	0	2(3*H*)-Furanone, dihydro-5-(3-pyridinyl)-
21040-45-9	0	1	0	2-Propen-1-ol, 3-phenyl-, acetate, (*E*)-
21056-52-0	0	1	0	β-*D*-Glucopyranose, 1-benzoate
21087-64-9	0	1	0	1,2,4-Triazin-5(4*H*)-one, 4-amino-6-*tert*-butyl-3-(methylthio)- {Metribuzin®}
21101-88-2	1	0	0	Pentanenitrile, 3-methyl-
21202-52-8	1	0	0	1*H*-Imidazole, 1-ethyl-2-methyl-
21291-36-1	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-α-*D*-glucopyranosyl-(1→6)-
21293-01-6	1	0	0	2,4-Hexadiene, 3,4-dimethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
21293-29-8	0	1	0	2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-, [S-(*Z,E*)]- [2 CAS Nos.] {abscisic
14375-45-2				acid}
21296-92-4	1	0	0	1*H*-Indole, 2,3,5-trimethyl-
21300-07-2	0	1	0	2-Furancarboxaldehyde, 5-methoxy-
21422-41-3	0	1	0	3,6-Pyridazinedione, 1,2-dihydro-, diethanolamine salt
5716-15-4				
21490-25-5	0	1	0	Ergosta-7,24(28)-dien-3β-ol, 4β-methyl-
21504-51-8	1	1	1	3-Heptene-2,5-dione, 6-methyl-
21511-31-9	1	1	1	Docosanoic acid, octacosyl ester
21535-97-7	1	0	0	Benzofuran, 3-methyl-
21548-32-3	0	1	0	1,3-Dithietan-2-ylidenephosphoramidic acid, diethyl ester {Fosthietan®}
21606-61-1	1	0	0	Pyridine, 2-(2-butenyl)-
21609-90-5	1	1	1	Phenylphosphonothioic acid, *O*-(4-bromo-2,5-dichlorophenyl)-, *O*-methyl ester {Phosvel®}
21637-25-2	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(β-*D*-glucofuranosyloxy)-5,7-dihydroxy- {isoquercetrin}
21662-09-9	0	1	0	4-Decenal, (*Z*)-
21693-51-6	0	1	0	Naphthalene, 1,2,3,4-tetrahydro-1,5,8-trimethyl-
21722-33-8	1	1	1	2*H*-Pyran-2-one, 5,6-dihydro-4-(1-methylethyl)-
21722-34-9	1	1	1	2*H*-Pyran-2-one, tetrahydro-6-methyl-3-(1-methylethyl)- {two isomers indicated}
21730-66-5	1	1	1	Benzene, methoxy-, 1-^{14}C, labeled with ^{14}C {anisole-1-^{14}C}
21754-22-3	0	1	0	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-, (±)-
21788-49-8	0	1	0	2-Butenedioic acid, 2,3-dimethyl-, (*E*)-
21789-36-6	1	0	0	Benzonitrile, 2,4-dimethyl-
21834-92-4	0	1	0	2-Hexenal, 5-methyl-2-phenyl-
21834-98-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,5-dimethyl-
21835-00-7	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl
21835-01-8	1	0	0	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- {ethylcyclopentenolone}
21850-61-3	1	0	0	Benzeneacetonitrile, 4-hydroxy-α-methyl-
21963-26-8	0	1	0	2(5*H*)-Furanone, 5-pentyl- [2 CAS Nos.]
1963-26-8				
21968-17-2	1	1	1	2-Propanamine, *N*-propyl- = 1-propanamine, *N*-(1-methylethyl)-
21978-49-4	1	1	1	5,9,13,17,21,25,29,33-Pentatriacontaoctaen-2-one, 6,10,14,18,22,26,30,34-octamethyl-, (all-*E*)-
21980-71-2	1	0	0	1,3-Hexadecadiene, 3,7,11,15-tetramethyl- {phytadiene}
21984-93-0	1	0	0	3-Furancarboxylic acid, 5-methyl-
21987-21-3	0	1	0	1-Tridecanol, 12-methyl-
22023-64-9	1	0	0	1-Propanamine, *N*-(1-methylethylidene)-
22029-76-1	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- [2 CAS Nos.] {β-ionol}
27008-60-2				
22047-25-2	1	1	1	Ethanone, 1-pyrazinyl- {acetylpyrazine}
22047-26-3	1	1	1	Ethanone, 1-(6-methylpyrazinyl)- {2-acetyl-6-methylpyrazine}
22047-27-4	1	1	1	Ethanone, 1-(5-methylpyrazinyl)- {2-acetyl-5-methylpyrazine}
22059-21-8	0	1	0	Cyclopropanecarboxylic acid, 1-amino-
22072-35-1	1	0	0	1*H*-indole, 2,3,6-trimethyl-
22083-74-5	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (±)-
22104-83-2	0	1	0	2-Hexadecen-1-ol
22104-85-4	0	1	0	2-Eicosen-1-ol
22122-36-7	1	1	1	2(5*H*)-Furanone, 3-methyl-
22223-61-6	1	0	0	Thionitrous acid (HNOS), S-methyl ester
22224-92-6	0	1	0	Phosphoramidic acid, (1-methylethyl)-, ethyl 3-methyl-4-(methylthio)phenyl ester {Fenamiphos®, Nemacur®}
22241-38-9	1	0	0	Pyridine, 4-(4-methylpentyl)-
22248-79-9	0	1	0	Phosphoric acid, 2-chloro-1-(2,4,5-trichlrophenyl)ethenyl-, dimethyl ester {DDVP, Tetrachlorvinphos®}
22271-04-1	1	0	0	Fluoranthene, 7,10-dimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
22303-81-7	1	0	0	1*H*-Inden-1-one, 3-methyl-
22323-97-3	1	0	0	2-Cyclopenten-1-one, 2-methoxy-
22343-28-8	0	1	0	2-Naphthalenol, decahydro-1-(5-hydroxy-3-methyl-3-pentenyl)-2,5,5,8a-tetramethyl-, [1R-(1α,2β,4aβ,8aα)]-
22349-59-3	1	0	0	Phenanthrene, 1,4-dimethyl-
22349-74-2	1	0	0	Benzene, 1-chloro-4-(2-chloro-1-phenylethenyl)-
22364-68-7	1	0	0	Benzeneacetonitrile, 2-methyl-
22382-94-1	1	0	0	Pyridine, 2-ethenyl-3-methyl-
22393-85-7	1	1	1	9-Octadecenoic acid (*Z*)-, tetradecyl ester
22393-86-8	1	1	1	9-Octadecenoic acid (*Z*)-, hexadecyl ester
22393-88-0	1	1	1	9-Octadecenoic acid (*Z*)-, eicosyl ester
22413-00-9	1	1	1	Tetradecanoic acid, eicosyl ester
22413-01-0	1	1	1	Hexadecanoic acid, eicosyl ester
22413-02-1	1	1	1	Octadecanoic acid, eicosyl ester
22413-03-2	1	1	1	Octadecanoic acid, docosyl ester
22413-04-3	1	1	1	Eicosanoic acid, tetradecyl ester
22413-05-4	1	1	1	Eicosanoic acid, hexadecyl ester
22422-34-0	0	1	0	Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl- {2,3-pinanediol}
22432-79-7	1	1	1	Eicosanoic acid, octadecyl ester
22432-80-0	1	1	1	Eicosanoic acid, eicosyl ester
22500-92-1	1	1	1	2,4-Hexadienoic acid, (*E,E*)- {sorbic acid}
110-44-1				
22509-02-0	1	0	0	1*H*-Imidazole, 1-methyl-2-(1-methylethyl)-
22537-07-1	1	0	0	4-Penten-1-amine
22537-22-0	0	1	0	Magnesium, ion
22537-38-8	0	1	0	Rubidium, ion
22541-54-4	1	1	1	Arsenic, arsenious state
22567-22-2	0	1	0	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, [1R-(1α,2α,5β)]-
22583-61-5	1	0	0	Ethanone, 1-[2-(1,1-dimethylethyl)phenyl]-
22639-24-3	1	0	0	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-6-methyl-
22663-55-4	0	1	0	Adenosine, *N*-(4-hydroxy-3-methylbutyl)-
22688-80-8	0	1	0	1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-[(2-*O*-β-*D*-glucopyranosyl-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-, chloride
22699-70-3	1	0	0	Ethanone, 1-(3-ethylphenyl)-
22732-83-8	0	1	0	Adenosine 5′-(trihydrogen pyrophosphate), mono-*D*-glucopyranosyl ester
22868-76-4	1	0	0	Pyrimidine, 2,5-dimethyl-
22884-95-3	1	0	0	Benzonitrile, 3,4-dimethyl-
22929-52-8	1	1	1	3(2*H*)-Furanone, dihydro-
22971-32-0	1	0	0	1-Butanone, 1-(2-pyridinyl)-
22986-69-2	1	0	0	17-Tritriacontanone
23007-29-6	0	1	0	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, (*E*)- {*trans*-linalool oxide}
23012-10-4	1	0	0	Oxazole, 2-methyl-
23012-11-5	1	0	0	Oxazole, 2,5-dimethyl-
23048-13-7	1	0	0	2-Cyclopenten-1-one, 2,4-dimethyl-
23069-00-3	1	1	1	2-Cyclohexen-1-one, 4-hydroxymethyl-3,5,5-trimethyl-
23074-10-4	1	0	0	2-Furancarboxaldehyde, 5-ethyl-
23103-98-2	0	1	0	Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester {Pirimicarb®}
23105-58-0	1	0	0	1*H*-Pyrrole, 1-acetyl-2,3-dihydro-
23120-57-2	1	0	0	3-Buten-2-one, 4-(5-methyl-2-furanyl)-
23135-22-0	0	1	0	Ethanimidothioic acid, 2-(dimethylamino)-*N*-[[(methylamino)carbonyl]oxy]-2-oxo-, methyl ester {Oxamyl®}
23245-64-9	1	0	0	1-Naphthalenecarbonitrile, 5-nitro-
23267-57-4	0	1	0	3-Buten-2-one, 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-
23283-97-8	0	1	0	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5β)- {isomenthol}
490-99-3				
23290-26-8	0	1	0	Stigmasta-7,24(28)-dien-3-ol, (3β,5α,24*Z*)-

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
23328-91-8	1	0	0	Ethanone, 1-(5-methyl-1*H*-imidazol-4-yl)-
23339-04-0	1	0	0	Fluoranthene, 2,3-dimethyl-
23339-05-1	1	0	0	Fluoranthene, 7-methyl-
23350-58-5	1	0	0	2-Butenamide, (*E*)- [2 CAS Nos.] {crotonamide}
625-37-6				
23350-60-9	1	0	0	2-Butenamide, *N*-ethyl-
23395-72-4	1	0	0	6-Quinolinecarbonitrile
23415-96-7	1	0	0	2-Cyclopenten-1-one, 4-methyl-
23445-11-6	0	1	0	β-*D*-Glucopyranose, 1-(2,5-dihydroxybenzoate)
23462-75-1	1	0	0	2*H*-Pyran-3(4*H*)-one, dihydro-
23470-00-0	1	0	0	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester {glyceryl 2-hexadecanoate}
23513-39-5	1	0	0	Piperidine, 2,3-dimethyl-, *cis*-
23526-45-6	0	1	0	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- (+) {Blumenol A}
23580-52-1	0	1	0	Pyridine, 3-ethyl-2,6-dimethyl-
23599-75-9	1	1	1	1-Butanol, 2-methyl-4-(1*H*-purin-6-ylamino)- {dihydrozeatin}
23605-13-2	0	1	0	2,6-Nonadienoic acid, (*E,Z*)-
23612-48-8	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, 2-methyl-
23675-06-1	0	1	0	α-*D*-Arabinohexopyranoside, 2-deoxy-α-*D*-arabino-hexopyranosyl 2-deoxy-
23696-85-7	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)- [2 CAS Nos.] {β-damascenone}
23726-93-4				
23713-49-7	0	1	0	Zinc, ion
23726-91-2	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-
23726-92-3	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)- [2 CAS Nos.] {β-damascone}
85949-43-5				
23726-93-4	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (*E*)- [2 CAS Nos.] {β-damascenone}
23696-85-7				
23733-91-7	0	1	0	Cyclohexene, 3-methylene-4-(1-methylethenyl)-, (R)-
23747-37-7	1	0	0	1,2-Cyclopentanedione, 3-propyl-
23747-46-8	1	1	1	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-methyl-
23747-47-9	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-
23747-48-0	1	1	1	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-methyl-
23770-92-3	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)- [3 CAS Nos.] {damascone}
35044-68-9				
80111-68-8				
23787-80-6	1	1	1	Ethanone, 1-(3-methylpyrazinyl)- {2-acetyl-3-methylpyrazine}
23811-18-9	0	1	0	3-Cyclohexen-1-ol, 3,5,5-trimethyl-, (±)-
23832-27-1	0	1	0	1,2-Cyclohexanediol, 4-methyl-
23838-16-6	1	1	1	Stigmasta-5,22-dien-3-ol, octadecanoate, (3β,22*E*)- {stigmasteryl stearate}
23839-47-6	0	1	0	Ergosta-8,14-dien-3-ol, (3β,5α)-
23938-71-8	1	0	0	2(3*H*)-Furanone, dihydro-3-(1-oxopropyl)-
23992-32-7	1	0	0	4*H*-Cyclopenta[*def*]triphenylene {4,5-methylenetriphenylene}
24017-47-8	0	1	0	Phosphorothioic acid, *O,O*-diethyl *O*-(1-phenyl-1*H*-1,2,4-triazol-3-yl) ester {Triazophos®}
24075-47-6	1	0	0	9*H*-Carbazole, 2,9-dimethyl-
24075-48-7	1	0	0	9*H*-Carbazole, 3,9-dimethyl-
24075-49-8	1	0	0	9*H*-Carbazole, 4,9-dimethyl-
24105-07-5	1	1	1	2-Cyclopenten-1-one, 2-propyl-
24156-95-4	1	0	0	2-Cyclopenten-1-one, 3.5.5-trimethyl-
24203-36-9	1	0	0	Potassium, ion
24218-00-6	0	1	0	*D*-erythro-2-Pentulose, 1,5-bis(dihydrogen phosphate)
24259-59-4	1	1	1	*L*-Ribose

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
24271-12-3	1	1	1	Docosanoic acid, octadecyl ester
24295-03-2	0	1	0	Ethanone, 1-(2-thiazolyl)- {2-acetylthiazole}
24321-18-4	0	1	0	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dioxo-1,5-cyclohexadien-1-yl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-
24380-92-5	1	1	1	Pyridine, 3-(1-methyl-2-piperidinyl)-, (S)- [2 CAS Nos.] {*N*-methylanabasine}
19730-04-2				
24405-16-1	0	1	0	2*H*-Pyran-2-one, tetrahydro-5,6-dimethyl- [2 CAS Nos.]
10413-18-0				
24427-77-8	1	0	0	2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {vomifoliol}
24471-47-4	1	0	0	Perylene, 3-methyl-
24587-25-5	1	0	0	1,3,5-Heptatriene
24587-26-6	1	0	0	1,3,5-Hexatriene, 3-methyl-
24623-20-9	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-6-methyl-
24624-61-5	0	1	0	2,4-Hexadienoic acid, potassium salt [2 CAS Nos.]
590-00-1				
24644-78-8	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-4-methyl-
24645-67-8	0	1	0	Cystine {propanoic acid, 2-amino-3,3′-dithiobis-}
24667-03-6	1	0	0	Oxazole, 2-ethyl-4-methyl-
24677-78-9	1	1	1	Benzaldehyde, 2,3-dihydroxy-
24683-00-9	0	1	0	Pyrazine, 2-methoxy-3-methylpropyl-
24696-05-7	0	1	0	Benzenepropanoic acid, 2-(β-*D*-glucopyranosyloxy)-
24753-52-4	0	1	0	9-Octadecenoic acid, 18-hydroxy-, (*Z*)-
24851-98-7	0	1	0	Acetic acid, 2-pentyl-3-oxo-1-cyclopentyl-, methyl ester {methyl dihydrojasmonate}
24861-47-0	0	1	0	Phorbine
24871-12-3	1	0	0	2(3*H*)-Benzofuranone, hexahydro-
6051-03-2				
24946-64-3	0	1	0	Plastochromenol {solanachromene isomer}
24950-44-5	1	0	0	Pyridine, 3,3′-(1,2-ethenediyl)bis-
24959-67-9	1	1	1	Bromide
24966-13-0	1	0	0	Methanone, cyclopropyl-3-pyridinyl-
25013-16-5	1	0	0	Phenol, 2-(1,1-dimethylethyl)-4-methoxy-
25016-16-4	0	1	0	Ethanone, 1-(1*H*-pyrazol-4-yl)-
25042-83-5	1	0	0	5*H*-Cyclopentapyrazine
25044-01-3	1	0	0	1-Penten-3-one, 2-methyl-
25057-77-6	1	0	0	Piperazine, 1,2-dimethyl-
25077-26-3	1	0	0	2,6-Piperidinedione, 4-methyl-
25110-79-6	1	0	0	2-Pyrrolidinol, 1-methyl-5-(3-pyridinyl)-
25127-16-6	0	1	0	*L*-Alanine, *N*-(1-deoxy-*D*-fructos-1-yl)-
16124-24-6				
25152-84-5	1	1	1	2,4-Decadienal, (*E,E*)-
25152-85-6	0	1	0	3-Hexen-1-ol, benzoate, (*Z*)-
25154-40-9	1	1	1	Thiophene, methyl-
25154-45-4	1	0	0	Ethanone, 1-(furanyl)-
25155-26-4	1	0	0	Phenol, dimethoxy-
25162-00-9	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (R)- {*d*-nicotine}
25167-67-3	1	0	0	Butene
25167-89-9	1	0	0	Benzo[*a*]pyrene, methyl- {at least two isomers in MSS}
25167-90-2	1	0	0	Benzo[*a*]pyrene, dimethyl- {at least two isomers in MSS}
25168-07-4	0	1	0	Cyclohexene, ethenyl-
25249-06-3	0	1	0	*D*-Galacturonic acid, homopolymer
25252-64-6	1	0	0	Ethanone, 1-(tetrahydro-2-furanyl)-
25264-93-1	1	0	0	Hexene
25269-17-4	1	1	1	2,7,11-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1R-(1R*,2*E*,4S*,7*E*,11*E*)]-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
25309-65-3	1	0	0	Benzonitrile, 4-ethyl-
25311-71-1	0	1	0	Phosphoramidothioic acid, *O*-ethyl *O*-2-(1-methylethyl)carbonylphenyl-, (1-methylethyl) ester {Isofenphos®}
25312-34-9	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-ionol}
472-78-6				
25322-68-3	0	1	0	Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-
25323-89-1	0	1	0	Ethane, 1,2,2-trichloro-
25339-57-5	1	0	0	Butadiene
25340-17-4	1	1	1	Benzene, diethyl-
25343-57-1	0	1	0	Ethanone, 1-[3-(1,4,5,6-tetrahydropyridinyl)]-
25346-59-2	0	1	0	Hexanal, 4-oxo-
25376-45-8	1	0	0	1,3-Benzenediamine, ar-methyl-
25376-49-2	0	1	0	2-Furancarboxaldehyde, (hydroxymethyl)-
25377-27-9	1	0	0	1,3-Benzenediol, dimethyl-
25377-46-2	1	1	1	Heptenoic acid
25377-52-0	1	1	1	Hexadecadienoic acid {palmitolenic acid}
25377-56-4	1	1	1	Hexadecatrienoic acid
25377-72-4	1	0	0	Pentene
25377-82-6	1	0	0	2-Tridecene, (*E*)-
25378-22-7	1	0	0	Dodecene
25395-31-7	1	1	1	1,2,3-Propanetriol, diacetate {diacetin}
25402-06-6	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 3-(2-butenyl)-2-methyl-4-oxo-2-cyclopenten-1-yl ester {Pyrethrin (natural), Cinerin I®}
25413-61-0	1	1	1	1-Propanamine, *N*-ethyl-*N*-nitroso-
25429-24-7	1	1	1	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, monohydroxy derivative, (*S*)-
25429-37-2	1	0	0	Phenol, ethyl-
25429-38-3	1	0	0	2-Propenoic acid, 3-(hydroxyphenyl)-
25447-95-4	1	1	1	Hexadecenoic acid
25448-01-5	0	1	0	Eicosadienoic acid
25448-03-7	0	1	0	Octadecatrienoic acid
25448-06-0	0	1	0	Octadecatetraenoic acid
25454-23-3	0	1	0	Ethanedioic acid, calcium salt [2 CAS Nos.]
563-72-4				
25457-49-2	1	0	0	Propanamide, *N*-methyl-*N*-(1-oxopropyl)-
25487-94-9	0	1	0	1(4*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)-
25496-14-4	1	0	0	Ethanone, 1-(ethylphenyl)-
25512-65-6	1	1	1	2*H*-Pyran, dihydro-
25522-33-2	1	0	0	2-Propenoic acid, 3-(3-hydroxy-4-methoxyphenyl)-, (*E*)-
25545-13-5	0	1	0	*D*-Glucopyranose, 4-(4-hydroxybenzoate)
25550-13-4	1	0	0	Benzene, diethylmethyl-
25550-14-5	1	0	0	Benzene, ethylmethyl-
25550-22-5	1	0	0	Benzonitrile, methyl-
25551-13-7	1	1	1	Benzene, trimethyl-
25551-35-3	1	0	0	Naphthalenecarbonitrile
25567-10-6	1	0	0	Benzoic acid, methyl- {toluic acid}
25570-03-0	1	0	0	Butanenitrile, 2-methyl [2 CAS Nos.]
18936-17-9				
25586-38-3	1	0	0	Benzofuran, methyl- {three isomers detected}
25586-39-4	1	0	0	Benzofuran, dimethyl- {three isomers detected}
25596-90-1	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy- (3R,4S)
25600-22-0	1	0	0	2(3*H*)-Furanone, dihydro-3-(1-oxopropoxy)-
25606-41-1	0	1	0	Carbamic acid, 3-(dimethylamino)propyl-, propyl ester, hydrochloride {Propamocarb hydrochloride®}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
25619-60-7	1	1	1	Benzene, tetramethyl-
25638-00-0	1	0	0	Pyridine, ethenylmethyl-
25659-22-7	1	0	0	4-Hexen-3-one
25680-58-4	0	1	0	Pyrazine, 2-ethyl-3-methoxy-
25683-11-8	0	1	0	1,5-Pentanediamide, 2-amino- {glutamine amide}
25684-04-2	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-propyl-
25684-05-3	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylpropyl)-
25692-13-1	0	1	0	9,19-Cyclolanost-24-en-3-ol, 24-methyl-, (3β)-
25704-73-8	1	1	1	Pyrazine, dimethyl-
25714-71-0	1	0	0	Butanal, 4-hydroxy-
25732-74-5	1	0	0	Cyclopenta[*cd*]pyrene, 3,4-dihydro-
25826-63-5	1	0	0	Naphtho[1,2-*b*]furan, 2-methyl-
25889-60-5	1	0	0	Fluoranthene, 1-methyl-
25889-63-8	1	0	0	Fluoranthene, 8,9-dimethyl-
25917-35-5	1	1	1	Hexanol
25954-44-3	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-*O*-β-*D*-glucopyranosyl-(1 → 6)-
25990-10-7	0	1	0	Galacturonic acid, homopolymer
25990-60-7	1	1	1	*DL*-Xylose
26040-98-2	0	1	0	1-Pentacosanol
26047-31-4	0	1	0	Ergost-7-en-3-ol, (3β)-
26093-31-2	0	1	0	2*H*-Benzopyran-2-one, 7-amino-4-methyl-
26140-60-3	1	0	0	1,1′:3′,1″-Terphenyl [2 CAS Nos.] {*m*-terphenyl}
92-06-8				
26148-68-5	1	0	0	1*H*-Pyrido[2,3-*b*]indol-2-amine {AαC}
26173-92-2	1	0	0	1*H*-Pyrrole-2-carbonitrile, 5-methyl-
26190-61-4	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-
26190-82-9	1	0	0	Quinoline, 2,5-dimethyl-
26225-79-6	0	1	0	7-Benzofuranol, 2,3-dihydro-3,3-dimethyl-2-ethoxy-, methanesulfonate {Ethofumesate®}
26265-99-6	1	1	1	Heptadecenoic acid
26266-05-7	1	1	1	Heptadecene
26329-68-0	1	0	0	2(5*H*)-Furanone, 5-ethyl-3-methyl-
26370-28-5	0	1	0	2,6-Nonadienal {leaf aldehyde violet}
26409-08-5	0	1	0	Lanost-9(11)-en-3-ol, 24,25-epoxy-, (3β)-
26444-03-1	1	1	1	Tetradecenoic acid
26444-04-2	1	1	1	Pentadecenoic acid
26444-18-8	1	0	0	Benzene, methyl (1-methylethenyl)-
26444-19-9	1	0	0	Ethanone, 1-(methylphenyl)- {methylacetophenone}
26445-05-6	1	0	0	Pyridinamine
26446-27-5	0	1	0	Decenoic acid {three isomers detected}
72881-27-7				
26446-35-5	1	1	1	1,2,3-Propanetriol, monoacetate {monoacetin}
106-61-6				
26447-28-9	1	1	1	Furancarboxylic acid
26519-91-5	1	0	0	1,3-Cyclopentadiene, methyl-
26519-92-6	1	0	0	1,3-Cyclopentadiene, ethyl-
26539-01-5	1	0	0	Benzenepropanoic acid, 3,5-dihydroxy-
26563-74-6	1	0	0	1,3-Dioxolane, 4-methyl-2-pentyl-, (*Z*)-
26624-13-5	1	1	1	Phenol, 2,6-dimethoxy-4-(1-propenyl)-, (*Z*)-
26626-89-1	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-propyl-, (3S-*trans*)-
26636-59-9	1	0	0	2,3′-Bipyridine, 2′(or 3)-methyl-
26638-03-9	1	0	0	Phenol, methoxy-
26655-34-5	1	1	1	α-*D*-Glucose

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
50-99-7				
26656-33-7	0	1	0	*D*-Galactopyranuronic acid, homopolymer
26741-29-7	1	0	0	2-Hexadecene, (*E*)-
26761-75-1	1	0	0	Phenol, (2-propen-1-yl)-
26764-25-0	1	1	1	Octadecadienoic acid
26764-26-1	1	1	1	Octadecenoic acid {oleic acid}
26764-41-0	1	1	1	Eicosenoic acid
26817-24-3	1	0	0	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-
26836-30-6	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitolinolein}
99431-70-6				
26836-32-8	0	1	0	9,12-Octadecadienoic acid, monoester with propanetriol monohexadecanoate and monooctadecanoate {palmitostearolinolein}
26836-35-1	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, ester with 1,2,3-propanetriol monohexadecanoate mono[(*Z*)-9-octadecenoate]
26836-36-2	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, diester with 1,2,3-propanetriol monohexadecanoate {palmitodilinolein}
26836-38-4	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol monooctadecanoate mono-9-octadecenoate, (*Z*)-
26844-80-4	1	1	1	2,3′-Bipyridine, 5-methyl-
26855-40-3	0	1	0	Octadecanoic acid, diester with 1,2,3-propanetriol dihexadecanoate {dipalmitostearin}?
26856-30-4	1	0	0	Hexyne
26894-49-5	0	1	0	6*H*-Dibenzo[*b,d*]pyran-6-one, 3,7(3,9 or 7,9)-dihydroxy-9(7 or 3)-methoxy-1-methyl-
26895-04-5	1	0	0	2-Furancarboxaldehyde, methyl-
26897-24-5	0	1	0	Benzene, methoxymethyl- {two isomers detected}
26912-31-2	0	1	0	Butanoic acid, hexenyl ester
26914-16-9	1	0	0	Acridine, 9,10-dihydro-9,9-dimethyl-(1-methylethyl)-
26914-17-0	1	1	1	9*H*-Fluorene, methyl-
26914-18-1	1	0	0	Anthracene, methyl-
26915-12-8	1	0	0	Benzenamine, ar-methyl-
26927-07-1	0	1	0	β,β-Carotene-3,3′-diol, 5,6:5′,6′-diepoxy-5,5′,6,6′-tetrahydro-, (3S,3′S,5R,5′R,6S,6′S,9-*cis*)-
26952-14-7	0	1	0	Hexadecene
26952-23-8	0	1	0	1-Propene, 1,2-dichloro- {Telone®}
26955-76-0	0	1	0	9,19-Cyclolanostan-3-ol, 24,25-epoxy-, (3β)-
26991-67-3	1	1	1	2*H*-Pyran-2-one, tetrahydro-6-methyl- {δ-hexalactone, δ-caprolactone}
823-22-3				
26998-80-1	1	0	0	Phenol, trimethyl-
73850-02-9				
27008-60-2	0	1	0	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)- [2 CAS Nos.] {β-ionol}
22029-76-1				
27013-25-8	1	0	0	Benzene, 1,1′-(2,2-dichloroethylidene)bis[chloro-
27013-35-0	1	0	0	Cyclohexane, methyl-(1-methylethenyl)-
27043-34-1	1	0	0	Benzenemethanol, methyl-
27044-07-1 1899-29-2	0	1	0	Cyclohexanecarboxylic acid, 1,3,4-trihydroxy-5-[[3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propenyl]oxy]-, (1α,3α,4α,5β)- [2 CAS Nos.] {3-*O*-feruloylquinic acid} Also listed as cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, monoester with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, (1α,3α,4α,5β)-
27070-58-2	1	0	0	Octadecene
27071-84-7	0	1	0	9-Octadecenoic acid, diester with 1,2,3-propanetriol monohexadecanoate {palmitodiolein}
27096-03-3	1	0	0	5*H*-Tribenzo[*a,f,l*]trindene, 10,15-dihydro- {5*H*-diindeno[1,2-*a*:1′,2′-*c*]fluorene, truxene}
548-35-6				
27104-13-8	0	1	0	Octadecenoic acid, (*Z*)-
27133-93-3	1	0	0	1*H*-Indene, 2,3-dihydromethyl- {four isomers detected}
27134-13-0	1	0	0	9*H*-Fluoren-9-one, dimethyl {five isomers detected}
27134-14-1	1	0	0	Fluoren-9-one, ethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
27134-15-2	1	0	0	Fluoren-9-one, ethylmethyl-
27135-78-0	1	0	0	1*H*-Indene, tetramethyl- {at least four isomers present in MSS}
27137-10-6	1	0	0	Isotetradecanoic acid, methyl ester
27137-41-3	1	0	0	Furan, methyl-
27138-10-9	1	0	0	Benzene, ethenylethylmethyl-
77220-33-8				
27138-19-8	1	0	0	Naphthalene, ethyl-
27147-71-3	0	1	0	Hexadecanoic acid, 2-methyl-
27154-43-4	1	0	0	Piperidinone
27154-67-2	1	0	0	Pentanone
27175-64-0	1	1	1	Pyridine, dimethyl- {lutidine}
27178-34-3	1	0	0	Phenol, (1,1-dimethylethyl)-
27185-77-9	0	1	0	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-
27185-80-4	0	1	0	2-Cyclohexen-1-ol, 3-(3-hydroxy-1-butenyl)-2,4,4-trimethyl-
27195-67-1	1	1	1	Cyclohexane, dimethyl-
27208-37-3	1	0	0	Cyclopenta[*cd*]pyrene
27213-43-0	0	1	0	Octadecatrienoic acid, (*Z,Z,Z*)-
27234-05-5	0	1	0	Octadecenoic acid, methyl ester
27251-68-9	1	1	1	Pentadecene
27252-25-1	0	1	0	Furan, ethyl-
27252-26-2	0	1	0	Furan, propyl-
27257-15-4	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, 1-methyl- {7-azaindole, *N*-methyl-}
27293-93-2	0	1	0	Pyridine, 3-(1,3-dimethyl-2-pyrrolidinyl)-
27296-76-0	1	0	0	3-Pyridinol, 2,4-dimethyl-
27296-77-1	1	0	0	3-Pyridinol, 4,6-dimethyl-
27300-27-2	0	1	0	Ethanone, 1-[3-(3,4,5,6-tetrahydropyridinyl)]-
27323-28-0	1	1	1	1*H*-Indole, methyl-
27323-29-1	1	0	0	9*H*-Carbazole, methyl-
27341-45-3	1	0	0	Pyridinol
27342-88-7	1	0	0	Dodecanol
27358-28-7	1	0	0	Anthracene, trimethyl-
27378-74-1	0	1	0	Naphthalene, propyl-
27400-77-7	1	0	0	Nonadecene
27400-78-8	1	0	0	Eicosene
27400-79-9	1	0	0	Heneicosene
27406-77-5	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3-methyl-
27410-97-5	1	0	0	1(2*H*)-Naphthalenone, 3,4-dihydro-4,5,7-trimethyl-
27417-39-6	1	0	0	1*H*-Pyrrole, methyl-
27442-42-8	0	1	0	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-, 5-(dihydrogen phosphate)
27505-78-8	1	0	0	1*H*-Indole, 2,3,7-trimethyl-
27516-53-6	1	0	0	Pentenoic acid
27519-02-4	0	1	0	9-Tricosene
27538-09-6	0	1	0	3(2*H*)-Furanone, 3-ethyl-4-hydroxy-5-methyl-
27548-56-7	0	1	0	3-Benzoxepin-7-methanol, 5a,6,7,8,9,9a-hexahydro-α,α,5,9a-tetramethyl-, (5aα,7α,9aα)-(–)-
27554-19-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-glucosyl]oxy]-5,7-dihydroxy-2-(4-hydroxy phenyl)-
27554-26-3	1	1	1	1,2-Benzenedicarboxylic acid, bis(6-methylheptyl) ester [2 CAS Nos.] {diisooctyl phthalate}
131-20-4				
27576-03-0	1	0	0	Benzene, ethenyl-dimethyl-
27577-90-8	1	0	0	Pyrene, methyl- {several isomers in MSS}
27582-20-3	1	0	0	1*H*-Imidazo[4,5-*b*]pyridine, 7-methyl-
27593-23-3	0	1	0	2*H*-Pyran-2-one, 6-pentyl- {6-amyl-α-pyrone}
27598-81-8	1	0	0	Benzene, dimethoxy-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
27601-00-9	1	0	0	Quinoline, methyl-
27610-27-1	1	1	1	2(3*H*)-Furanone, dihydro-5-(1-hydroxyethyl)-
27610-38-4	1	1	1	Pyrazine, 2-(2-furanyl)-5-methyl-
27656-76-4	0	1	0	2,3-Naphthalenediol, 1,2α,3β,4,5,6,7,8-octahydro-7α-isopropenyl-1α-methyl-
27664-65-9	0	1	0	ψ,ψ-Carotene, 7,7′,8,8′,11,12-hexahydro- {phytofluene}
540-05-6				
27744-95-2	1	0	0	Oxazole, 4-methyl-5-propyl-
27770-23-6	1	0	0	2,4-Oxazolidinedione, 5-methyl-
27783-00-2	1	1	1	6-Oxabicyclo[3.2.1]octan-7-one, 1,3,4-trihydroxy-, (exo,exo)-
27816-52-0	1	0	0	1*H*-Indole, 1,4-dimethyl-
27816-53-1	1	0	0	1*H*-Indole, 1,5-dimethyl-
27817-67-0	1	0	0	1-Propene, 3-(propylthio)-
27836-87-9	0	1	0	Isopentadecanoic acid
27936-34-1	1	0	0	9,10-Anthracenedione, methyl-
27936-41-0	0	1	0	Pentanoic acid, methyl-
27987-10-6	1	1	1	Pyridine, ethyl methyl- {four isomers}
27987-13-9	1	0	0	Benzene, chloromethyl-
27992-31-0	1	0	0	2-Pyridinol, 5,6-dimethyl-
28013-11-8	1	1	1	1,1′-Biphenyl, ar,ar′-dimethyl-
28017-62-1	1	0	0	2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-
28039-99-8	0	1	0	Hexadecenoic acid, (Z)-
28056-87-3	1	0	0	1-Hexanamine, 2-ethyl-*N,N*-dimethyl-
28059-64-5	1	0	0	Benzenamine, ?-phenylmethyl- {aniline, ?-benzyl-}
28061-47-4	0	1	0	Octadecadienoic acid, methyl ester
28069-72-9	0	1	0	2,6-Nonadien-1-ol, (*E,Z*)-
28098-80-8	0	1	0	2-Butenedioic acid, 2-ethyl-3-methyl-, (*E*)-
28098-82-0	0	1	0	2,5-Pyrrolidinedione, 3-ethylidene-4-methyl-, (*E*)-
28106-30-1	1	0	0	Benzene, ethenylethyl-
28115-37-9	1	0	0	2-Pyrrolidinemethanol, 5-methyl-, *cis*-
28217-95-0	1	0	0	Pyrazine, 2-phenylmethyl-
28231-03-0	0	1	0	Cedrenol
28258-64-2	1	0	0	Naphthalenamine, *N*-phenyl-
28261-03-2	0	1	0	Hexenol
28261-54-3	1	0	0	Pyrrolidinone
28343-22-8	1	1	1	Phenol, 2,6-dimethoxy-4-ethenyl-
28350-87-0	1	0	0	1*H*-Pyrrole, dihydro- {pyrroline}
28351-04-4	1	0	0	Quinoline, dimethyl-
28368-08-3	0	1	0	β,ε-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,6′R)-
28384-26-1	0	1	0	1-Butanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
28401-39-0	0	1	0	6,8-Dioxabicyclo[3.2.1]octane, 1,5-dimethyl- {frontalin}
28409-91-8	0	1	0	9,12-Octadecadienoic acid-, diester with 1,2,3-propanetriol mono-9-octadecenoate {oleodilinolein}?
28409-94-1	0	1	0	9-Octadecenoic acid-, monoester with 1,2,3-propanetriol dihexadecanoate {dipalmitoolein}
28446-58-4	1	0	0	3-Butenamide
28467-88-1	1	0	0	2-Hexenal, 2-methyl-
28473-29-2	1	0	0	Cyclopentanedione {two isomers}
28522-57-8	1	0	0	Tricycloquinazoline, 3-methyl-
28542-78-1	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-
28564-83-2	1	1	1	4*H*-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
28570-28-7	1	1	1	Octacosanoic acid, tetradecyl ester
28631-77-8	1	0	0	Pyridine, ethyl-
28631-88-1	1	0	0	Cyclopentanone, methyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
28638-58-6	1	0	0	Cyclopentene, 1-ethenyl-
28641-62-5	1	0	0	5*H*-Dibenzo[*c,g*]carbazole
28652-72-4	1	1	1	1,1′-Biphenyl, methyl-
28652-74-6	1	1	1	Naphthalene, tetramethyl- {at least four isomers in MSS}
28652-77-9	1	1	1	Naphthalene, trimethyl- {at least 10 isomers in MSS}
28664-35-9	0	1	0	2(5*H*)-Furanone, 3-hydroxy-4,5-dimethyl-
28679-05-2	0	1	0	Eicosanol
28712-62-1	1	0	0	Quinoline, 3-methyl-5,6,7,8-tetrahydro-
28715-26-6	1	0	0	Benzofuran, 2,3-dimethyl-
28729-54-6	1	0	0	Benzene, methylpropyl-
28743-04-6	1	1	1	2*H*-Pyran-3(4*H*)-one
28750-51-8	1	1	1	3-Cyclopentene-1,2-dione
28761-27-5	1	0	0	Undecene
28777-67-5	1	0	0	Hexane, dimethyl-
28779-32-0	1	0	0	Pyrene, dihydro-
28790-86-5	1	0	0	2-Cyclopenten-1-one, 2,3,4-trimethyl-
28801-93-6	1	1	1	Hexadecanoic acid, methyl-
28802-49-5	1	0	0	Furan, dimethyl-
28804-88-8	1	1	1	Naphthalene, dimethyl-
28843-39-2	1	0	0	2,5-Furandione, 3,4-diethyl-
28880-78-6	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol bis[(*Z*)-9-octadecenoate]
28882-68-0	1	0	0	Pyrrolidinecarboxylic acid
28902-93-4	0	1	0	Lysine, hydroxy-
1190-94-9				
28905-07-9	0	1	0	α-*D*-Glucuronic acid, methyl ester
28905-12-6	1	1	1	β-*D*-Glucose
28930-19-0	1	0	0	1,2-Benzenediol, methyl-
28930-20-3	1	0	0	1,2-Benzenediol, ethyl-
28949-66-8	0	1	0	Stigmasta-5,24-dien-3-ol, (β)-
28962-27-8	1	0	0	Octenoic acid
28965-86-8	1	0	0	Benzoic acid, hydroxymethyl-
28973-74-2	1	1	1	9,12,15-Octadecatrienoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecatrienoate}
28977-67-5	1	1	1	β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylvalerate) β-*D*-Glucopyranose, 6-acetate 2,3,4-tris((+)-3-methylpentanoate)
28982-58-3	1	0	0	Cyclopentenone
28984-67-0	1	1	1	Heneicosenoic acid
28984-77-2	0	1	0	Octadecadienoic acid, (Z,Z)-
29011-62-9	1	0	0	Pyridine, dimethylethenyl-
29031-84-3	1	0	0	1,2-Benzenediol, propyl-
29036-02-0	1	0	0	Quaterphenyl
29036-25-7	1	0	0	1*H*-Indene, methyl- {at least three isomers are present in MSS}
29044-06-2	0	1	0	2,5-Hexanediol, 2-methyl-
29062-95-1	1	0	0	Dibenzofuran, dimethyl-
29062-98-4	1	0	0	Phenanthrene, dimethyl-
29063-00-1	1	0	0	Anthracene, dimethyl-
29093-90-1	0	1	0	5-Undecen-2-one, 10-hydroxy-6,10-dimethyl-
29118-61-4	0	1	0	*D*-Fructose, 1-(2-carboxy-1-pyrrolidinyl)-1-deoxy-, (S)-
29134-29-0	1	0	0	1-Pyrrolidineacetonitrile
29144-38-5	1	1	1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, acetate, stereoisomer {solanesyl
58000-93-4				acetate}
29210-91-1	1	0	0	2(1*H*)-Naphthalenone, 3,4-dihydro-4,4,7-trimethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
29224-55-3	1	0	0	Benzene, dimethylethyl-
29232-93-7	0	1	0	Phosphorothioic acid, *O*-[2-(diethylamino)-6-methyl-4-pyrimidinyl] *O*,*O*-dimethyl ester {Pirimiphos-methyl®}
29239-89-2	1	0	0	1*H*-Imidazole, 4-ethyl-2-methyl-
29253-36-9	1	1	1	Naphthalene, (1-methylethyl)-
29275-82-9	1	0	0	Phenol, 2-methoxy-6-(1-propenyl)-, (*Z*)-
29275-83-0	1	0	0	Phenol, 2-methoxy-6-(1-propenyl)-, (*E*)-
29344-95-4	0	1	0	Benzaldehyde, 2,3,4,5-tetramethyl-
29348-63-8	1	0	0	1*H*-Indene, dimethyl-
29350-67-2	1	1	1	2,3-Butanedione [2 CAS Nos.] {diacetyl, biacetyl}
431-03-8				
29350-73-0	0	1	0	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)- {δ-cadinene}
29393-32-6	1	1	1	2(3*H*)-Furanone, 5-acetyldihydro-
29414-56-0	1	0	0	1,5,7-Octatrien-3-ol, 2,6-dimethyl-
29444-46-0	1	0	0	Pyrazine, 2-methyl-6-propyl-
29444-53-9	1	0	0	Pyrazine, 2-methyl-3-phenyl-
29460-90-0	0	1	0	Pyrazine, (1-methylethyl)-
29460-91-1	1	0	0	Pyrazine, butyl-
29460-93-3	1	1	1	Pyrazine, 2-(2-butenyl)-
29460-97-7	1	1	1	Pyrazine, phenyl-
29460-98-8	1	1	1	Pyrazine, 3-furanyl-
29461-03-8	1	0	0	Pyrazine, 2-methyl-5-propyl-
29461-10-7	1	0	0	Pyrazine, 2-(3-furanyl)-5-methyl-
29472-68-2	0	1	0	β,β-Carotene-3,3′-diol {zeaxanthin}
29484-46-6	0	1	0	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl-, [2S-(2α,4aβ,8aβ)]-
29548-30-9	1	1	1	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, acetate {farnesyl acetate}
29553-51-3	1	0	0	2,6-Piperidinedione, 3-methyl-
29554-26-5	0	1	0	2-Propenamide, *N*-(4-aminobutyl)-3-(3,4-dihydroxyphenyl)- {caffeoylputrescine}
29564-66-7	0	1	0	Docosadienoic acid, (*Z*,*Z*)-
29565-44-4	0	1	0	Octadecatrienoic acid, methyl ester
29584-92-7	1	0	0	Oxazole, 5-ethyl-4-methyl-
29590-02-1	0	1	0	9,12-Octadecadienoic acid-, diester with 1,2,3-propanetriol monooctadecanoate {stearodilinolein}
29611-84-5	1	1	1	Pyridine, trimethyl- {collidine}
29709-08-8	1	1	1	Heptadecanoic acid, 15-methyl-
29720-92-1	1	1	1	1*H*-Pyrrole-2,5-dione, ethylmethyl-
29730-67-4	1	0	0	Docosene
29732-48-7	0	1	0	Flavylium, 3-[[*O*-(6-deoxymannosyl)-*D*-glucosyl]oxy]-3′,4′,5,5′,7-pentahydroxy-, chloride
29736-33-2	0	1	0	2-Buten-1-ol, 2-methyl-4-[[2-(methylthio)-1*H*-purin-6-yl]amino]-, (*E*)-
29752-43-0	0	1	0	6*H*-Dibenzo[*b*,*d*]pyran-6-one, 9-methoxy-4a-methyl-2,3,4,4a-tetrahydro-2,3,7-trihydroxy- (2α,3β,4aβ)-
29760-89-2	1	0	0	Phenol, 3-ethyl-2-methoxy-
29790-29-2	0	1	0	2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-, (1*E*)-
29797-09-9	1	0	0	Cyclohexadiene
29798-72-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-butyl)-
29798-73-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylpropyl)-
29813-44-3	1	1	1	1*H*-Pyrrole-2-carboxaldehyde, 5-(hydroxymethyl)-1-methyl-
29828-28-2	1	0	0	Naphthalene, dihydro-
29832-78-8	1	0	0	Isoquinoline, tetrahydro-
29833-69-0	1	1	1	1-Pentadecene, 2-methyl-
29848-46-2	1	0	0	3-Furanol, tetrahydro-5,5-dimethyl-
29859-91-4	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxy-*L*-mannosyl)-*D*-galactosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-
29887-60-3	0	1	0	Cyclohexane, 1,2-dimethoxy-, (*E*)
29930-57-2	1	0	0	1*H*-Indole, dimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
29943-42-8	1	0	0	4*H*-Pyran-4-one, tetrahydro-
29960-49-4	0	1	0	Hexadecenoic acid, methyl ester
29961-54-4	0	1	0	Hexadecadienoic acid, methyl ester
29968-14-7	1	0	0	Quinoline, dihydro-
29973-13-5	0	1	0	Methylcarbamic acid, 2-((ethylthio)methyl)phenyl ester {Ethiofencarb®}
29988-76-9	1	1	1	Furancarboxamide
30084-91-4	1	0	0	1*H*-Indene-5-carboxaldehyde, 2,3-dihydro-
30086-02-3	0	1	0	3,5-Octadien-2-one, (*E,E*)-
30221-44-4	0	1	0	1-Hexadecene, 3,7,11,15-tetramethyl- {phytene 1}
30230-52-5	1	0	0	Phenol, ethylmethyl-
30232-26-9	1	0	0	Phenanthrene, trimethyl- {at least three isomers in MSS}
30233-85-3	1	0	0	Cyclopentene, ethyl-
30256-45-2	1	0	0	Pyridine, 4-methyl-2-propyl-
30283-95-5	0	1	0	Picene, methyl-
30286-23-8	1	0	0	Indenone, dihydro-
30303-65-2	0	1	0	Docosanol
30304-58-6	1	0	0	1*H*-Benzimidazole, methyl-
30310-80-6	0	1	0	*L*-Proline, 4-hydroxy-1-nitroso-, *trans*- {NHPRO}
30310-81-7	1	1	1	2-Piperidinecarboxylic acid, 1-nitroso- {*N*-nitrosopipecolic acid (NPIC)}
4515-18-8				
30311-61-6	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-
30315-34-5	0	1	0	2-Pyridinamine, 5-(1-methyl-2-pyrrolidinyl)-, (S)-
30316-22-4	1	0	0	1-Naphthalenol, 1,2,3,4-tetrahydro-3,5,8-trimethyl-
30316-36-0	0	1	0	Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-
30326-99-9	1	0	0	Tricosenoic acid
30364-38-6	1	1	1	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-
30390-50-2	0	1	0	4-Decenal
30402-14-3	1	0	0	Dibenzofuran, tetrachloro-
30402-15-4	1	0	0	Dibenzofuran, pentachloro-
30414-55-2	0	1	0	Hexanoic acid, 5-methyl-3-oxo-, methyl ester
30414-57-4	0	1	0	6-Heptenoic acid, 3-oxo-, methyl ester
30434-64-1	1	0	0	2-Cyclopenten-1-one, 3,4-dimethyl-
30434-65-2	0	1	0	2-Cyclopenten-1-one, 3,4,4-trimethyl-
30434-68-5	1	0	0	2-Cyclopenten-1-one, 4-ethyl-3-methyl-
30450-17-0	0	1	0	Naphtho[2,1-*b*]furan-2(1*H*)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aS- (3aα,5aα,9aβ,9bα)]-
30452-68-7	1	0	0	9,12,15-Octadecatrienoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E,Z,Z,Z*)]]-
30498-64-7	1	0	0	Cyclopentane, trimethyl-
30533-08-5	1	0	0	Ethanamine, *N*,1-dimethyl-*N*-nitroso-
30551-31-6	1	0	0	Pentacosene
30560-19-1	0	1	0	Phosphoramidothioic acid, *N*-acetyl-, *O*,S-dimethyl ester {Orthene®, Acephate®}
30567-26-1	1	0	0	2-Heptenal, 2-methy-
56161-68-3				
30581-97-6	1	0	0	1,1′-Biphenyl, trimethyl- {three isomers detected}
30582-01-5	1	1	1	9*H*-Fluorene, dimethyl- {at least five isomers in MSS}
30582-02-6	1	0	0	9*H*-Fluorene, trimethyl-
30582-03-7	1	0	0	Pyrene, dimethyl- {at least three isomers in MSS}
30642-36-5	1	0	0	1*H*-Indole, trimethyl-
30642-38-7	1	0	0	9*H*-Carbazole, dimethyl-
30677-34-0	1	0	0	Cyclohexane, ethylmethyl-
30743-41-0	0	1	0	β,β-Carotene, 6,7-didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-3,3′,5-trihydroxy-, (3S,3′S,5R,5′R,6R,6′S)-
30777-18-5	1	0	0	Benzo[*a*]fluorene

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
243-18-5	1	0	0	5*H*-Benzo[*b*]fluorene
30777-19-6				
30790-23-9	0	1	0	Tetradecatrienoic acid
30810-51-6	0	1	0	1,2,3-Propanetricarboxylic acid, 1-hydroxy- {isocitric acid}
30889-50-0	1	0	0	2-Naphthalenol, 3,5,8-trimethyl-
30907-88-1	0	1	0	6*H*-Benzo[*c*]pyrido[3,2,1-*jk*]carbazole
30917-33-0	1	0	0	1,3-Hexadecadiene, 2,6,10,14-tetramethyl-
100210-90-0				
30923-59-2	0	1	0	Benzenemethanol, 2-hydroxy-, α-benzoate
30934-97-5	1	0	0	Ethanol, 2,2-dimethoxy-
30987-48-5	0	1	0	Spiro[furan-2(3*H*),2′(1′*H*)-naphtho[2,1-*b*]furan]-5(4*H*)-one, decahydro-3,3′a,6′,6′,9′a-pentamethyl- {α-levantenolide}
5989-24-2				
30995-64-3	1	1	1	Dibenzothiophene, methyl- {at least four isomers detected}
30997-38-7	1	0	0	Phenanthrene, ethyl-
30997-39-8	1	0	0	Fluoranthene, methyl-
31032-91-4	1	1	1	Naphthalene, 1-ethyl-6-methyl-
31032-92-5	1	1	1	Naphthalene, 1-ethyl-7-methyl-
31032-94-7	1	1	1	Naphthalene, 2-ethyl-3-methyl-
31082-90-3	1	0	0	2-Propenoic acid, 3-(2,3-dihydroxyphenyl)-
31089-17-5	1	0	0	2-Cyclopenten-1-one, 2-methyl-5-(1-methylethyl)-
31093-11-5	1	0	0	Benzenamine, ar,ar,ar-trimethyl-
31093-57-9	1	0	0	Furan, ethenyl-
31103-86-3	1	1	1	Mannose
31105-02-9	0	1	0	*L*-Aspartic acid *N*-(1-deoxy-*D*-fructos-1-yl)-
31105-03-0	0	1	0	*L*-Phenylalanine, *N*-(1-deoxy-*D*-fructos-1-yl)-
31110-30-2	1	0	0	2-Butenamide, (*Z*)-
31135-62-3	1	0	0	Quinolinamine
31149-06-1	0	1	0	2-Naphthalenol, 1-[5-(acetyloxy)-3-methyl-3-pentenyl]decahydro-2,5,5,8a-tetramethyl-, [1R-[1α(*E*),2β,4aβ,8aα]]-
31162-45-5	1	1	1	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butynyl)-3,5,5-trimethyl- [2 CAS Nos.]
58023-72-6				
31178-70-8	0	1	0	α-*D*-Xylose
31178-71-9	0	1	0	β-*d*-Xylose
31212-21-2	0	1	0	1*H*-Indoleacetamide
31253-95-9	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)
31257-96-2	1	0	0	Phenol, ethenyl-
31291-71-1	1	1	1	Naphthalene, methyl-1,2,3,4-tetrahydro-
31297-30-0	1	0	0	2,3-Benzofurandione, 2,3-dihydro-4,7-dimethyl-
31388-09-7	1	0	0	Pyridine, butyl-
31391-42-1	1	0	0	Naphthalene, ethylmethyl-
31393-23-4	1	0	0	Benzo[*b*]thiophene, methyl- {four isomers reported}
31422-28-3	0	1	0	Pentadecenoic acid, methyl ester
31424-04-1	1	0	0	Pentenal
31424-16-5	0	1	0	Heptadecenoic acid, methyl ester
31501-11-8	0	1	0	Hexanoic acid, *cis*-3-hexenyl ester
31502-14-4	0	1	0	2-Nonen-1-ol
31519-22-9	0	1	0	2-Naphthalenecarboxylic acid, 1,4-dihydroxy-
31556-45-3	1	1	1	Octadecanoic acid, tridecyl ester
31577-86-3	0	1	0	Ethanone, 1-[3-(1-methylethenyl)cyclopentyl]- [2 CAS Nos.] {two isomers}
43219-68-7				
31613-73-7	0	1	0	5-Undecene, 5-methyl-
31615-93-7	1	1	1	Stigmasta-5,22-dien-3-ol, 9-octadecenoate, [3β(*Z*),22*E*]- {stigmasteryl oleate}

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
31632-62-9	1	0	0	Benz[*a*]anthracene, ethyl-
31642-67-8	0	1	0	8-Nonenoic acid
31704-79-7	1	0	0	2-Propenal, 2-methyl-3-(5-methyl-2-furanyl)-
31711-53-2	1	1	1	Phenanthrene, methyl-
31831-35-3	0	1	0	Naphthalene, diethyl-
31883-01-9	1	0	0	Thiazole, 5-ethyl-4-methyl-
31927-64-7	1	0	0	Dibenzo[*def,mno*]chrysene, 6-methyl-
31983-22-9	0	1	0	Naphthalene, 4,7-dimethyl-1,2,4a,5,6,8a-hexahydro-1-(1-methylethyl)- {α-muurolene}
32040-41-8	0	1	0	2-Butenoic acid, 4-(formylamino)-4-oxo-, (Z)-
32073-24-8	1	0	0	Phenol, 2-methoxy-propyl-
32142-31-7	0	1	0	Benzoic acid, 4-(β-*D*-glucopyranosyloxy)-3-methoxy-
32184-51-3	1	1	1	Pyrazine, 2-cyclopentyl-6-methyl-
32190-57-1	0	1	0	*L*-Threonine, *N*-[2-amino-4-(3-hydroxy-2-oxo-3-azetidinyl)-1-oxobutyl]-
32214-82-7	1	1	1	β-*D*-Glucopyranoside, (3β)-ergost-5-en-3-yl- {campesteryl glucoside}
32214-91-8	0	1	0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, acetate {β-caryophyllene acetate}
32222-21-2	0	1	0	Androsta-3,5-dien-7-one
32272-48-3	1	0	0	Thiazole, 4-ethyl-2-methyl-
32272-49-4	1	0	0	Thiazole, 2,4-diethyl-
32304-17-9	1	1	1	5,9,13,17,21,25-Heptacosahexaen-2-one, 6,10,14,18,22,26-hexamethyl-, (all-*E*)-
32378-60-2	0	1	0	Pregnan-20-one, 3-[(1-oxohexadecyl)oxy]-, (3β,5α)-
32389-40-5	0	1	0	Pyrrolidinecarboxylic acid, oxo-, (S)-
32391-38-1	1	1	1	Phenol, methoxymethyl-
32449-92-6	0	1	0	*D*-Glucurono-3,6-lactone
32529-53-6	1	1	1	2-Furancarboxaldehyde, 5-acetyl-
32536-43-9	0	1	0	1*H*-Indoleacetic acid
32736-91-7	1	0	0	Pyrazine, 2,5-diethyl-3-methyl-
32736-95-1	1	1	1	Pyrazine, 2-furanyl-
32737-01-2	1	1	1	Pyrazine, 2-(2-furanyl)-3-methyl-
32737-03-4	1	1	1	Pyrazine, 2-(2-furanyl)-6-methyl-
32737-06-7	1	0	0	Pyrazine, 2-methyl-3-(3-methylbutyl)-
32740-01-5	1	0	0	Benz[*c*]acridine, 7,11-dimethyl-
32743-35-4	1	0	0	2-Pyridinecarboxamide, 4-ethyl-
32793-37-6	1	0	0	2-Butenamide, 2-methyl-
32809-16-8	0	1	0	1,2-Cyclopropanedicarboximide, *N* (3,5-dichlorophenyl)-1,2-dimethyl- {Procymidone®}
32811-40-8	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*E*)-
32821-70-8	0	1	0	2*H*-Pyran-2-one, tetrahydro-3-(1-methylethyl)-
32833-96-8	0	1	0	Acetic acid, (dimethylamino)oxo-
32839-24-0	0	1	0	Hexadecatrienoic acid, (*Z,Z,Z*)-
32974-92-8	0	1	0	Ethanone, 1-(5-ethylpyrazinyl)-
33073-01-7	1	0	0	1*H*-Purine-2,6-dione, 3,9-dihydro-1,9-dimethyl-
33124-69-5	0	1	0	threo-2,3-Hexodiulosonic acid, γ-lactone {2,3-diketogulonic acid, γ-lactone}
33213-65-9	1	1	1	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aα,6β,9β,9aα)- {β-Endosulfan®}
33240-56-1	1	0	0	Hexane, 1-chloro-5-methyl-
33318-74-0	1	0	0	Oxazole, 2,4-dimethyl-5-ethyl-
33320-27-3	1	0	0	1,3-Cyclopentadiene-1-carboxaldehyde
33342-48-2	1	0	0	2-Furancarboxaldehyde, 3-methyl-
33393-93-0	1	1	1	Benzenepropanoic acid, 3-hydroxy-
621-54-5				
33414-49-2	1	0	0	Ethanone, 1-(3-hydroxy-4-methylphenyl)-
33425-47-7	1	0	0	2,5-Pyrrolidinedione, 3,4-dimethyl-
33467-73-1	0	1	0	3-Hexen-1-ol, formate, (*Z*)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
33467-76-4	0	1	0	2-Hepten-1-ol (*E*)
33488-51-6	1	1	1	2(5*H*)-Furanone, 3,4,5-trimethyl-
33504-66-4	1	0	0	Pyrazine, ethylmethyl-
33527-93-4	1	0	0	Pyrrolidine, 1-(1-oxobutyl)-
33543-31-6	1	1	1	Fluoranthene, 2-methyl-
33601-06-8	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-, (R)-(+)-
33629-47-9	0	1	0	Benzenamine, 4-(1,1-dimethylethyl)-2,6-dinitro-*N*-(1-methylpropyl)- {Butralin®}
33691-73-5	1	0	0	2*H*-Pyran-2-one, tetrahydro-5-hydroxy-
33698-49-6	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methylbutyl)-
33698-87-2	1	0	0	3-Pentenoic acid, (*Z*)-
33759-63-6	0	1	0	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-
33765-37-6	0	1	0	2,5-Furandione, 3,4-diethyldihydro-, (*E*)-
33774-71-9	1	1	1	Benzaldehyde, dihydroxy-
33794-61-5	1	0	0	3(2*H*)-Furanone, dihydro-2,5-dimethyl-, (*Z*)-
33818-21-2	1	0	0	α-*D*-Galactofuranose, 1,6-anhydro-
33820-53-0	0	1	0	Benzenamine, 2,6-dinitro-*N,N*-dipropyl-4-(1-methylethyl)- {Isopropalin®}
33860-48-9	0	1	0	Ergost-8-en-3-ol, 14-methyl-, (3β,5α)-
33880-83-0	0	1	0	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, (1α,2β,4β)-
33886-74-7	0	1	0	Ergosta-8,24(28)-dien-3-ol, 14-methyl-, (3β,5α)-
33909-95-4	1	0	0	3(2*H*)-Furanone, dihydro-2,5-dimethyl-, (*E*)-
33942-93-7	1	0	0	Benz[*c*]acridine, 9-methyl-
33978-17-5	0	1	0	1-Benzopyrylium, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-, chloride
33986-27-5	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, 3-methyl-*N*-(3-methyl-2-butenyl)-
33986-28-6	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methylbutyl)-
34044-64-9	0	1	0	1,5,9,13,17,21,25,29,33-Pentatriacontanonaene, 2,6,10,14,18,22, 26,30,34-nonamethyl- {norsolanesene}
34786-54-4				
34047-39-7	1	1	1	2-Butanone, 4-(methylthio)-
34083-18-6	1	0	0	2,6,10,14-Hexadecatetraene, 2,6,10,14-tetramethyl-
34098-52-7	0	1	0	*D*-xylo-Hept-2-enaric acid, 2,6-anhydro-3-deoxy- {2*H*-pyran-2,4-dicarboxylic acid, 3,4-dihydro-3,4-dihydroxy-}
34136-53-3	0	1	0	2-Propenamide, *N*-(4-aminobutyl)-3-(4-hydroxyphenyl)-
34136-57-7	1	0	0	Benzonitrile, 3-ethyl-
34136-59-9	1	0	0	Benzonitrile, 2-ethyl-
34137-25-2	1	1	1	Stigmast-5-en-3-ol, octadecanoate, (3β)- {β-sitosteryl stearate}
34137-26-3	0	1	0	Pyridine, 5-fluoro-3-(1-methyl-2-pyrrolidinyl)-, (S)-
34150-36-2	0	1	0	*D*-Galacturonic acid, anhydro-
34214-77-2	1	1	1	Cyclohexanecarboxylic acid, 4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,3,5-trihydroxy-, (1α,3α,4α,5β)-
34232-31-0	0	1	0	1*H*-Pyrazolo[4,3-*d*]pyrimidin-7-amine, *N*-(3-methyl-2-butenyl)-
34314-83-5	1	1	1	Furan, 2,3-dihydro-4-methyl-
34318-21-3	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- {4-keto-α-ionol, 4-oxo-α-ionol}
65017-80-3				
34336-18-0	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-
34347-58-5	0	1	0	9,19-Cycloergostan-3-ol, 14-methyl-, (3β,5α,9β)-
34347-65-4	0	1	0	Stigmasta-8,14-dien-3-ol, (3β,5α)-
34350-85-1	0	1	0	Stigmasta-8,14,24(28)-trien-3-ol, (3β,5α)-
34366-21-7	1	0	0	Pyridine, 3-(2-piperidinyl)-, (R)- {*d*-anabasine}
34375-89-8	1	0	0	Pyrrolidine, 3-methyl-
34393-22-1	0	1	0	*L*-Tyrosine, *N*-(1-deoxy-*D*-fructos-1-yl)-
34393-27-6	0	1	0	*D*-Fructose, 1-[(3-amino-1-carboxy-3-oxopropyl)amino]-1-deoxy-, (S)-
34413-35-9	1	1	1	Quinoxaline, 5,6,7,8-tetrahydro-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
34419-76-6	1	1	1	1-Propanamine, *N*,2-dimethyl-*N*-nitroso- [2 CAS Nos.]
2504-18-9				
34425-19-9	1	0	0	Isotriacontane
34441-14-0	0	1	0	1-Azetidinebutanoic acid, α-[(3-amino-3-carboxypropyl)amino]-2-carboxy-, [2S-[1[αR*(R*)],2R*]]- {nicotianamine}
34442-52-9	1	0	0	1*H*-Dibenzo[*a,c*]carbazole
34443-88-4	0	1	0	9,19-Cycloergost-24(28)-en-3-ol, 14-methyl-, (3β,5α)-
34465-46-8	1	0	0	Dibenzo[*b,e*][1,4]dioxin, hexachloro-
34514-52-8	1	0	0	Pyrazine, methyl(1-methylethyl)-
34521-51-2	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dioctadecanoate
34522-32-2	0	1	0	Arginine, *N*2-(1-carboxyethyl)- [2 CAS Nos.]
1069-09-6				
34540-66-4	0	1	0	Naphthalene, methylpropyl-
34598-80-6	1	0	0	1,3-Cyclopentanedione, 2,4-dimethyl-
34671-89-1	1	0	0	2,3′-Bipyridine, 5-ethyl-
34764-22-2	1	0	0	Butanal, 3,4-dihydroxy-
34786-54-4	0	1	0	1,5,9,13,17,21,25,29,33-Pentatriacontanonaene, 2,6,10,14,18,22, 26,30,34-nonamethyl- {norsolanesene}
34044-64-9				
34879-87-3	0	1	0	1*H*-Indazole, 1,6-dimethyl-
34883-01-7	1	1	1	Phenol, 2,3-dimethyl-5-methoxy-
34916-78-4	1	0	0	4(1*H*)-Pyrimidinone, 5,6-dimethyl- = 6-pyrimidinol, 4,5-dimethyl-
34939-17-8	1	0	0	2(1*H*)-Pyrimidinone, 4,5-dimethyl- = 2-pyrimidinol, 4,5-dimethyl-
34945-05-6	1	0	0	2(3*H*)-Furanone, dihydro-4-hydroxy-4-methyl-
35044-68-9	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)- [3 CAS Nos.] {damascene}
80111-68-8				
23770-92-3				
35194-36-6	1	1	1	4-Hexenoic acid
35194-37-7	1	1	1	4-Heptenoic acid
35256-85-0	0	1	0	Propanamide, dimethyl-*N*-(1-methylethyl)-*N*-(phenylmethyl) {Butam®}
35285-68-8	0	1	0	Benzoic acid, 4-hydroxy-, ethyl ester, sodium salt
35285-69-9	0	1	0	Benzoic acid, 4-hydroxy-, propyl ester, sodium salt
35322-84-0	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-3,4,7-trimethyl-
35323-45-6	0	1	0	Pyridinium, 3-carboxy-1-β-*D*-glucopyranosyl-, hydroxide {trigonelline}
35355-35-2	0	1	0	Benzofuran, 5-methoxy-6,7-dimethyl-
35367-38-5	1	1	1	Urea, 1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)- {Diflubenzuron®}
35381-83-0	0	1	0	Galactose, diether with 1,2,3-propanetriol (1:2)
35392-77-9	0	1	0	Butanedioic acid, 2,3-diethyl-, (R*,R*)-(±)- {succinic acid, 2,3-diethyl-}
35543-25-0	1	0	0	1-Pyrrolidinebutyronitrile
35549-47-4	1	0	0	2-Pyridinepropanenitrile
35576-91-1	1	0	0	Nitrosamide
35602-69-8	0	1	0	Cholest-5-en-3-ol (3β)-, octadecanoate, (3β,22*E*)- {cholesteryl stearate}
35656-49-6	0	1	0	1*H*-Indolepropanoic acid, α-oxo-
35674-33-0	0	1	0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-4-methyl-3-oxo-
35688-48-3	0	1	0	*D*-Serine, *N*-(carboxyacetyl)-
35692-98-9	0	1	0	2-Cyclohexene-1,4-dione, 2-hydroxy-3,5,5-trimethyl-
35694-08-7	1	0	0	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′-octachloro-
35734-61-3	1	1	1	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-
35734-62-4	1	0	0	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-
35737-86-1	1	0	0	Naphthalene, 2-ethenyl-1-methyl-
35794-11-7	1	0	0	Piperidine, 3,5-dimethyl-
35822-46-9	1	1	1	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,8-heptachloro-
35897-16-6	0	1	0	Acetic acid, 2-methyl-3-pentyl ester
35909-01-4	1	1	1	*L*-Proline, 1-nitroso-, methyl ester

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
35951-50-9	0	1	0	Spiro[4.5]decane-6-carboxaldehyde, 8-hydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,10β]]-
35953-18-5	1	0	0	2-Cyclopenten-1-one, 3-propyl-
35953-21-0	1	1	1	3-Nonene-2,8-dione, 5-(1-methylethyl)-, [S-(*E*)]- [2 CAS Nos.] {oxysolanone}
60619-46-7				
101159-09-5				
35953-53-8	1	0	0	2-Tetradecene, (*E*)-
35953-54-9	1	0	0	2-Tetradecene, (*Z*)-
35980-18-8	1	0	0	Pyrene, 1-butyl-
36078-10-1	1	1	1	9-Octadecenoic acid (*Z*)-, dodecyl ester
36088-22-9	1	0	0	Dibenzo[*b,e*][1,4]dioxin, pentachloro-
36119-15-0	0	1	0	*D*-Fructose, mono(dihydrogen phosphate)
36127-43-2	1	0	0	Pyridine, 3-(1,3,3-trimethyl-2-pyrrolidinylyl)-
36151-02-7	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl-, [R-(R*,R*)]-
36203-31-3	0	1	0	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-
515-00-4				
36211-21-9	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-
36232-37-8	1	0	0	6-Pentadecene, 2,6,10,14-tetramethyl-
36232-38-9	1	0	0	Hexadecane, 2,6,10-trimethyl-14-methylene-
36232-39-0	1	0	0	2-Heptadecene, 4-methylene-8,12,16-trimethyl-
36238-34-3	1	1	1	Pyrazine, 5-(2-furanyl)-2,3-dimethyl- = pyrazine, 2-(2-furanyl)-5,6-dimethyl-
36238-36-5	1	0	0	Pyridine, 2,4-dimethyl-5-(1-methylethyl)-
36267-71-7	0	1	0	Thieno(3,4-*d*)pyrimidine, 5,7-dihydro-2-methyl-
36330-90-2	1	0	0	2-Pyridinol, 3,4-dimethyl- {2(1*H*)-pyridinone, 3,4-dimethyl-}
95907-02-1				
36332-93-1	1	1	1	Eicosanoic acid, 18-methyl-
36332-94-2	1	1	1	Heneicosanoic acid, 19-methyl-
36332-95-3	0	1	0	Docosanoic acid, 20-methyl-
36332-96-4	1	1	1	Tricosanoic acid, 21-methyl-
36340-49-5	0	1	0	3-Buten-2-one, 4-(1,2-epoxy-2,6,6-trimethylcyclohexyl)-, (E)-
36357-32-1	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-methyl-, (3R-*trans*)-
19943-28-3				
36357-38-7	1	1	1	Ethanone, 1-(6-methyl-3-pyridinyl)-
36413-60-2	0	1	0	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, (1α,3α,4α,5β)-
36508-80-2	1	0	0	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-, 1-oxide {cotinine 1-oxide}
15569-85-4				
36541-17-0	1	0	0	Benzofuran, trimethyl-
36541-18-1	1	0	0	1*H*-Indene, 2,3-dihydrotrimethyl-
36541-21-6	1	0	0	Acenaphthylene, 1,2-dihydromethyl-
36541-24-9	1	0	0	Benzonitrile, dimethyl-
36541-26-1	1	0	0	Pyridinecarbonitrile, methyl-
36541-27-2	1	0	0	Pyridinecarbonitrile, dimethyl-
36541-30-7	1	0	0	Pyrazine, methylpropyl-
36556-06-6	1	0	0	Isoquinoline, 5,6,7,8-tetrahydro-
36588-48-4	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, octahydro-
6708-06-1				
36610-45-4	1	1	1	Octadecanoic acid, nonadecyl ester
36610-47-6	1	1	1	Nonadecanoic acid, tridecyl ester
36610-48-7	1	1	1	Nonadecanoic acid, tetradecyl ester
36610-49-8	1	1	1	Nonadecanoic acid, pentadecyl ester
36610-50-1	1	1	1	Nonadecanoic acid, hexadecyl ester
36610-51-2	1	1	1	Nonadecanoic acid, heptadecyl ester

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
36610-52-3	1	1	1	Nonadecanoic acid, octadecyl ester
36610-53-4	1	1	1	Nonadecanoic acid, nonadecyl ester
36610-54-5	1	1	1	Nonadecanoic acid, eicosyl ester
36610-55-6	1	1	1	Eicosanoic acid, tridecyl ester
36610-58-9	1	1	1	Eicosanoic acid, heptadecyl ester
36610-60-3	1	1	1	Eicosanoic acid, nonadecyl ester
36617-18-2	1	1	1	Dodecanoic acid, eicosyl ester
36617-26-2	1	1	1	Tridecanoic acid, eicosyl ester
36617-27-3	1	1	1	Tetradecanoic acid, tridecyl ester
36617-28-4	1	1	1	Tetradecanoic acid, nonadecyl ester
36617-30-8	1	1	1	Pentadecanoic acid, tridecyl ester
36617-31-9	1	1	1	Pentadecanoic acid, tetradecyl ester
36617-32-0	1	1	1	Pentadecanoic acid, pentadecyl ester
36617-33-1	1	1	1	Pentadecanoic acid, hexadecyl ester
36617-34-2	1	1	1	Pentadecanoic acid, heptadecyl ester
36617-35-3	1	1	1	Pentadecanoic acid, octadecyl ester
36617-36-4	1	1	1	Pentadecanoic acid, nonadecyl ester
36617-37-5	1	1	1	Pentadecanoic acid, eicosyl ester
36617-38-6	1	1	1	Hexadecanoic acid, tridecyl ester
36617-44-4	1	1	1	Hexadecanoic acid, nonadecyl ester
36617-46-6	1	1	1	Heptadecanoic acid, tridecyl ester
36617-47-7	1	1	1	Heptadecanoic acid, tetradecyl ester
36617-48-8	1	1	1	Heptadecanoic acid, pentadecyl ester
36617-49-9	1	1	1	Heptadecanoic acid, hexadecyl ester
36617-50-2	1	1	1	Heptadecanoic acid, heptadecyl ester
36617-51-3	1	1	1	Heptadecanoic acid, octadecyl ester
36617-52-4	1	1	1	Heptadecanoic acid, nonadecyl ester
36617-53-5	1	1	1	Heptadecanoic acid, eicosyl ester
36618-49-2	1	0	0	Benzofuran, tetramethyl-
36653-82-4	1	1	1	1-Hexadecanol
124-29-8				
36665-69-7	1	1	1	Eicosanoic acid, pentadecyl ester
36679-81-9	1	1	1	2(3*H*)-Furanone, dihydro-4-(hydroxymethyl)-
36724-24-0	1	0	0	Benzofuran, 3-ethyl-
36734-19-7	0	1	0	1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-2,4-dioxo- {Iprodione®}
36917-36-9	1	0	0	Pyridine, 2,6-dimethyl-4-ethyl-
36947-68-9	1	0	0	1*H*-Imidazole, 2-(1-methylethyl)-
37112-31-5	1	1	1	6,8-Dioxabicyclo[3.2.1]oct-2-en-4-one, (1S)- {levoglucosenone}
37147-17-4	0	1	0	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-, (R)
37205-35-9	0	1	0	Synthetase, arginyl-transfer ribonucleate
37205-42-8	0	1	0	Decarboxylase, α-ketoglutaric acid
37205-61-1	0	1	0	Proteinase inhibitor
37205-63-3	0	1	0	Synthetase, adenosine triphosphate
37208-05-2	0	1	0	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [1R-(1α,3β,4β,4aα,6α)]-
37209-50-0	0	1	0	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, acetate, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberin}
37211-77-1	0	1	0	Synthase, 5-dehydroquinate
37250-19-4	0	1	0	Dehydrogenase, malate (nicotinamide adenine dinucleotide phosphate)
37256-31-8	0	1	0	Dehydrogenase, nicotine
37256-36-3	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide (quinone)
37256-37-4	0	1	0	Dehydrogenase, reduced nicotinamide adenine dinucleotide phosphate (quinone)
37256-44-3	0	1	0	Reductase, ferredoxin–nitrite
37259-57-7	0	1	0	Aminotransferase, serine–glyoxylate

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
37259-58-8	0	1	0	Protease
37259-67-9	0	1	0	Decarboxylase, glycine
37259-79-3	0	1	0	Oxidase, methylputrescine
37275-41-5	1	0	0	Pentene, methyl-
37275-48-2	1	0	0	Bipyridine
37277-74-0	0	1	0	Pyrophosphorylase, nicotinate mononucleotide (carboxylating) {phosphoribosyltransferase, quinolinate}
37277-82-0	0	1	0	Aminopropyltransferase, putrescine
37289-33-1	0	1	0	Pyrophosphatase, nicotinamide adenine dinucleotide
37290-89-4	0	1	0	Synthase, cysteine {acetylserine sulfhydrylase}
37294-28-3	1	1	1	Glucoxylan
37297-20-4	0	1	0	Phytoalexins
37317-38-7	0	1	0	Glucuronoxylan
37318-64-2	0	1	0	Synthetase, methenyltetrahydrofolate
37332-51-7	0	1	0	Synthetase, *p*-coumaroyl coenzyme A
37340-89-9	0	1	0	Diaphorase
37341-54-1	0	1	0	Carboxylase, phosphopyruvate
37341-58-5	0	1	0	Phosphatase, phytate
37347-76-5	0	1	0	Glyoxalase
37414-44-1	1	0	0	1*H*-Indene-2-carboxaldehyde, 2,3-dihydro-
37455-52-0	1	0	0	1*H*-Imidazole, 2-methyl-4-(1-methylethyl)-
37455-55-3	1	0	0	1*H*-Imidazole, 4-methyl-2-propyl-
37455-56-4	1	0	0	1*H*-Imidazole, 4-ethyl-2-propyl-
37455-58-6	1	0	0	1*H*-Imidazole, 4-methyl-2-(1-methylethyl)-
37455-59-7	1	0	0	1*H*-Imidazole, 4-ethyl-2-(1-methylethyl)-
37455-73-5	1	0	0	1*H*-Imidazole, 1,4-dimethyl-2-(1-methylethyl)-
37526-88-8	0	1	0	2-Butenoic acid, 2-methyl-, phenylmethyl ester {benzyl tiglate}
37531-06-9	0	1	0	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-, (*Z*)-
37531-07-0	0	1	0	2(3*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-, (*E*)-
37551-73-8	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]-
37551-74-9	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aα,6aβ,10aα,10bβ)]-
37574-03-1	0	1	0	2-Naphthalenemethanol, 1,2,3,4,4a,8a-hexahydro-α,α,4a,8-tetramethyl- {*trans*-occidentalol}
37574-48-4	1	0	0	Benzo[*a*]pyren-4-ol
37620-20-5	1	1	1	Pyridine, 3-(1-nitroso-2-piperidinyl)-, (*S*)- [2 CAS Nos.] {NAB}
1133-64-8				
37645-61-7	1	0	0	Thiazole, 2-butyl-
37680-65-2	1	0	0	1,1′-Biphenyl, 2,2′,5-trichloro-
37687-18-6	1	0	0	Ethanone, 1-(1-methyl-1*H*-pyrazol-4-yl)-
37704-28-2	0	1	0	Propanoic acid, 2-methyl-, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-3-cyclohexen-1-yl ester
37822-76-7	0	1	0	Nonenoic acid, methyl ester
37822-80-3	0	1	0	Heptadecadienoic acid, methyl ester
37822-81-4	0	1	0	Hexadecatrienoic acid, methyl ester
37822-82-5	0	1	0	Heptadecatrienoic acid, methyl ester
37846-06-3	1	0	0	Benzenamine, 4-ethyl-*N*-methyl-
37871-00-4	1	0	0	Dibenzo[*b,e*][1,4]dioxin, heptachloro-
37920-25-5	1	0	0	Ethanone, 1-(4-butylphenyl)-
37924-13-3	0	1	0	Methanesulfonamide, trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl) {Perfluidone®}
38017-17-3	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl- {8,13-epoxylabd-14-en-12-one}
38043-97-9	1	1	1	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-4-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-, (4aR-*cis*)- {1-keto-α-cyperone}
38044-00-7	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-
38048-87-2	1	0	0	Fluoranthene, 7,8-dimethyl-
38073-89-1	0	1	0	3-Cyclohexene-1-carboxylic acid, 6-(1-methylethyl)-, *cis*-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
38076-78-7	1	0	0	3-Pyridinecarbonitrile, 2-amino-5-methyl-
38205-61-7	1	0	0	Thiazole, 5-ethyl-2,4-dimethyl-
38205-66-2	1	0	0	Ethanone, 1-(4-thiazolyl)- {4-acetylthiazole}
38207-11-3	1	1	1	1*H*-Pyrrole, 1-acetyl-2-methyl-
38232-01-8	1	0	0	Hentriacontanoic acid
38232-03-0	1	0	0	Tritriacontanoic acid
38232-04-1	1	0	0	Tetratriacontanoic acid
38260-27-4	1	0	0	2(5*H*)-Furanone, 4-acetyl-
38273-97-1	0	1	0	2(3*H*)-Furanone, dihydro-3,3-dimethyl-5-(2-oxopropyl)-
38284-11-6	0	1	0	7-Oxabicyclo[4.1.0]heptane-2,5-dione, 1,3,3-trimethyl-
38284-27-4	0	1	0	3,5-Octadien-2-one
38284-28-5	0	1	0	2,5,8-Nonanetrione
38372-56-4	1	1	1	3-Nonene-2,8-dione {norsolanadione}
38411-22-2	1	0	0	1,1′-Biphenyl, 2,2′,3,3′,6,6′-hexachloro-
38419-69-1	0	1	0	6*H*-3,10b-Epoxy-1*H*-naphtho[2,1-*b*]pyran, decahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aβ,6aα,10aβ,10bα)]-
38445-24-8	1	0	0	4*H*-1-Benzopyran-4-one, 6-hydroxy-
38462-22-5	0	1	0	Cyclohexanone, 2-(1-mercapto-1-methylethyl)-5-methyl-
38477-23-5	0	1	0	7*H*-Purin-6-amine, 7-*D*-glucofuranosyl-*N*-(phenylmethyl)-
38527-91-2	1	0	0	Phosphorothioic acid, 2-(2,4-dichlorophenyl) *O*-ethyl *S*-propyl ester {Ethaphos®}
38552-75-9	0	1	0	Ethanone, 1-[2-(1-methylethenyl)cyclopentyl]-
38624-29-2	0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-
38638-41-4	1	0	0	1*H*-Indene, phenyl-
38655-27-5	0	1	0	Cyclopentanecarboxylic acid, 1-methyl-3-(1-methylethenyl)-
38713-11-0	0	1	0	1,2-Cyclohexanediol, 1,3,3-trimethyl-
38713-12-1	0	1	0	3,7-Nonadien-1-ol, 4,8-dimethyl- {homogeraniol}
38713-13-2	0	1	0	2-Undecanol, 6,10-dimethyl-
38713-24-5	0	1	0	2-Propanone, 1-[tetrahydro-3-(1-methylethyl)-2-furanyl]-, *trans*-
38713-26-7	0	1	0	1-Oxaspiro[4.5]dec-2-en-8-one, 2,6,6,10-tetramethyl-
38713-41-6	1	1	1	Pyrazine, (1-methylethenyl)-
38725-47-2	0	1	0	2(4*H*)-Benzofuranone, tetrahydro-4,4,7a-trimethyl-
19432-05-4				
38738-60-2	1	0	0	Cyclohexene, 1-methyl-3-(1-methylethenyl)- {sylvestrene}
10	1	0	0	2-Cyclohexene-1,4-dione, 2,5,5-trimethyl-
38806-26-7	1	0	0	Acetamide, *N*-ethyl-*N*-methyl-
38818-55-2	1	1	1	2-Cyclohexen-1-one, 4-(1,3-butadienyl)-3,5,5-trimethyl-, (*E*)-
38840-03-8	1	1	1	1-Pyrrolidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)- {*N*′-formylnornicotine} [2 CAS Nos.]
3000-81-5				
38840-05-0	1	1	1	2,3′-Bipyridine, 4-methyl-
38840-06-1	0	1	0	3,3′-Bipyridine, 4-methyl-
38854-09-0	1	1	1	Pyrrolidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-
38854-10-3	1	1	1	Pyrrolidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-
38877-21-3	1	0	0	4*H*-Pyran-4-one, 2,3-dihydro-5-hydroxy-6-methyl-
38895-88-4	1	0	0	2-Butanone, 3,3-dimethyl-4-hydroxy-
38917-60-1	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-2-ethyl-
38917-63-4	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-2,3-dimethyl-
38917-65-6	1	0	0	Quinoxaline, 2-methyl- 5,6,7,8-tetrahydro-
38963-41-6	1	0	0	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-2-cyclohexen-1-yl)- {4-hydroxy-α-ionone}
38998-75-3	1	0	0	Dibenzofuran, heptachloro-
39001-02-0	1	0	0	Dibenzofuran, octachloro-
39006-52-5	0	1	0	Stigmasta-7,24(28)-diene-3-ol, 4-methyl- (3β,4α,5α,24*E*)-
39012-18-5	1	1	1	5,7-Nonadien-2-one, 8-methyl-5-(1-methylethyl)- {isosolanone}
39029-41-9	0	1	0	Naphthalene, 7-methyl-4-methylene-1-(1-methylethyl)- 1,2,3,4,4a,5,6,8a-octahydro-, (1α,4aβ,8aα)- {γ-cadinene}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
39099-23-5	1	0	0	1-Butanamine, *N*-(1-methylethyl)-
39161-19-8	0	1	0	3-Penten-1-ol
39212-***23-2***	0	1	0	2(3*H*)-Furanone, 5-butyldihydro-4-methyl-
39227-28-6	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,7,8-hexachloro-
39276-09-0	1	0	0	Furancarboxaldehyde
39280-21-2	0	1	0	(1 → 2)-*L*-Rhamno-(1 → 4)-α-*D*-galacturonan
39292-53-0	1	0	0	Naphthalene, dihydromethyl- {at least three isomers in MSS}
39300-45-3	0	1	0	2-Butenoic acid, 2-(1-methylheptyl)-4,6-dinitrophenyl ester {Dinocap®}
39327-16-7	1	0	0	Benzoquinoline
39335-11-0	0	1	0	Oxygenase, ribulose diphosphate
39341-47-4	0	1	0	Starch, labeled with ^{13}C {starch-^{13}C}
39341-90-7	0	1	0	Synthetase, indoleacetate
39434-01-0	0	1	0	Phosphodiesterase, nucleotide
39515-41-8	1	1	1	Cyclopropanecarboxylic acid, 2,2,3,3-tetramethyl cyano(3-phenoxyphenyl)methyl ester {Fenpropathrin®, Danitol®}
39815-65-1	0	1	0	Nonacosanoic acid, 4-(2-hydroxyethyl)phenyl ester
39815-66-2	0	1	0	2,4,9,13-Cyclotetradecatetraen-1-ol, 3,9,13-trimethyl-6-(1-methylethyl)-
39815-67-3	0	1	0	6-Benzofuranol, octahydro-4,4,7a-trimethyl-
39815-68-4	1	1	1	2-Propanone, 1-[tetrahydro-6-methyl-3-(1-methylethyl)-2*H*-pyran-2-yl]- {two isomers reported}
39815-69-5	1	1	1	2-Propanone, 1-[tetrahydro-4-(1-methylethyl)-2-furanyl]-
39815-70-8	0	1	0	6(2*H*)-Benzofuranone, hexahydro-4,4,7a-trimethyl-
39815-71-9	0	1	0	2*H*-Inden-2-one, 1,4,5,6,7,7a-hexahydro-1-hydroxy-1,4,4,7a-tetramethyl-
39815-73-1	0	1	0	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-
39815-74-2	0	1	0	2(3*H*)-Naphthalenone, 4,6,7,8-tetrahydro-4,4,7-trimethyl-
39815-78-6	0	1	0	Heptanoic acid, 3-oxo-, methyl ester
39954-19-3	0	1	0	2(1*H*)-Pyridinone, 3,6-dihydroxy- {2,3,6-pyridinetriol}
40000-89-3	1	0	0	1,8-Naphthyridin-2(1*H*)-one, 3-methyl-
40186-72-9	1	0	0	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6-nonachloro-
40222-77-3	1	0	0	3-Pyridinol, 6-hydroxymethyl- {2-pyridinemethanol, 5-hydroxy-}
40286-47-3	0	1	0	6,8-Nonadien-2-one, 8-methyl-5-(methylethyl)-
40309-49-7	0	1	0	Hexanoic acid, 3-hydroxy-5-methyl-
40311-00-0	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(1-methylethyl)-
40314-06-5	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 5-methyl-
40316-88-9	1	1	1	2(1*H*)-Pyridinone, 3-(1-methyl-2-pyrrolidinyl)-, (S)- {nicotone}
40321-76-4	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,7,8-pentachloro-
40460-44-4	0	1	0	1,1,2-Ethanetriol
40487-42-1	0	1	0	Benzenamine, 3,4-dimethyl-2,6-dinitro-*N*-(1-ethylpropyl)- {Pendimethalin®}
40525-38-0	1	1	1	6,8-Nonadien-2-ol, 8-methyl-5-(1-methylethyl)- {solanol}
40529-54-2	1	0	0	1-Naphthalenol, dimethyl-
40529-66-6	1	0	0	1,1′-Biphenyl, ethyl-
40596-69-8	1	1	1	2,4-Dodecadienoic acid, 11-methoxy-3,7,11-trimethyl-, 1-methylethyl ester, (*E,E*)- {Methoprene®, Altosid®}
40626-35-5	1	0	0	Phosphorothioic acid, *O*-ethyl *O*-phenyl S-propyl ester {Heterophos®}
40654-82-8	0	1	0	Butanal, 2-methyl-4-phenyl-
40678-46-4	1	0	0	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-1-methyl-, (1S-*cis*)-
40688-28-6	1	0	0	1*H*-Imidazole, 2,4-dimethyl-5-(1-methylethyl)-
40793-85-9	1	0	0	Benzene, 2-methoxy-1-methyl-4-(1-propenyl)-
40795-25-3	1	0	0	Furanmethanol
40811-89-0	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *N*-(phenylmethyl)-
40861-87-8	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-propyl-
40922-97-2	0	1	0	Adenosine 5′-(tetrahydrogen triphosphate), *N*-(phenylmethyl)-
41005-65-6	1	1	1	Stigmast-5-en-3-ol, dodecanoate, (3β)- {β-sitosteryl laurate}
41050-31-1	1	1	1	Pentadiene

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
41055-68-9	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, labeled with ^{13}C
41059-93-2	0	1	0	2-Heptanone, 6-methyl-5-(4-methyl-2-furanyl)- {solanofuran}
41059-94-3	0	1	0	1,6-Dioxaspiro[4.5]dec-3-en-2-one, 3,4,7-trimethyl-
51607-05-7				
41114-00-5	0	1	0	Pentadecanoic acid, ethyl ester
41198-08-7	0	1	0	Phosphorothioic acid, *O*-(4-bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl ester {Profenophos®}
41233-72-1	1	0	0	1,3,5-Hexatriene, 2-methyl-
41239-48-9	0	1	0	Furan, 2,3-diethyl-tetrahydro-
41429-54-3	1	1	1	2,6,11-Cyclotetradecatrien-1-one, 13-hydroxy-3,7,13-trimethyl-10-(1-methylethyl)- = 4,8,13-cyclotetradecatrien-1-ol-3-one,-1,5,9-trimethyl-12-(1-methylethyl)-,
41429-55-4	0	1	0	3,7,12-Pentadecatriene-2,14-dione, 4,8-dimethyl-11-(1-methylethyl)-, (*E,Z,E*)-
41496-77-9	1	1	1	2-Cyclopenten-1-one, 3-ethyl-2-methyl-
41577-83-7	1	0	0	2-Cyclohexen-1-one, 3-ethyl-2-hydroxy-
41593-24-2	1	0	0	Fluoranthene, dihydro-
41637-86-9	1	0	0	Anthracene, ethyl-
41637-87-0	1	0	0	Fluoranthene, trimethyl-
41637-88-1	1	0	0	Pyrene, trimethyl- {at least three isomers in MSS}
41637-89-2	1	0	0	Triphenylene, methyl-
41637-90-5	1	0	0	Chrysene, methyl-
41637-91-6	1	0	0	2,2′-Binaphthalene, methyl-
41637-92-7	1	0	0	Chrysene, dimethyl- {at least three isomers in MSS}
41637-93-8	1	0	0	Benzo[*k*]fluoranthene, methyl-
41637-94-9	1	0	0	Benz[*e*]acephenanthrylene, methyl-
41653-89-8	0	1	0	Nonanoic acid, 7-methyl-
41653-93-4	0	1	0	3-Pentenoic acid, 3-methyl-, (*E*)-
41653-94-5	0	1	0	3-Pentenoic acid, 3-methyl-, (*Z*)
41653-95-6	0	1	0	4-Heptenoic acid, (*Z*)-
41653-96-7	0	1	0	2-Hexenoic acid, 5-methyl-
41653-97-8	0	1	0	5-Octenoic acid, (*Z*)-
41653-98-9	0	1	0	3-Nonenoic acid, (*Z*)-
41653-99-0	0	1	0	6-Nonenoic acid, (*Z*)-
41654-03-9	0	1	0	Pentanoic acid, 4-hydroxy-3-methyl-
41654-04-0	0	1	0	Hexanoic acid, 5-methyl-4-oxo-
41654-06-2	0	1	0	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)-
41654-07-3	0	1	0	4-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (*E*)-
41654-08-4	0	1	0	4-Octenoic acid, 6-ethyl-3-hydroxy-3,7-dimethyl-
41654-09-5	0	1	0	2-Butenedioic acid, 2-ethyl-3-methyl-, (*Z*)-
41678-34-6	0	1	0	Tridecatrienoic acid
41682-52-4	0	1	0	β-*D*-Glucopyranose, 1-(3-phenyl-2-propenoate)
41699-04-1	1	0	0	Benzo[*e*]pyrene, methyl- {at least two isomers in MSS}
41699-06-3	1	0	0	Benzo[*e*]pyrene, dimethyl- {at least two isomers in MSS}
41699-07-4	1	0	0	Indeno[1,2,3-*cd*]fluoranthene, methyl-
41699-09-6	1	0	0	Benzo[*ghi*]perylene, methyl- {at least two isomers in MSS}
41699-10-9	1	0	0	Dibenzo[*def,mno*]chrysene, methyl- {at least two, possibly three, isomers in MSS}
41720-93-8	0	1	0	1(2*H*)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-3-hydroxy-4,4a-dimethyl-6-(1-methylethenyl)-, [3R-(3α,4α,4aβ,6β)]-
41744-75-6	1	0	0	1-Heptadecanol, 16-methyl-
41903-57-5	1	0	0	Dibenzo[*b,e*][1,4]dioxin, tetrachloro-
41981-60-6	1	0	0	Thiazole, 4-propyl-
41981-71-9	1	0	0	Thiazole, 2,5-diethyl-4-methyl-
42126-84-1	1	0	0	11*H*-Benzo[*cd*]fluoranthene [2 CAS Nos.]
16135-81-2				
42172-35-0	0	1	0	Hexadecanoic acid, 3-methyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
42201-30-9	0	1	0	6-Hepten-2-ol, 4-methylene-
42218-21-3	1	1	1	Tetradecanoic acid, heneicosyl ester
42218-25-7	1	1	1	Heptadecanoic acid, docosyl ester
42218-26-8	1	1	1	Eicosanoic acid, heneicosyl ester
42232-05-3	1	1	1	Tetradecanoic acid, docosyl ester
42232-06-4	1	1	1	Tetradecanoic acid, tricosyl ester
42232-14-4	1	1	1	Pentadecanoic acid, dodecyl ester
42232-22-4	1	1	1	Pentadecanoic acid, heneicosyl ester
42232-23-5	1	1	1	Pentadecanoic acid, docosyl ester
42232-24-6	1	1	1	Pentadecanoic acid, tricosyl ester
42232-29-1	1	1	1	Hexadecanoic acid, dodecyl ester
42232-32-6	1	1	1	Hexadecanoic acid, heneicosyl ester
42232-33-7	1	1	1	Hexadecanoic acid, docosyl ester
42232-34-8	1	1	1	Hexadecanoic acid, tricosyl ester
42232-35-9	1	1	1	Hexadecanoic acid, tetracosyl ester
42232-43-9	1	1	1	Heptadecanoic acid, dodecyl ester
42232-52-0	1	1	1	Heptadecanoic acid, heneicosyl ester
42232-53-1	1	1	1	Heptadecanoic acid, tricosyl ester
42232-54-2	1	1	1	Heptadecanoic acid, tetracosyl ester
42232-59-7	1	1	1	Octadecanoic acid, heneicosyl ester
42232-60-0	1	1	1	Octadecanoic acid, tricosyl ester
42232-61-1	1	1	1	Octadecanoic acid, tetracosyl ester
42232-66-6	1	1	1	Nonadecanoic acid, dodecyl ester
42232-75-7	1	1	1	Nonadecanoic acid, heneicosyl ester
42232-76-8	1	1	1	Nonadecanoic acid, docosyl ester
42232-77-9	1	1	1	Nonadecanoic acid, tricosyl ester
42232-82-6	1	1	1	Eicosanoic acid, dodecyl ester
42232-87-1	1	1	1	Eicosanoic acid, docosyl ester
42232-88-2	1	1	1	Eicosanoic acid, tricosyl ester
42232-89-3	1	1	1	Eicosanoic acid, tetracosyl ester
42232-93-9	1	1	1	Heneicosanoic acid, dodecyl ester
42232-94-0	1	1	1	Heneicosanoic acid, tridecyl ester
42232-95-1	1	1	1	Heneicosanoic acid, tetradecyl ester
42232-96-2	1	1	1	Heneicosanoic acid, pentadecyl ester
42232-97-3	1	1	1	Heneicosanoic acid, hexadecyl ester
42232-98-4	1	1	1	Heneicosanoic acid, heptadecyl ester
42232-99-5	1	1	1	Heneicosanoic acid, nonadecyl ester
42233-00-1	1	1	1	Heneicosanoic acid, eicosyl ester
42233-01-2	1	1	1	Heneicosanoic acid, heneicosyl ester
42233-02-3	1	1	1	Heneicosanoic acid, docosyl ester
42233-03-4	1	1	1	Heneicosanoic acid, tricosyl ester
42233-04-5	1	1	1	Heneicosanoic acid, tetracosyl ester
42233-07-8	1	1	1	Docosanoic acid, dodecyl ester
42233-08-9	1	1	1	Docosanoic acid, tridecyl ester
42233-09-0	1	1	1	Docosanoic acid, tetradecyl ester
42233-10-3	1	1	1	Docosanoic acid, pentadecyl ester
42233-11-4	1	1	1	Docosanoic acid, hexadecyl ester
42233-12-5	1	1	1	Docosanoic acid, heptadecyl ester
42233-13-6	1	1	1	Docosanoic acid, nonadecyl ester
42233-14-7	1	1	1	Docosanoic acid, eicosyl ester
42233-15-8	1	1	1	Docosanoic acid, heneicosyl ester
42233-16-9	1	1	1	Docosanoic acid, tricosyl ester

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
42233-17-0	1	1	1	Docosanoic acid, tetracosyl ester
42233-27-2	1	1	1	Tricosanoic acid, dodecyl ester
42233-28-3	1	1	1	Tricosanoic acid, tridecyl ester
42233-29-4	1	1	1	Tricosanoic acid, tetradecyl ester
42233-30-7	1	1	1	Tricosanoic acid, pentadecyl ester
42233-31-8	1	1	1	Tricosanoic acid, hexadecyl ester
42233-32-9	1	1	1	Tricosanoic acid, heptadecyl ester
42233-33-0	1	1	1	Tricosanoic acid, octadecyl ester
42233-34-1	1	1	1	Tricosanoic acid, nonadecyl ester
42233-35-2	1	1	1	Tricosanoic acid, eicosyl ester
42233-36-3	1	1	1	Tricosanoic acid, heneicosyl ester
42233-37-4	1	1	1	Tricosanoic acid, docosyl ester
42233-38-5	1	1	1	Tricosanoic acid, tricosyl ester
42233-39-6	1	1	1	Tricosanoic acid, tetracosyl ester
42268-60-0	1	0	0	1*H*-Benzimidazole, 2-(1-naphthalenylmethyl)-
42315-22-0	1	0	0	Cyclopenta[*a*]pyrene
42330-36-9	0	1	0	Heptanoic acid, 5-methyl-, (S)-
42348-12-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-ethyl-4-methyl-
42369-86-8	0	1	0	2-Propenamide, *N,N′*-1,4-butanediylbis[3-(4-hydroxy-3-methoxyphenyl)-
42370-41-2	0	1	0	3-Cyclohexene-1-methanol, 5-hydroxy-α,α,4-trimethyl-, *trans*-
42397-64-8	1	0	0	Pyrene, 1,6-dinitro-
42397-65-9	1	0	0	Pyrene, 1,8-dinitro-
42400-32-8	0	1	0	*D*-Arabinohexonic acid, 2-deoxy-, γ-lactone
42438-90-4	1	0	0	1*H*-Pyrido[3,4-*b*]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-, (S)-
42448-85-2	1	0	0	2-Eicosene, (*E*)-
42451-07-0	1	0	0	3-Pyridinol, 6-ethyl-2-methyl-
42463-54-7	1	0	0	Oxazole, 2-ethyl-5-methyl-
42508-10-1	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-5-methyl-
42545-63-1	1	0	0	3-Pyridineacetaldehyde
42569-63-1	1	0	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-1,3-pentadienyl)-, [1R-[1α(1*E*,3*E*),2β,4aβ,8aα]]-
42569-64-2	0	1	0	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1R-[1α(*E*),2β,4aβ,8aα]]-
42617-16-3 479-61-8	0	1	0	Magnesium, [3,7,11,15-tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-*N*23,*N*24,*N*25,*N*26]-, [*SP*-4-2-[3S-[3α(2*E*,7S*,11S*),4β,21β]]]- [2 CAS Nos.] {chlorophyll a}
42732-49-0	1	0	0	3-Pyridinol, 5-methyl-
42885-14-3	1	0	0	3-Pyridinecarbonitrile, 5-methyl-
42933-00-6 54869-11-3	1	1	1	Furan, 3-(4,8,12-trimethyltridecyl)- [2 CAS Nos.] {phytofuran}
42972-46-3	1	1	1	Ethanone, 1-(5-methyl-3-pyridinyl)-
43000-45-9	1	1	1	1-Buten-1-ol, 3-methyl-
43052-87-5	0	1	0	2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- {α-damascone}
43058-40-8	1	1	1	Ethanedioic acid, labeled with ^{14}C {oxalic acid-^{14}C}
43121-43-3	0	1	0	2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl) {Triadimefon®}
43133-95-5	1	0	0	Pentane, methyl-
43152-89-2	1	0	0	2*H*-Pyran-3(4*H*)-one, dihydro-6-methyl-
43178-07-0	1	0	0	Benz[*a*]anthracene, dimethyl-
43178-22-9	1	0	0	Benz[*a*]anthracene, methyl-
43205-82-9	1	0	0	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)- {dihydrocarvone}
43219-68-7 31577-86-3	0	1	0	Ethanone, 1-[3-(1-methylethenyl)cyclopentyl]- [2 CAS Nos.] {two isomers}
45009-62-9	0	1	0	Hexoses
45803-83-6	1	0	0	Phenol, 4-ethenyl-2-methyl-
46175-80-8	0	1	0	Benzenamine, 2-(cyclohexen-1-yl)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
46864-87-3	1	0	0	Fluoranthene, 8-ethyl-
47018-25-7	1	0	0	2-Propenoic acid, 3-phenyl-, 2-phenylethenyl ester
49741-70-0	0	1	0	*D*-myo-Inositol, *O*-*D*-glucopyranosyl-
49749-17-9	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-, (2α,4aα,8aβ)-(±)-
50281-40-8	0	1	0	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1R-[1α(*E*),4β,6α]]-
50281-41-9	0	1	0	3-Buten-2-one, 4-[4-(acetyloxy)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl]-, [1S-[1α(*E*),4α,6α]]-
50281-42-0	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1S-[1α(*E*),4α,6α]]-
50313-71-8	0	1	0	1-Tetradecanol, 12-methyl-
50471-44-8	0	1	0	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- {Vinclozolin®}
50598-50-0	0	1	0	2(5*H*)-Furanone, 3,5,5-trimethyl-
50609-61-5	1	0	0	4*H*-Pyrido[1,2-*a*]pyrimidine-3-acetic acid, 9-hydroxy-4-oxo-, ethyl ester
50671-50-6	1	0	0	4*H*-Pyran-4-one, 3-methyl-
50672-03-2	1	0	0	2-Propanone, 1-[5-(hydroxymethyl)-2-furanyl]-
50691-29-7	1	0	0	1*H*-Pyrrole, 1-(2-phenylethyl)-
50691-30-0	1	0	0	1*H*-Pyrrole, 1-butyl-2-methyl-
50767-76-5	0	1	0	3-Hepten-2-one, 5-ethyl-6-methyl-, (*E*)-
50767-77-6	0	1	0	2-Butanone, 4-(2-ethenyl-2,6,6-trimethylcyclohexyl)-
50768-69-9	1	0	0	2(3*H*)-Furanone, dihydro-5-hydroxy-
50790-93-7	1	0	0	1*H*-Imidazole, 2-butyl-
50812-10-7	0	1	0	Aminotransferase, glutamate–glyoxylate
50812-18-5	0	1	0	β-*D*-Glucosyltransferase, uridine diphosphoglucose-flavonol 3-*O*-glucoside
50812-37-8	0	1	0	Transferase, glutathione *S*-
50851-69-9	1	0	0	Phenol, ethenylethyl-
50868-72-9	1	1	1	Benzenamine, 2-methoxy-5-methyl-
50874-76-5	0	1	0	Cyclohexanone, trimethyl-
50906-50-8	0	1	0	9,19-Cyclostigmast-24(28)-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24Z)-
50936-45-3	0	1	0	Methyltransferase, caffeate
50966-74-0	1	0	0	Pyridine, 3-(1*H*-pyrrol-1-yl)-
72692-99-0				
50976-21-1	1	0	0	Benzene, ethenyltrimethyl-
77220-32-7				
50984-45-7	1	0	0	Phenol, dimethyl-ethenyl-ethyl-
51001-44-6	1	0	0	Benzo[*ghi*]fluoranthene, methyl-
51013-77-5	0	1	0	31-Norlanosterol
51020-10-1	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4a,8,8-tetramethyl-, (4aR-*trans*)- {isonordrimenone}
51025-25-3	1	0	0	Pyridinol, dimethyl-
51064-12-1	1	0	0	Pentadiene, methyl-
51064-37-0	0	1	0	Phenylalanine, ar,ar-dihydroxy-
51064-38-1	1	1	1	β-*D*-Glucopyranoside, (3β,24S)-stigmast-5-en-3-yl- {γ-sitosteryl glucoside}
51088-90-5	0	1	0	2*H*-Pyrrol-2-one, 1,5-dihydro-3,5-dimethyl-
51109-34-3	0	1	0	Nonadienoic acid
51171-72-3	1	0	0	2-Cyclohexen-1-one, 4-phenyl-
51207-31-9	1	0	0	Dibenzofuran, 2,3,7,8-tetrachloro-
51218-45-2	0	1	0	Acetamide, 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)- {Metolachlor®}
51276-47-2	0	1	0	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®}
53369-07-6				
51297-34-8	0	1	0	Oxiranemethanol, 3-(1-ethyl-2-methylpropyl)-α,α-dimethyl-
51297-35-9	0	1	0	Ethanone, 1-[3-(1-ethyl-2-methylpropyl)oxiranyl]-
51297-36-0	0	1	0	8,10-Undecadien-4-one, 2,10-dimethyl-7-(1-methylethyl)-, (*E*)-(±)-
51327-73-2	0	1	0	9,12,15-Octadecatrienoic acid, 18-hydroxy-, (*Z,Z,Z*)-
51366-52-0	1	0	0	Quinoline, trimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
51424-01-2	0	1	0	2-Hexenoic acid, 5-methyl-, (*E*)-
51542-52-0	0	1	0	3,6-Pyridazinedione, 1,2-dihydro-, potassium salt
51592-59-7	0	1	0	3,6,9,12,15-Octadecapentaenoic acid, (all-*Z*)-
51607-05-7	0	1	0	1,6-Dioxaspiro[4.5]dec-3-en-2-one, 3,4,7-trimethyl-
41059-94-3				
51630-58-1	1	1	1	Benzeneacetic acid, 4-chloro- α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Fenvalerate®}
51655-64-2	1	0	0	Nonane, 3-methylene-
51767-72-7	0	1	0	*D*-Fructose, labeled with ^{13}C {*D*-Frucrose-^{13}C}
51769-21-2	0	1	0	1-Butanone, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (±)-
51771-56-3	1	1	1	2-Cyclohexen-1-one, 3,5,5-trimethyl-2-(1-methylethenyl)-
51772-30-6	1	0	0	1-Propanone, 1-(3-methylphenyl)-
51773-45-6	0	1	0	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, [1R-(1α,2α,5α)]-
51787-42-9	1	0	0	Benz[*c*]acridine, 7,9,11-trimethyl-
51806-25-8	0	1	0	4-Hexadecene, 3-methylene-7,11,15-trimethyl-
51848-43-2	0	1	0	Retine
51855-29-9	1	0	0	Naphthalene, dimethyl-1,2,3,4-tetrahydro- [2 CAS Nos.] {at least five isomers in MSS}
65338-07-0				
51863-60-6	0	1	0	Ethanone, 1-(3,5-dihydroxyphenyl)-
51945-98-3	0	1	0	1,5-Heptadiene-3,4-diol
51953-03-8	0	1	0	9*H*-Purine
51961-51-4	1	0	0	Pyridine, 3-ethenyl-5-methyl-
52049-48-6	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*Z*)-
52115-69-2	0	1	0	1*H*-Pyrrole-2-carboxaldehyde, 5-[(acetyloxy)methyl]-
52126-90-6	1	1	1	2(3*H*)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-
52210-15-8	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-
52227-92-6	0	1	0	Phosphatase, phosphorylcholine
52254-38-3	1	0	0	1-Tetradecene, 2-methyl-
52254-50-9	1	0	0	1-Nonadecene, 2-methyl-
52315-07-8	1	1	1	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {Cypermethrin®}
52414-89-8	1	0	0	Thiazole, 2,4-diethyl-5-methyl-
52414-91-2	1	0	0	Thiazole, 4-ethyl-5-methyl-
52458-35-2	0	1	0	Heptadecanoic acid, 16-methyl-, ethyl ester
52517-53-0	1	0	0	5*H*-Cyclopentapyrazine, 6,7-dihydro-5-ethyl-
52536-09-1	1	1	1	3-Pyridinol
109-00-2				
58064-43-0				
52617-99-9	0	1	0	1-Naphthalenemethanol, decahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [1S-(1α,2β,4aβ,8aα)]-
52642-07-6	1	0	0	Butanediol, monoacetate
52645-53-1	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-dichloroethenyl-, (3-phenoxyphenyl)methyl ester {Permethrin®, Spartan®}
52655-10-4	0	1	0	Isoeicosanol
52690-42-3	0	1	0	2-Butanone, 4-[2,2,6-trimethyl-6-(methylethylene)cyclohexyl]-
52701-70-9	0	1	0	Isopentacosane
52712-05-7	1	0	0	1,1′-Biphenyl, 2,2′,3,4,5,5′,6,-heptachloro-
52756-25-9	0	1	0	*DL*-Alanine, *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-, methyl ester {Flamprop-methyl®}
52783-43-4	1	0	0	Nonadecanol
52786-29-5	1	0	0	1,4-Pentanedione, 1-(2-furanyl)-
52808-97-6	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,5-diethyl-
52811-22-0	1	1	1	7*H*-1-Benzopyran-7-one, 2,3,5,6,8,8a-hexahydro-5,5,8a-trimethyl-
52811-58-2	1	1	1	*3H*-Naphtho[2,1-*b*]pyran-3-one, 4a,5,6,6a,7,8,9,10,10a,10b-decahydro-4a,7,7,10a-tetramethyl-, [4aR-(4aα,6aβ,10aα,10bβ)]- {dehydroambreinolide}
52811-59-3	1	1	1	Naphtho[2,1-*b*]furan-2(3a*H*)-one, 4,5,5a,6,7,8,9,9a-octahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα)]-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
52811-60-6	1	1	1	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl-
52811-61-7	1	0	0	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-
52811-62-8	0	1	0	Naphtho[2,1-*b*]furan-2-ol, dodecahydro-3a,6,6,9a-tetramethyl- {sclaral}
52812-41-6	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-
102518-81-0				
52812-43-8	0	1	0	2-Heptanone, 5-[3-(1-hydroxy-1-methylethyl)oxiranyl]-6-methyl-
52812-44-9	1	0	0	2-Heptanone, 5-(3-acetyloxiranyl)-6-methyl-
52844-21-0	1	1	1	1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- {β-cyclocitral}
432-25-7				
52845-07-5	1	0	0	Isoeicosane
52845-08-6	1	0	0	Eicosane, 2-methyl- {isoheneicosane}
1560-84-5				
52886-15-4	0	1	0	2,9-Dioxabicyclo[3.3.1]nonan-4-ol, 1,3,3-trimethyl-6-(1-methylethyl)- {two isomers reported}
52918-63-5	1	1	1	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dibromoethenyl)-, cyano(3-phenoxyphenyl)methyl ester {Deltamethrin®}
52936-69-3	0	1	0	Ergosta-5,25-dien-3-ol, (3β)-
52945-87-6	1	0	0	2(5*H*)-Furanone, 5-ethyl-4-methyl-
52992-36-6	0	1	0	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-
53046-97-2	0	1	0	3,6-Nonadien-1-ol, (*Z,Z*)-
53093-94-0	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-, (*Z*)- (±)-
53093-95-1	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-, (*E*)- (±)-
53093-96-2	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethyl)-, (*Z*)- (±)-
53093-97-3	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethyl)-, (*E*)- (±)-
53109-18-5	0	1	0	1-Cyclopentene-1-pentanoic acid, δ-hydroxy-3,5-bis(1-methylpropyl)-β-oxo-
53123-73-2	1	0	0	Quinoline, ethyl-
53155-68-3	0	1	0	2(3*H*)-Furanone, dihydro-3,4,5-trimethyl-, (3α,4α,5α)-
53163-43-2	0	1	0	2-Naphthalenol, decahydro-1,2,5,5,8a-pentamethyl-, [1R-(1α,2β,4aβ,8aα)]-
53254-53-8	1	1	1	Nonadecanoic acid, 17-methyl-
53263-58-4	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-5-ethyl-3-methyl-
53274-45-6	0	1	0	Adenosine, *N*-(4-hydroxy-3-methyl-2-butenyl)-2-(methylthio)-, (*E*)-
53366-54-4	1	0	0	Cyclopentane, (2-methylbutylidene)-
53366-58-8	1	0	0	Cyclopentane, (2-methylpropylidene)-
53369-07-6	0	1	0	Butanoic acid, 2-amino-4-(hydroxymethylphosphinyl)- {Glufosinate®}
51276-47-2				
53392-07-7	1	0	0	Benzenebutanol, 4-methyl-
53398-09-7	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(1-oxo-2-butenyl)-
53398-17-7	0	1	0	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethycyclohexanyl)- {4-hydroxydihydro-β-damascone}
53428-02-7	1	0	0	2(1*H*)-Pyridinone, 3,6-dimethyl-
53448-06-9	0	1	0	3-Pentenal, (*Z*)-
53452-65-6	1	0	0	Quinoline, butyl-
53498-30-9	1	0	0	Thiazole, 4,5-dimethyl-2-(1-methylethyl)-
53498-32-1	1	0	0	Thiazole, 4,5-dimethyl-2-(2-methylpropyl)-
53516-76-0	0	1	0	Ammonium chloride, alkyldimethylbenzyl- {Benzalkonium chloride®}
53535-33-4	0	1	0	Heptanol
53561-62-9	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl- {two isomers}
53563-67-0	1	0	0	1*H*-Indene, 2,3-dihydrodimethyl- {four isomers detected}
53566-37-3	1	0	0	2-Hexyne, 5-methyl-
53587-16-9	1	0	0	Phenol, 2-methoxy-4-(1-methylethyl)-
53598-99-5	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-4-methyl-
53833-20-8	1	0	0	Oxazole, 4-ethyl-2-methyl-
53833-28-6	1	0	0	Oxazole, 4-ethyl-5-methyl-
53833-29-7	1	0	0	Oxazole, 5-ethyl-2-methyl-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
53833-30-0	1	0	0	Oxazole, 4,5-dimethyl-2-ethyl-
53833-31-1	1	0	0	Oxazole, 5-methyl-2-propyl-
53837-34-6	1	1	1	5,9-Undecadien-2-ol, 6,10-dimethyl-
53844-44-3	1	1	1	Pyridine, 3-(2-pyrrolidinyl-2-^{14}C)-, (S)-, labeled with ^{14}C
53844-45-4	1	1	1	Pyridine, 3-(1-nitroso-2-pyrrolidinyl-2-^{14}C)-, (S)-, label with ^{14}C
53872-97-2	1	0	0	2-Butanone, 3-methyl-1-(3-pyridinyl)-
53897-27-1	1	0	0	Butanamide, 4-cyano-
53950-58-6	1	1	1	Hexadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
53950-59-7	1	0	0	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-
53951-50-1	0	1	0	Benzaldehyde, ethyl-
53596-04-0	0	1	0	2-*O*-β-*D*-Glucopyranuronysyl-α-*D*-glucopyranosiduronic acid, ammoniated (3β,20β)-20-carboxy-11-oxo-30-norolean-12-en-3-yl-, ammoniated {glycyrrhizic acid ammoniated, glycyrrhizin ammoniated}
53966-53-3	1	0	0	3-Nonene, 2-methyl-
54007-33-9	1	0	0	Pentanamide, *N*-ethyl-
54020-53-0	1	0	0	1*H*-Indole, 3,7-dimethyl-
54031-97-9	0	1	0	Pentanoic acid, 2-hydroxy-4-oxo-
54036-77-0	1	0	0	2*H*-Pyrrol-2-one
54116-90-4	1	0	0	Acridine, methyl-
54140-30-**6**	1	0	0	Cyclopentene, ethenyl-
54340-99-7	1	0	0	1*H*-Indole, 5,6,7-trimethyl-
54344-76-2	0	1	0	Butanoic acid, 4-(2,6,6-trimethylcyclohexen-1-yl)-
54345-38-9	0	1	0	2-Buten-1-one, 1-(2,3,6-trimethylphenyl)-, (*E*)-
54356-27-3	1	0	0	2-Propenenitrile, 3-(3-pyridinyl)-, (*E*)-
54356-28-4	1	0	0	2-Propenenitrile, 3-(3-pyridinyl)-, (*Z*)-
54362-49-1	1	0	0	1,2-Cyclopentanedione, 3,5-diethyl-
54365-40-1	1	1	1	Isoheptacosane
54467-53-7	0	1	0	2(5*H*)-Furanone, 4-ethyl-5-methyl-
54538-20-4	0	1	0	7*H*-Purin-6-amine, 7-*D*-glucosyl-*N*-(phenylmethyl)-
54541-18-3	1	0	0	1,2-Propanediol, 2-propanoate
54557-54-9	0	1	0	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-, (*E*)-
54557-55-0	0	1	0	4,6-Heptadienoic acid, 6-methyl-3-(1-methylethyl)-, (*E*)-
54557-57-2	0	1	0	4,6-Heptadienoic acid, 6-methyl-3-(1-methylethyl)-, methyl ester, (*E*)-
80114-59-6				
54562-24-2	1	0	0	2-Cyclopenten-1-one, 2,3,5-trimethyl-
54621-96-4	1	0	0	2(5*H*)-Furanone, 5-(1-hydroxyethyl)-, [R-(R*,S*)]-
54612-24-7	1	0	0	Hexadiene, dimethyl-
54621-96-4	1	0	0	2(5*H*)-Furanone, 5-(1-hydroxyethyl)-, [R-(R*,S*)]-
54656-80-3	0	1	0	3-Buten-2-one, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1α(*E*),2α,4aβ,8aα]-(±)-
54657-94-2	1	0	0	2*H*-Pyran-2-one, 3,4-dihydro-5-methyl-
54703-51-4	1	0	0	2-Naphthalenol, 1,8-dimethyl-
54724-00-4	0	1	0	Callose [2 CAS Nos.] {1,3-β-*D*-glucan}
9064-51-1				
54774-28-6	0	1	0	2-Furanmethanol, 5-methyltetrahydro-
54789-23-0	1	1	1	1*H*-Inden-1-one, 2,3-dihydro-3,3,5,7-tetramethyl-
54811-53-9	1	0	0	11*H*-Benzo[*a*]fluorene, 9-methyl-
54824-90-7	1	0	0	Acetamide, *N*-(2-methylbutyl)-
54835-70-0	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-4-hydroxy-3,5,5-trimethyl-, [R-[R*,S*-(*E*)]]-
54846-63-8	0	1	0	Benzoic acid, 3-methylbutyl ester
54868-48-3	0	1	0	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, (*E*)-
54869-11-3	1	1	1	Furan, 3-(4,8,12-trimethyltridecyl)- [2 CAS Nos.] {phytofuran}
42933-00-6				
54878-25-0	0	1	0	Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-2-(1-methylethenyl)-, [2R-[2α,5α(R*)]]-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
54906-44-4	1	1	1	8(5*H*)-Indolizinone, 5,6,7,8-tetrahydro- {5-oxocyclohexa[*a*]pyrrole}
54911-63-6	1	0	0	2(3*H*)-Benzofuranone, hexahydro-4-hydroxy-
54993-31-6	0	1	0	1,4-Cyclohexanediol, 2,2,6-trimethyl-
55007-08-4	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-pentyl-
55023-52-4	0	1	0	6-Nonen-2-one, 8-hydroxy-5-(1-methylethyl)-
55023-53-5	1	1	1	3-Nonene-2,8-diol, 5-(1-methylethyl)-
55023-54-6	0	1	0	2-Nonanone, 8-hydroxy-5-(1-methylethyl)-
55023-56-8	1	1	1	2,8-Nonanediol, 5-(1-methylethyl)-
55023-57-9	1	1	1	2,8-Nonanedione, 5-(1-methylethyl)- {norsolanadione}
55023-59-1	0	1	0	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-
55030-93-8	0	1	0	Adenosine 5′-(trihydrogen diphosphate), *N*-(3-methyl-2-butenyl)-
55041-85-5	1	1	1	Ethanone, 1-(2,3-dihydro-1*H*-pyrrolizin-5-yl)-
55041-88-8	0	1	0	8(5*H*)-Indolizinone, 6,7-dihydro-2-methyl-
55044-97-8	1	0	0	Benzene, 1,1′-[oxy(methylene)]bis[4-ethyl-
55051-94-0	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-3-hydroxy-4-methyl-6-(1-methylethenyl)-, [3R-(3α,4β,4aβ,6α)]-
55066-56-3	1	1	1	Butanoic acid, 3-methyl-, 4-methylphenyl ester
55087-82-6	1	0	0	Ethanone, 1-[5-(hydroxymethyl)-2-furanyl]-
55100-07-7	0	1	0	2*H*-Pyran-2-one, 5,6-dihydro-4-hydroxy-
55136-76-0	0	1	0	4*H*-1-Benzopyran-4-one,3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-
55136-77-1	1	1	1	Docosanoic acid, hexacosyl ester
55138-67-5	0	1	0	Pyrazine, 2-methyl-6-(1-propenyl)-
55191-12-3	1	0	0	1*H*-Indole, 1,3-dibutyl-
55219-65-3	0	1	0	1*H*-1,2,4-Triazol-1-ethanol, 8-(4-chlorophenoxy)-α-(1,1-dimethylethyl)- {Triadimenol®}
55220-69-4	1	0	0	Fluoranthene, propyl-
55220-72-9	1	0	0	Fluoranthene, ethyl-
55270-47-8	1	0	0	Pyridine, 5-methoxy-2-methyl-
55277-47-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(1-methylethyl)-
55285-14-8	0	1	0	Methylcarbamic acid, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl [(di-*N*-butylamino)thio] ester {Carbosulfan®}
55309-61-0	1	1	1	Eicosanoic acid, octacosyl ester
55310-49-1	1	0	0	2-Cyclohexen-1-one, 2-hydroxy-3-propyl-
55326-39-1	0	1	0	Oxidase, isopentenyladenosine
55454-22-3	0	1	0	2-Hepten-1-ol (*Z*)
55484-04-3	1	0	0	Furan, 2-(4-pyridyl)-
55497-93-3	0	1	0	1(2*H*)-Naphthalenone, octahydro-2-hydroxy-2,5,5,8a-tetramethyl-, [2R- (2α,4aα,8aβ)]-
55520-40-6	0	1	0	Tyrosine
55556-98-4	0	1	0	2-Azetidinecarboxylic acid, 1-nitroso-
55557-02-3	0	1	0	3-Pyridinecarboxylic acid, 1,2,5,6-tetrahydro-1-nitroso-, methyl ester
55591-08-7	0	1	0	1-Naphthalenol, 1,2,3,4-tetrahydro-2,5,8-trimethyl-
55615-04-8	0	1	0	5-Hexen-2-one, 4,5-dimethyl-
55635-13-7	0	1	0	Cyclohexanecarboxylic acid, 2,2-dimethyl-2,4-dioxo-3-(1-((2-propenyloxy)amino)butylidene)-, methyl ester, sodium salt {Alloxydim-sodium®}
55664-77-2	0	1	0	2-Furanmethanol, methyl-
55673-89-7	1	0	0	Dibenzofuran, 1,2,3,4,7,8,9-heptachloro-
55682-88-7	0	1	0	11,14,17-Eicosatrienoic acid, methyl ester
55682-90-1	1	0	0	Pyrene, 1-decyl-
55684-94-1	1	0	0	Dibenzofuran, hexachloro-
55696-57-6	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1 → 6)]-β-*D*-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-
55713-38-7	0	1	0	8(5*H*)-Isoquinolinone, 6,7-dihydro-1,3,6,6-tetramethyl- [6,7-dihydro- or 5,6,7,8-tetrahydro-?]
55713-43-4	0	1	0	7*H*-2-Pyrindin-7-one, 5,6-dihydro-3,6,6-trimethyl-
55713-44-5	0	1	0	Cyclopentanone, 2,2-dimethyl-4-(2-oxopropyl)-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
55733-01-2	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4,4a,8,8-pentamethyl-, (4aS-*trans*)-
55738-21-1	1	0	0	Pyridinedicarbonitrile
55751-83-2	1	0	0	Acridine, 2-ethyl-
55784-90-2	0	1	0	Spiro[4.5]decane-6-carboxaldehyde, 8,9-dihydroxy-10-methyl-2-(1-methylethenyl)-, [5S-[5α(S*),6β,8β,9α,10β]]-
55804-74-5	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(*O*-6-deoxy-α-*L*-mannopyranosyl-(1→2)-*O*-[6-deoxy-α-*L*-mannopyranosyl-(1 → 6)]-β-*D*-glucopyranosyl)oxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-
55976-13-1	0	1	0	1,4-Undecadiene, (*E*)-
56057-93-3	1	1	1	Pyridine, 2-methyl-5-(1-methylethenyl)-
56057-96-6	1	0	0	Pyridine, 2-methyl-5-(1-propenyl)-
56078-08-1	1	1	1	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)-
56078-09-2	1	1	1	1-Piperidinecarboxylic acid, 2-(3-pyridinyl)-, methyl ester, (S)-
56084-94-7	0	1	0	2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-(4,8,12,16,20,24,28,32-octamethyl-3,7,11,15,19,23,27,31-tritriacontaoctaenyl)- [3*E*,7*E*,11*E*,15*E*,19*E*,23,*E*,27*E*] {solanochromene, solanachromene}
56100-19-7	1	0	0	2,2′-Bipyridine, 4-methyl-
56142-09-7	1	0	0	Pyrene, propyl-
56142-12-2	1	0	0	Pyrene, 1-ethyl-
56159-42-3	0	1	0	7*H*-Purin-6-amine, 7-β-*D*-glucopyranosyl-*N*-(phenylmethyl)-
56161-68-3	1	0	0	2-Heptenal, 2-methy-
30567-26-1				
56169-12-1	0	1	0	1-Cyclopentene-1-carboxylic acid, 2-methyl-5-(1-methylethyl)-
56219-06-8	0	1	0	9-Tetradecenoic acid, methyl ester, (*Z*)-
56375-33-8	1	0	0	1-Butanamine, *N*-nitroso-
56554-87-1	0	1	0	16-Octadecenal
56625-04-8	1	0	0	Formamide, *N*-(3-pyridinylmethyl)-
56631-57-3	1	0	0	1*H*-Indenol [1*H*-Inden-4-ol]
56681-06-2	0	1	0	3-Buten-2-one, 4-(2,3,6-trimethylphenyl)-
56682-25-8	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2R-[2α(R*),3aβ,5aα,9aβ,9bα]]-
56691-69-1	0	1	0	2-Cyclohexen-1-one, 5-[1-(acetyloxy)-1-methylethyl]-2-methyl-, (R)-
56711-38-7	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2R-[2α(S*),3aβ,5aα,9aβ,9bα]]-
56711-39-8	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(S*),3aα,5aβ,9aα,9bβ]]-
56711-40-1	0	1	0	Naphtho[2,1-*b*]furan-2-methanol, α-ethenyldodecahydro-α,3a,6,6,9a-pentamethyl-, [2S-[2α(R*),3aα,5aβ,9aα,9bβ]]-
56717-33-0	1	0	0	Quinoline, 2-ethyl-5,6,7,8-tetrahydro-
56745-61-0	1	0	0	2-Hexanone, 5-hydroxy-
56797-42-3	0	1	0	8,11-Heptadecadienal, (*Z,Z*)-
56797-44-5	0	1	0	8,11,14-Heptadecatrienal, (*Z,Z,Z*)-
56803-04-4	0	1	0	Synthase, flavanone
56805-23-3	0	1	0	3,6-Nonadien-1-ol
56832-73-6	1	0	0	Benzofluoranthene
56842-43-4	1	0	0	Pyridine, diphenyl-
56847-03-1	1	0	0	Octadecadienoic acid, methyl ester
56857-64-8	0	1	0	3a*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, 5,5a,6,7,8,9-hexahydro-α,α,3a,5a-tetramethyl-, [3aR-(3aα,5aβ,8β,9aR*)]- {phytuberol}
56859-02-0	0	1	0	1,2-Cyclohexanediol, 2-(3-hydroxy-1-butenyl)-1,3,3-trimethyl-
56879-46-0	0	1	0	2-Pyrrolidineacetic acid
56908-81-7	1	1	1	Naphthalene, pentamethyl-
56915-02-7	1	1	1	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-damascone}
56941-16-3	0	1	0	Dehydrogenase, malate (decarboxylating) (nicotinamide adenine dinucleotide (phosphate))
56947-55-8	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-(1-methylethyl)-
56986-88-0	1	0	0	Pyridine, 2-ethyl-3-methyl-
57011-15-1	1	0	0	2-Butanone, 3,4-dihydroxy-
57117-31-4	1	0	0	Dibenzofuran, 2,3,4,7,8-pentachloro-
57117-41-6	1	0	0	Dibenzofuran, 1,2,3,7,8-pentachloro-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
57117-44-9	1	0	0	Dibenzofuran, 1,2,3,6,7,8-hexachloro-
57147-25-8	1	0	0	2(1*H*)-Pyridinone, 3,4-dihydro-
57213-51-1	0	1	0	2(3*H*)-Furanone, dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-
57276-33-2	1	0	0	Ethanone, 1-cyclopropyl-2-(3-pyridinyl)-
57283-79-1	0	1	0	3-Hepten-2-one, 5-ethyl-6-methyl-
57295-30-4	1	0	0	Benzaldehyde, 3-hydroxy-4-methyl-
57523-93-0	0	1	0	4*H*-1-Benzopyran-4-one, octahydro-2,5,5,7a-tetramethyl-
57567-06-3	0	1	0	1-Naphthalenepropanol, α-ethenyldecahydro-7-hydroxy-α,5,5,8a-tetramethyl-2-methylene-
57567-07-4	0	1	0	2(1*H*)-Naphthalenone, 8-(3-hydroxy-3-methyl-4-pentenyl)-octahydro-4,4,8a-trimethyl-7-methylene-
57568-60-2	0	1	0	Benzeneacetaldehyde, α-(2-furanylmethylene)-
57601-69-1	0	1	0	1(4*H*)-Naphthalenone, 2-hydroxy-4,4,7-trimethyl-
57605-80-8	1	1	1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-
57605-81-9	1	1	1	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,8*E*,12S*,13*E*)]-
57633-59-7	1	0	0	Pyrene, 1,2,6,7-tetrahydro-
57646-30-7	0	1	0	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(2-furanylcarbonyl)-, methyl ester {Furalaxyl®}
57653-85-7	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,6,7,8-hexachloro-
57688-98-9	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol,1,5-dimethyl-11-methylene-8-(1-methylethyl)-,[1R-(1R*,2*E*,5S*,6*E*,8R*,10S*)]-
57688-99-0	1	0	0	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)- [2 CAS Nos.]
59284-87-6				
57760-47-1	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol,1,5-dimethyl-11-methylene-8-(1-methylethyl)-,[1R-(1R*,2*E*,5R*,6*E*,8S*,12S*)]-
57760-48-2	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol,1,5,11-trimethyl-8-(1-methylethyl)-,[1R-(1R*,2*E*,5S*,6*E*,8S*,10*E*,12S*)]-
57760-50-6	0	1	0	3,7,12-Pentadecatriene-2,14-dione, 4,8-dimethyl-11-(1-methylethyl)-, [S-(*E,E,E*)]-
57782-60-2	0	1	0	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)-
57782-61-3	0	1	0	6-Hepten-2-ol, 5-(1-methylethyl)-7-(tetrahydro-2-methyl-2-furanyl)-
57827-84-6	1	0	0	Benzochrysene
57835-92-4	1	0	0	Pyrene, 4-nitro-
57837-19-1	0	1	0	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-, methyl ester {Ridomil®}
57840-35-4	1	0	0	9-Octadecenoic acid (*Z*)-, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-
57878-30-5	0	1	0	1*H*-Inden-1-one, 2,3-dihydro-5-hydroxy-3-methyl-
57893-27-3	0	1	0	1-Oxaspiro[4.5]decane, 6-acetoxy-2,6,10,10-tetramethyl- {6-acetoxydihydrotheaspirane}
57934-85-7	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-, (exo,exo)-(±)-
102518-82-1				
57934-86-8	0	1	0	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (*E*)-(±)-
57935-33-8	0	1	0	4,6-Heptadien-1-ol, 6-methyl-3-(1-methylethyl)-, (*E*)-
57966-95-7	0	1	0	Acetamide, 2-cyano-2-methoxyimino-*N*-(ethylcarbamoyl)- {Cymoxanil®}
58000-93-4	1	1	1	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, acetate, {solanesyl acetate}
29144-38-5				
58001-00-6	0	1	0	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,5-dimethyl- [1α,2β,5α,7α(R*)]
58001-10-8	0	1	0	6,8-Dioxabicyclo[3.2.1]octane-7-methanol, 2-(1-methylethyl)-α,α,5-trimethyl-, (2-endo,7-exo)-(±)-
58002-07-6	0	1	0	2-Nonanone, 6,7-epoxy-8-hydroxy-5-(1-methylethyl)-
58023-72-6	1	1	1	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butynyl)-3,5,5-trimethyl- [2 CAS Nos.]
31162-45-5				
58064-43-0	1	1	1	3-Pyridinone
52536-09-1				
109-00-2				
58074-25-2	0	1	0	3*H*-Indol-3-one, 2,3,4,5,6,7-hexahydro- {4,5,6,7-tetrahydro-3-indolinone}
58200-70-7	1	0	0	Dibenzo[*b,e*][1,4]dioxin, 1,2,3,4,6,7,9-heptachloro-
58228-72-1	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-ethyl-5-methyl-
58239-50-2	0	1	0	2-Naphthalenol, decahydro-5,5,8a-trimethyl-, [2R-(2α,4aα,8aβ)]-
58308-53-5	0	1	0	1,2,3-Propanetricarboxylic-1,3-$^{14}C_2$ acid, 2-hydroxy-, labeled with ^{14}C {citric acid-^{14}C}
58315-84-7	0	1	0	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, [S-(*E,E*)]-
58430-01-6	1	0	0	Benz[*c*]acridine, 7,9,10-trimethyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
58461-27-1	1	0	0	4-Hexen-1-ol, 5-methyl-2-(1-methylethyl)-
58467-27-9	1	0	0	2,5-Pyrrolidinedione, 3-ethyl- [2 CAS Nos.]
58474-80-9	0	1	0	3-Decenal
58501-92-1	1	1	1	2,5-Pyrrolidinedione, 3-ethyl-4-methyl-
58539-27-8	1	0	0	Phenol, 2-methoxy-5-propyl-
58539-65-4	1	0	0	3-Pyridinecarboxamide, 2-methyl-
58548-38-2	1	0	0	Acenaphthylene, methyl-
58548-39-3	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene, methyl-
58548-40-6	1	0	0	Acenaphthylene, diphenyl-
58615-36-4	1	0	0	Dibenzopyrene
58628-98-1	1	0	0	2,4-Oxazolidinedione, 4,5-dimethyl-
58650-48-9	1	0	0	1*H*-Imidazole, 4-(1-methylethyl)-
58720-40-4	0	1	0	2-Butanone, 4-(2,3,6-trimethylphenyl)-
58853-80-8	1	0	0	Isoquinoline, methyl- {several isomers detected in MSS}
58861-90-8	1	0	0	Pyrazine, 2-methyl-5-phenyl-
58879-40-6	0	1	0	1,13-Tetradecadien-3-one
58886-94-5	1	1	1	Octadecanoic acid, hexacosyl ester
58924-34-8	1	0	0	Benzofuran, ethyl-
58924-35-9	1	0	0	1*H*-Indene, ethyl-
58927-84-7	0	1	0	4-Hepten-2-ol, 6-methyl-, (*E*)-
58934-57-9	0	1	0	4*H*-1-Benzopyran-4-one, 3-[[*O*-(6-deoxymannosyl)glucosyl]oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-
58947-96-9	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-2-one, 8-hydroxy-8,12-dimethyl-5-(1-methylethyl)-
58994-15-3	0	1	0	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-, monoamide with *N*-(3-aminopropyl)-1,4-butanediamine {caffeoylspermidine}
59001-33-1	0	1	0	2-Propenamide, 3-(3,4-dihydroxyphenyl)-*N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]- {dicaffeoylspermidine}
59017-02-6	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, 1,2,3,5a,8,10a-hexahydro-, (5aS-*cis*)-
59056-32-5	0	1	0	2*H*-Pyran-2-one, tetrahydro-6,6-dimethyl-4-(1-methylethyl)-
59170-14-8	1	1	1	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3β,4aβ,6aα,10aβ,10bα)]- {labd-14-ene, 8,13-epoxy-12α-hydroxy-, 12α-hydroxy-13-epimanoyl oxide}
59239-12-2	1	0	0	Pyridine, 2-ethyl-6-phenyl-
59262-52-1	0	1	0	2,7-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*E,E*)-
59262-53-2	0	1	0	Heptanoic acid, 3-(1-methylethyl)-6-oxo-, (S)-
59284-87-6	1	0	0	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)- [2 CAS Nos.]
57688-99-0				
59284-88-7	1	1	1	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, (1S, 2*E*, 5R, 6*E*, 8S, 11*E*) {β-3,8,13-duvatriene-1,5-diol}
59286-28-1	0	1	0	2,4-Decadienoic acid, 3-methyl-6-(1-methylethyl)-9-oxo-, (*Z,E*)-
59409-91-5	1	0	0	Pyridine, 2-(1-methyl-3-butenyl)-
59471-80-6	0	1	0	Cyclohexanone, 2-methyl-5-(1-methylethyl)-
499-70-7				
59534-35-9	1	0	0	1-Naphthalenol, methyl-
59534-36-0	1	0	0	2-Naphthalenol, methyl-
59551-02-9	1	0	0	5-Quinolinecarbonitrile
59573-83-0	0	1	0	5,10,12-Tridecatrien-2-one, 6,12-dimethyl-9-(1-methylethyl)-, [S-(*E,E*)]-
59576-26-0	1	0	0	Ethanone, 1-(4-methyl-2-pyridinyl)-
59576-31-7	1	0	0	Ethanone, 1-(4,6-dimethyl-2-pyridinyl)-
59576-98-6	0	1	0	2-Propenamide, 3-(4-hydroxyphenyl)-
59578-62-0	1	1	1	1-Butanone, 4-hydroxy-1-(3-pyridinyl)-
59578-66-4	1	1	1	3-Pyridinebutanol, δ-(methylnitrosoamino)- [2 CAS Nos.] {NNAL}
76014-81-8				{1-butanol, 4-(*N*-methylnitrosoamino)-1-(3-pyridinyl)-, 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-}
59615-45-5	1	0	0	1,1′-Binaphthalene, methyl-
59632-87-0	0	1	0	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*E*)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
59632-88-1	0	1	0	1,4-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-, 1-acetate, (*Z*)-
59669-26-0	0	1	0	Ethanimidothioic acid, *N*′,*N*′-(thiobis((methylimino)carbonyloxy))bis-, dimethyl ester {Thiodicarb®}
59708-73-5	0	1	0	Eicosanoic acid, 19-methyl-
59708-74-6	0	1	0	Docosanoic acid, 21-methyl-
59780-40-4	0	1	0	9,19-Cycloergostan-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-
59832-90-5	1	0	0	1,4-Naphthalenedione, 2,6,7-trimethyl-
59832-96-1	1	0	0	Phenol, 4-butyl-2-methoxy-
59977-50-3	0	1	0	Nuclease, mammalian deoxyribonucleate-nicking endo-
60007-87-6	1	1	1	Hexadecanoic acid, hexacosyl ester
60016-73-1	1	1	1	2(3*H*)-Furanone, dihydro-(2-oxopropyl)-
60026-07-5	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylethyl)-
60026-08-6	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(1-methylpropyl)-
60026-09-7	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-(2-methylpropyl)-
60026-10-0	1	1	1	2,6-Nonadienoic acid
60026-11-1	0	1	0	2,7,12-Cyclotetradecatrien-1-ol, 1,7-dimethyl-11-methylene-4-(1-methylethyl)-
60026-12-2	1	1	1	Benzofuran, 5-hydroxy-6,7-dimethyl-
60026-13-3	0	1	0	4-Penten-2-ol, 5-(tetrahydro-2-methyl-2-furanyl)-
60026-14-4	0	1	0	3-Tridecene-2,8-diol, 4,8,12-trimethyl-
60026-15-5	0	1	0	3-Pyrrolidinecarboxaldehyde, 2-methyl-
60026-16-6	0	1	0	Cyclohexenylideneacetaldehyde, 4-oxo-2,6,6-trimethyl-
60026-17-7	0	1	0	Pyrrolidine, 1-(3-methyl-1-oxobutyl)-
60026-18-8	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,11-dimethyl-5-methylene-8-(1-methylethyl)-
60026-19-9	0	1	0	1*H*-Pyrrole-2,5-dione, 3-propyl-
60026-20-2	1	1	1	Ethanone, 1-(2-pyrrolidinyl)- {2-acetylpyrrolidine}
60026-21-3	0	1	0	Cyclohexanone, 3,3,5-trimethyl-4-(3-oxo-1-butenyl)-
60026-22-4	1	0	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)- {6-epicyperone-1}
60026-23-5	0	1	0	1,3(2*H*,5*H*)-Naphthalenedione, 6,7,8,8a-tetrahydro-4,8a-dimethyl-6-(1-methylethenyl)-
60026-24-6	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-
60026-25-7	1	1	1	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(1-propenyl)-
60026-26-8	0	1	0	7-Hexadecen-6-one, 3,7,11,15-tetramethyl-
60026-27-9	0	1	0	Furo[3,2-*b*]furan-2(3*H*)-one, tetrahydro-3a-methyl-
60026-28-0	0	1	0	1*H*-Pyrrolo[2,1-*c*][1,4]oxazine-6-carboxaldehyde, 3,4-dihydro-3-oxo-4-(phenylmethyl)-
60026-30-4	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-methyl-
60046-87-9	1	1	1	1-Hexadecen-3-ol, 3,7,11,15-tetramethyl- {isophytol}
505-32-8				
60047-16-7	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 1,5-dimethyl-11-methylene-8-(1-methylethyl)-
60047-17-8	0	1	0	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-
60047-18-9	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-trien-5-ol, 1,5,11-trimethyl-8-(1-methylethyl)-
60047-19-0	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl- {4-ketodihydro-α-ionol}
60054-55-9	0	1	0	1-Hexadecanol, 7,11,15-trimethyl-3-methylene-
60091-00-1	0	1	0	2*H*-1-Benzopyran-2-one, 7-[(6-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]-6-methoxy-
60153-49-3	1	1	1	Propanenitrile, 3-(methylnitrosoamino)- {MNPN}
60308-81-8	0	1	0	Hexanoic acid, 4,5-dimethyl-
60321-02-0	0	1	0	Hydroxycinnamyl-CoA, quinate {hydroxycinnamyl transferase, quinate}
60382-88-9	1	0	0	Dibenzofluoranthene {at least two isomers in MSS}
60386-55-2	1	0	0	1,2-Cyclopentanedione, 3-(1-methylethyl)-
60393-63-7	0	1	0	2*H*-Pyran-2-one, tetrahydro-6-methyl-5-(1-methylethyl)-
60484-66-4	1	0	0	Benzonitrile, 4-propyl-
60485-38-3	0	1	0	9,19-Cyclocholest-24-en-3-ol, 4,14-dimethyl-, (3β,4α,5α)-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
60517-74-0	0	1	0	β-*D*-Glucopyranose, 1-(2-hydroxybenzoate)
60593-18-2	0	1	0	3,8-Tridecadiene-2,12-dione, 8-methyl-5-(1-methylethyl)-, [S-(*E,E*)]-
60619-46-7	1	1	1	3-Nonene-2,8-dione, 5-(1-methylethyl)-, [S-(*E*)]- [2 CAS Nos.] {oxysolanone}
35953-21-0				
101159-09-5				
60646-31-3	1	0	0	2(3*H*)-Furanone, dihydro-5-methyl-5-(1-methylethyl)-, (S)-
60655-87-0	0	1	0	Pyridinium, 1-α-*L*-arabinopyranosyl-3-carboxy-
60676-86-0	0	1	0	Silica, vitreous
60714-16-1	0	1	0	6,8-Nonadien-2-one, 6-methyl-5-(1-methylethenyl)-
60738-11-6	0	1	0	*L*-Tryptophan, labeled with ^{14}C
60759-94-6	0	1	0	Cyclohexanol, 1-(3-hydroxy-1-butenyl)-2,2-dimethyl-6-methylene-
60761-23-1	0	1	0	2-Butanone, 4-(2,2,6-trimethylcyclohexyl)-, *cis*- {tetrahydroionone}
60826-61-1	1	0	0	1*H*-Indene, trimethyl- {at least three isomers present in MSS}
60826-62-2	1	0	0	Dibenzofuran, methyl-
60826-63-3	1	0	0	1*H*-Benz[*f*]indene, methyl-
60826-64-4	1	0	0	11*H*-Benzo[*a*]fluorene, methyl-
60826-65-5	1	0	0	11*H*-Benzo[*b*]fluorene, methyl-
60826-66-6	1	0	0	7*H*-Benzo[*c*]fluorene, methyl-
60826-67-7	1	0	0	Benzo[*j*]fluoranthene, methyl-
60826-68-8	1	0	0	Acenaphthylene, dimethyl-
60826-69-9	1	0	0	Acenaphthylene, 1,2-dihydrotrimethyl-
60826-70-2	1	0	0	Acenaphthylene, trimethyl-
60826-71-3	1	0	0	1*H*-Benz[*f*]indene, dimethyl-
60826-72-4	1	0	0	Acenaphthylene, 1,2-dihydrotetramethyl-
60826-73-5	1	0	0	Acenaphthylene, tetramethyl-
60826-75-7	1	0	0	Pyrene, tetramethyl- {at least four isomers in MSS}
60826-77-9	1	0	0	Chrysene, trimethyl-
60826-78-0	1	0	0	Benz[*a*]anthracene, trimethyl-
60684-29-9	1	0	0	Acenaphthylene, 1,2-dihydrodimethyl-
60825-46-9	1	0	0	Phenol-$^{14}C_6$, 2-methoxy- {guaiacol-$^{14}C_6$}
60826-70-2	1	0	0	Acenaphthylene, trimethyl-
60826-73-5	1	0	0	Acenaphthylene, tetramethyl-
60826-74-6	1	0	0	Fluoranthene, dimethyl- {at least four isomers in MSS}
60826-75-7	1	0	0	Pyrene, tetramethyl- {at least four isomers in MSS}
60826-76-8	1	0	0	Triphenylene, dimethyl-
60826-77-9	1	0	0	Chrysene, trimethyl-
60826-78-0	1	0	0	Benz[*a*]anthracene, trimethyl-
60826-79-1	1	0	0	Triphenylene, trimethyl-
60828-13-9	0	1	0	6-Nonen-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-, (6*E*)-
60851-34-5	1	0	0	Dibenzofuran, 2,3,4,6,7,8-hexachloro-
60858-07-3	1	0	0	Furan, 2-(3-hexenyl)-5-methyl-
60918-47-0	1	0	0	Benzofluorene, methyl- {at least four isomers in MSS}
60918-97-0	0	1	0	1,3,4-Oxadiazol-2-amine, *N*-(4-bromophenyl)-5-(1-naphthalenylmethyl)-
60922-91-0	1	0	0	Hexadecane, mixture with pentane
60924-66-5	0	1	0	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-
60924-86-9	0	1	0	2,6,10,14,18,22,26,30,33-Hexatriacontanonaene-1,35-diol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)-
60924-87-0	0	1	0	2,6,10,14,18,22,26,30,35-Hexatriacontanonaene-1,34-diol, 3,7,11,15,19,23,27,31,35-nonamethyl-, (all-*E*)-
60976-73-0	1	1	1	1-Pentadecene, 2,6,10,14-tetramethyl- [3 CAS Nos.] {norphytene}
2140-82-1				
100404-00-0				
61010-32-0	0	1	0	Isoquinoline, 1-[(4-methoxy-3-nitrophenyl)methyl]-, mononitrate
61089-87-0	1	0	0	Benzofluorene

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
61116-99-2	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, [1R-[1α(*E*),4β,6α]]-
61128-87-8	1	0	0	Phenanthrene, methoxy-
61141-66-0	0	1	0	1,1′-Biphenyl, 3,4-diethyl-
61142-00-5	1	0	0	Cyclohexane, 1,2,4,5-tetraethyl-
61185-25-9	0	1	0	Bicyclo[3.3.1]non-6-en-2-one, 4,4,9-trimethyl-8-methylene-, anti-
61190-74-7	1	1	1	2-Furancarboxamide, *N*-(2-furanylmethyl)-
61193-19-9	1	0	0	Octane, methyl-
61193-21-3	1	0	0	Decane, methyl-
61205-39-8	1	0	0	2-Cyclopenten-1-one, ethyl-2-hydroxy-
61205-40-1	1	1	1	2-Cyclopenten-1-one, 2-hydroxypropyl-
61261-04-9	1	0	0	Cyclopentaphenanthrene
61263-48-7	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,8-tetramethyl-, acetate, (R)-
61364-95-2	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,4-diethyl-
61391-07-9	1	0	0	3-Pyridinecarbonitrile, 5-ethyl-
61434-67-1	0	1	0	Ethene, 1-(4-hydroxyphenyl)-2-(3,5-dihydroxyphenyl)-, (*Z*)- {*cis*-resveratrol}
61445-55-4 133201-39-5	1	1	1	Butanoic acid, 4-(methylnitrosoamino)- = butanoic acid, 4-[(nitrosomethyl)amino]- [2 CAS Nos.] {NMBA}
61480-97-5	1	0	0	1*H*-Pyrrole, 1-(1-oxobutyl)-
61480-98-6	0	1	0	2-Pyrrolidinecarboxaldehyde
61480-99-7	1	0	0	Pyrrolidine, 1-[(5-methyl-2-furanyl)methyl]-
61481-02-5	1	0	0	2-Furanmethanol, 5-(1-pyrrolidinylmethyl)-
61653-41-6	0	1	0	*D*-lyxo-Hexonic acid, 2-deoxy-, γ-lactone
61679-89-8	1	0	0	2,5-Furandione, 3-propyl-
61771-67-3	1	0	0	3-Pyridinamine, 6-methoxy-*N*-methyl-
61837-35-2	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α-hexyl-
61837-36-3	0	1	0	1*H*-Pyrrole-1-propanoic acid, 2-formyl-β-methyl-
61837-37-4	0	1	0	1*H*-Pyrrole-1-propanoic acid, β-ethyl-2-formyl-
61837-38-5	0	1	0	1*H*-Pyrrole-1-butanoic acid, 2-formyl-
61837-39-6	0	1	0	1*H*-Pyrrole-1-butanoic acid, 2-formyl-γ-methyl-
61837-40-9	0	1	0	1*H*-Pyrrole-1-hexanoic acid, 2-formyl-
61837-41-0	0	1	0	1*H*-Pyrrole-1-octanoic acid, 2-formyl-
61837-42-1	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-formyl-α,5-dimethyl-
61837-43-2	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-ethyl-5-formyl-α-(2-methylpropyl)-
61837-44-3	0	1	0	1*H*-Pyrrole-1-butanoic acid, 2-formyl-5-methyl-
61868-19-7	1	0	0	1-Hexadecene, 2-methyl-
61868-20-0	1	0	0	1-Octadecene, 2-methyl-
61886-71-3	1	1	1	Naphthalene, 1-ethyl-8-methyl-
61891-55-2	1	0	0	β-*D*-Glucopyranose, 1,6-anhydro-, monoacetate
61891-57-4	1	0	0	5*H*-Cyclopentapyrazine, dimethyl-
61891-65-4	1	0	0	2-Piperidinone, methyl-
61891-74-5	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, tetrahydro-
61891-76-7	1	0	0	Ethanone, 1-(dihydro-3,4-dimethylpyrrol-2-yl)-
61892-42-0	1	0	0	2(5*H*)-Furanone, 3-acetyl-4-methyl-
61892-43-1	1	0	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-4-hydroxy-
61892-44-2	1	0	0	2(3*H*)-Furanone, 5-(acetyloxy)dihydro-4-hydroxy-
61892-45-3	1	0	0	2(3*H*)-Furanone, dihydro-4-hydroxy-3-(hydroxymethyl)-
61892-46-4	1	0	0	2(3*H*)-Furanone, dihydro-4-ethynyl-5-hydroxy-3-methyl-
61892-47-5	1	0	0	2(3*H*)-Furanone, dihydro-5-hydroxy-4-methyl-
61892-48-6	1	0	0	2(3*H*)-Benzofuranone, hexahydro-3a-hydroxy-
61892-49-7	1	0	0	2(3*H*)-Furanone, dihydro-5-(1-oxopropyl)-
61892-50-0	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-5-methyl-

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
61892-51-1	1	0	0	Hexonic acid, 3,6-dideoxy-, γ-lactone
61892-52-2	1	0	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-(2-hydroxyethyl)-
61892-53-3	1	0	0	2(5*H*)-Furanone, 5-acetyl-
61892-54-4	1	1	1	2(5*H*)-Furanone, 3-methyl-5-methylene-
61892-55-5	1	0	0	2(3*H*)-Furanone, dihydro-5-(hydroxymethyl)-4-methyl-
61892-56-6	1	0	0	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-
61892-57-7	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-5-(hydroxymethyl)-4-methyl-
61892-58-8	1	0	0	2(3*H*)-Furanone, 3-(hydroxymethyl)-5-methyl-
61892-59-9	1	0	0	1,2,3-Propanetriol, 1-acetate 2-formate
61892-60-2	1	1	1	Acetic acid, hydroxy-, 2-hydroxypropyl ester
61892-61-3	1	1	1	2-Furancarboxylic acid, 2-(acetyloxy)ethyl ester
61892-62-4	0	1	0	2,3-Oxiranedimethanol, monopropanoate
61892-63-5	1	0	0	2-Propenamide, *N*-(1-oxopropyl)-
61892-64-6	1	1	1	2,3′-Bipyridine, 1-acetyl-1,2,3,6-tetrahydro-, (S)- {*N*′-acetylanatabine}
61892-65-7	1	1	1	[2,3′-Bipyridine]-1(2*H*)-carboxaldehyde, 3,6-dihydro-, (S)- {*N*′-formylanatabine}
61892-66-8	1	0	0	Butanamide, 3-cyano-3-methyl-
61892-67-9	1	0	0	2-Pentenamide, *N*-methyl-
61892-68-0	1	0	0	Propanamide, 3-cyano-
61892-69-1	1	0	0	Pentanamide, 3-methyl-
61892-70-4	1	0	0	2,6-Piperidinedione, 4-methoxy-
61892-71-5	1	1	1	1*H*-Pyrrole-2,5-dione, 3,4-bis(hydroxymethyl)-1-methyl-
61892-72-6	1	1	1	1*H*-Pyrrole-2,5-dione, 3-ethyl-4-(hydroxymethyl)-
61892-73-7	1	0	0	1*H*-Pyrrole-2,5-dione, 3-(hydroxymethyl)-
61892-74-8	1	0	0	2,5-Pyrrolidinedione, 3-ethylidene-1-methyl-
61892-75-9	1	0	0	4*H*-Imidazol-4-one, 1,5-dihydro-1-methyl-
61892-76-0	1	0	0	2(1*H*)-Pyridinone, 5-acetyl-3,4-dihydro-
61892-77-1	1	0	0	2(1*H*)-Pyridinone, 3,6-dihydro-
61892-78-2	1	0	0	2,5-Piperazinedione, 3-(2-propenyl)-
61892-79-3	1	0	0	1*H*,7*H*-Pyrazolo[1,2-*a*]pyrazole-1,7-dione, tetrahydro-
61892-80-6	1	0	0	2*H*-Pyrrol-2-one, 1-acetyl-3-ethyl-1,5-dihydro-4-methyl-
61892-81-7	1	0	0	1-Butanone, 1-pyrazinyl-
61892-82-8	1	0	0	3-Buten-2-one, 4-(4-hydroxy-1-cyclohexen-1-yl)-
61892-83-9	1	0	0	2-Cyclopenten-1-one, 2-methyl-4-(1-methylethyl)-
61892-84-0	1	0	0	2-Cyclopenten-1-one, 2-(2-oxopropyl)-
61892-85-1	1	0	0	2,5-Hexanedione, 3-hydroxy-
61892-86-2	1	0	0	4*H*-Pyran-4-one, 3,5-dihydroxy-2,6-dimethyl-
61892-87-3	1	0	0	4*H*-Pyran-4-one, 2-hydroxy-5-methyl-
61892-88-4	1	0	0	4*H*-Pyran-4-one, 2-hydroxy-3-methyl-
61892-89-5	1	0	0	3-Pyrrolidinone, 1-methyl-5-(2-oxopropyl)-
61892-90-8	1	0	0	2-Pyrrolidinone, 1-(2-oxopropyl)-
61892-91-9	1	0	0	Pyrazinebutanol, 3-methyl-
61892-92-0	1	1	1	Pyrazineethanol, 3-methyl-
61892-93-1	1	1	1	Pyrazineethanol, 6-methyl-
61892-94-2	1	0	0	3,4-Furandiol, tetrahydro-3-methyl-
61892-95-3	1	1	1	Pyrazinemethanol, 5-methyl- = pyrazinemethanol, 3-methyl-
61892-96-4	1	0	0	2*H*-Pyran-6-methanol, 3,4-dihydro-3-hydroxy-
61892-97-5	1	0	0	2-Pyrrolidinemethanol, 5-methyl-
61892-98-6	1	0	0	2,3′-Bipyridine, 1-ethyl-1,2,3,6-tetrahydro-, (S)-
61892-99-7	1	0	0	2(1*H*)-Pyridinone, 6-ethyl-
61893-00-3	1	0	0	3-Pyridinol, 5,6-dimethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
61893-01-4	1	0	0	3-Pyridinol, 6-ethyl-4-methyl-
61893-02-5	1	1	1	3-Pyridinol, 2-ethyl-
61893-03-6	1	0	0	3-Pyridinol, 4-propyl-
61893-04-7	1	0	0	3-Pyridinol, 5-propyl-
61893-05-8	1	0	0	1*H*-Furo[2,3-*d*]imidazole, 2-methyl-
61893-06-9	1	0	0	1*H*-Imidazole, 2-(1-methylpropyl)-
61893-07-0	1	0	0	1*H*-Imidazole, 4-methyl-2-(1-methylpropyl)-
61893-08-1	1	0	0	1*H*-Imidazole, 4-(2-methylpropyl)-
61893-09-2	1	0	0	2,4-Imidazolidinedione, 1-ethyl-
61893-10-5	1	0	0	2,4-Imidazolidinedione, 1-(1-methylethyl)-
61893-11-6	1	0	0	1*H*-Pyrido[2,3-*b*]indole, 2-ethyl-
61893-12-7	1	0	0	Pyrrolidine, 1-(2-furanylmethyl)-
61893-13-8	1	0	0	2,4(1*H*,3*H*)-Pyrimidinedione, 3-ethyldihydro-5-methyl-
61893-14-9	0	1	0	2-Cyclopenten-1-one, 2,3-dimethyl-5-(1-methylethyl)-
61927-07-9	1	0	0	Bicyclo[4,3,0]non-6-en-8-one, 3-hydroxy-9-oxo-1,5,5-trimethyl-
61929-05-3	1	0	0	5*H*-Cyclopentapyrazine, 2,3-dimethyl-
61949-26-6	1	0	0	1-Hexanol, methyl-
61949-29-9	1	0	0	Pyrrolo[1,2-*a*]pyrazine-1,4-dione, hexahydro-3-propyl-
61989-58-0	1	0	0	2(3*H*)-Furanone, dihydro-5-(1,2-dihydroxyethyl)-
61989-59-1	1	0	0	Hexonic acid, 2,3-dideoxy-, γ-lactone, monoacetate
61989-60-4	1	0	0	Pentonic acid, 2,3-anhydro-, γ-lactone
62003-47-8	1	0	0	2*H*-Pyrrol-2-one, 1,3-dihydro-5-(3-pyridinyl)-
62003-48-9	1	0	0	2-Pyridinol, 5-ethyl-
62060-10-0	1	0	0	2-Tridecene, 2-methyl-
62121-32-8	0	1	0	2-Naphthalenol, decahydro-2,5,5,8a-tetramethyl-1-[(3-methyl-2-furanyl)methyl]-, [1R-(1α,2β,4aβ,8aα)]-
62137-28-4	0	1	0	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-
62137-29-5	0	1	0	*L*-Proline, 4-[(*O*-β-*L*-arabinofuranosyl-(1→3)-*O*-β-*L*-arabinofuranosyl-(1→2)-*O*-β-*L*-arabinofuranosyl-(1→2)-β-*L*-arabinofuranosyl)oxy]-, *trans*-
62168-75-6	0	1	0	Deacylase
62172-52-5	1	0	0	Tetradecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
62172-54-7	1	0	0	Octadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
62213-14-3	0	1	0	Glucanase, endo-1,3(4)-β-
62238-29-3	1	0	0	Cyclohexane, 1-ethyl-1,3-dimethyl-, (*E*)-
62238-30-6	1	0	0	Cyclohexane, 1-ethyl-1,4-dimethyl-, (*Z*)-
62238-31-7	1	0	0	Cyclohexane, 1-ethyl-1,3-dimethyl-, (*Z*)-
62238-32-8	1	0	0	Cyclohexane, 1-ethyl-1,4-dimethyl-, (*E*)-
62238-33-9	1	0	0	Cyclohexane, 1-ethyl-2-propyl-
62244-24-0	1	0	0	1,2,3-Propanetriol, 1-propanoate, (R)-
62338-07-2	1	0	0	1,3-Hexadiene, 2,5-dimethyl-3-ethyl-
62376-15-2	1	0	0	Cycloundecane, 1,1,2-trimethyl-
62446-36-0	0	1	0	Hexuronic acid
62450-06-0	1	0	0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1,4-dimethyl- {Trp-P-1}
62450-07-1	1	0	0	5*H*-Pyrido[4,3-*b*]indol-3-amine, 1-methyl- {Trp-P-2}
62498-80-0	0	1	0	15-Oxabicyclo[9.3.1]pentadeca-2,6-diene-5,12-diol,1,5,11-trimethyl-8-(1-methylethyl)-,[1R-(1R*,2*E*,5S*,6*E*,8R*,11S*,12S*)]-
62504-27-2	0	1	0	*L*-Histidine, *N*-(1-carboxyethyl)-, (R)-
62512-22-5	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-
62512-23-6	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butyl]-3,5,5-trimethyl-
62512-25-8	0	1	0	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-
62512-96-3	0	1	0	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)butyl-
62574-25-8	0	1	0	Spiro[4.5]dec-6-en-8-one, 9-(β-*D*-glucopyranosyloxy)-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]-
62574-27-0	0	1	0	Spiro[4.5]dec-6-en-8-one, 2-[1-[(β-*D*-glucopyranosyloxy)methyl]ethenyl]-6,10-dimethyl-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
62574-29-2	0	1	0	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-
62623-87-4	0	1	0	Spiro[4.5]dec-6-en-8-one, 2-[2-(β-*D*-glucopyranosyloxy)-1-hydroxy-1-methylethyl]-6,10-dimethyl-
62623-88-5	0	1	0	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6,10-dimethyl-2-(1-methylethenyl)-, [5S-[5α(S*),9α,10β]]-
62660-03-1	0	1	0	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-
62672-96-2	1	0	0	1*H*-Pyrrole, 1-(1-cyclohexen-1-yl)-
62726-14-1	1	0	0	Benzenediol, nitro- {at least four isomers in MSS}
62744-64-3	1	0	0	Phenol, methylpropyl-
62783-95-3	1	0	0	Piperidine, 1-(1-oxopentyl)-2-(3-pyridinyl)-, (S)-
62784-01-4	1	0	0	Piperidine, 1-(1-oxohexyl)-2-(3-pyridinyl)-, (S)-
62813-37-0	1	0	0	Anthracenamine
62924-70-3	0	1	0	Benzenemethanamine, 2-chloro-*N*-(2,6-dinitro-4-(trifluoromethyl)phenyl)-*N*-ethyl-6-fluoro- {Flumetralin®}
62930-75-0	0	1	0	Glucuronomannan
63042-66-0	1	0	0	Benzo[*h*]quinoline,2,3,4-trimethyl-
63072-44-6	0	1	0	Pentanone, methyl-
63100-39-0	0	1	0	Hemicellulose A
63100-40-3	0	1	0	Hemicellulose B
63194-18-3	1	0	0	Benzanthracene, methyl-
63231-63-0	0	1	0	Ribonucleic acid
63316-28-9	0	1	0	Pentanoic acid, 5-amino-3-hydroxy-
63316-29-0	0	1	0	Pentanoic acid, 5-amino-2-hydroxy-, (R)-
63316-30-3	0	1	0	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (R)-
63317-82-8	1	1	1	Octadecanoic acid, octacosyl ester
63317-83-9	1	1	1	Octadecanoic acid, triacontyl ester
63346-81-6	1	1	1	1,2,3-Propanetriol, labeled with ^{13}C {glycerol-^{13}C}
63372-50-9	1	0	0	9*H*-Fluorene, tetramethyl-
63450-36-2	0	1	0	Nonadien-1-ol
63451-42-3	1	0	0	Acridine, 9,10-dihydro-9,9-dimethyl-2-(1-methylethyl)-
63455-19-6	1	0	0	Benzo[*a*]pyrenol
63626-79-9	1	0	0	3-Oxabicyclo[3.3.1]nonan-2-one, 9-hydroxy-5-methyl-
63637-90-1	1	0	0	2,4-Imidazolidinedione, 3-(1-methylethyl)-
63648-83-9	0	1	0	α-*D*-Glucopyranoside, 3-*O*-acetyl-β-*D*-fructofuranosyl-
63668-37-1	1	0	0	2-Pyridinecarboxamide, 6-methyl-
63700-30-1	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dihydroxy-3-methyl-
63785-24-0	0	1	0	1-Pentacosanol, 24-methyl-
63785-25-1	0	1	0	1-Hexacosanol, 24-methyl-
63785-26-2	0	1	0	1-Heptacosanol, 26-methyl-
63863-33-2	1	0	0	Cinnoline, dihydro-
63871-00-1	1	0	0	Hexadecatrien-1-ol, 3,7,11,15-tetramethyl-
63889-75-8	0	1	0	Decadienoic acid {sebacic acid}
63892-00-2	0	1	0	5-Octenoic acid
63892-02-4	0	1	0	Pentanedioic acid, 2-(1-methylethyl)-, (S)-
63892-03-5	0	1	0	2-Heptenoic acid, 3-(1-methylethyl)-6-oxo-, (Z)-
63892-04-6	0	1	0	2,7,9-Decatrienoic acid, 3,9-dimethyl-6-(1-methylethyl)-, (*E,E*)-
63907-54-0	0	1	0	1-Tricosanol, 22-methyl-
64031-89-6	1	0	0	Naphthalene, 2-ethenylmethyl- {at least two isomers in MSS}
64031-90-9	1	0	0	1*H*-Benz[*e*]indene, methyl-
64031-91-0	1	0	0	Perylene, methyl- {at least two isomers in MSS}
64079-00-1	0	1	0	Furan, butyl-
64079-01-2	0	1	0	Furan, pentyl-
64083-16-5	1	0	0	Naphthofuran
64090-50-2	0	1	0	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-
64091-90-3	1	1	1	3-Pyridinebutanal, γ-(methylnitrosoamino)- {NNA}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
64091-91-4	1	1	1	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- [3 CAS Nos.] {NNK}
126165-82-0				{1-Butanone, 4-[(nitrosomethyl)amino]-1-(3-pyridinyl)-}
110053-55-9				
121268-99-3				
64114-31-4	1	1	1	Pyridine, 2-methyl-3-(1-methyl-2-pyrrolidinyl)- {2-methylnicotine}
64130-24-1	1	1	1	6,8-Nonadien-2-ol, 8-methyl-5-(1-methylethyl)- {solanol isomer}
64142-45-6	1	1	1	3-Pyridinebutanal, γ-(methylnitrosoamino)-, (*Z*)-
64158-98-1	1	0	0	Indeno[1,2,3-*cd*]pyrene, methyl- {at least two isomers present in MSS}
64158-99-2	1	0	0	Indeno[1,2,3-*cd*]pyrene, dimethyl- {at least two isomers present in MSS}
64291-81-2	0	1	0	2(3*H*)-Furanone, dihydrodimethyl-
64294-96-8	1	0	0	9*H*-Fluorenamine
64350-07-8	1	0	0	Hexanenitrile, 2-hydroxy-
64389-08-8	1	0	0	Pyridine, 2-(1,5-dimethyl-1*H*-pyrrol-2-yl)-
64401-21-4	1	0	0	Pyrene, 1,3-dimethyl-
64461-84-3	0	1	0	β-*D*-Glucopyranose, 6-(3-phenyl-2-propenoate)
64502-89-2	1	0	0	2-Pentanone, 1-hydroxy-
64681-69-2	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2R-(2α,3α,4aα,6aβ,10aα,10bβ)]-
64681-70-5	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2S-(2α,3α,4aβ,6aα,10aβ,10bα)]-
64760-14-1	1	0	0	Benzo[*ghi*]fluoranthene, dimethyl-
64760-15-2	1	0	0	Coronene, dimethyl-
64760-18-5	1	0	0	Cyclopenta[*cd*]pyrene, 3,4-dihydromethyl-
64760-19-6	1	0	0	Perylene, dimethyl-
64760-20-9	1	0	0	Benzo[*b*]triphenylene, methyl-
64760-21-0	1	0	0	Benzo[*e*]pyrene, trimethyl-
64760-22-1	1	0	0	Benzo[*ghi*]perylene, dimethyl- {at least three isomers in MSS}
64760-23-2	1	0	0	Benzo[*ghi*]perylene, trimethyl- {at least two isomers in MSS}
64760-24-3	1	0	0	Dibenzo[*def,mno*]chrysene, dimethyl- {at least two isomers in MSS}
64808-91-9	1	0	0	Hexacosene
64811-57-0	1	0	0	Pyridine, dihydro-3-(1-methyl-I*H*-pyrrol-2-yl)-
64811-58-1	1	0	0	Quinoxaline, dihydro-
64811-59-2	1	0	0	Quinazoline, dihydro-
64828-44-0	1	0	0	Acridine, ethyl-
64828-45-1	1	0	0	Acridine, propyl-
64828-46-2	1	0	0	Quinoxaline, ethyl-
64828-47-3	1	0	0	Quinazoline, ethyl-
64828-48-4	1	0	0	Quinazoline, methyl-
64828-49-5	1	0	0	Isoquinoline, (1-methylethyl)-
64828-50-8	1	0	0	Isoquinoline, butyl-
64828-51-9	1	0	0	Isoquinoline, ethyl-
64828-52-0	1	0	0	Quinoline, propyl-
64828-53-1	1	0	0	Pyrenamine, *N*-methyl-
64828-54-2	1	0	0	Pyridine, methylphenyl-
64828-55-3	1	0	0	Pyridine, phenylpropyl-
64828-56-4	1	0	0	Quinoxaline, methyl-
64844-44-6	1	0	0	1*H*-Indole, propyl-
64844-45-7	1	0	0	1*H*-Indole, ethylmethyl-
64844-46-8	1	0	0	1*H*-Indole, methylpropyl-
64844-47-9	1	0	0	1*H*-Indole, dimethylethyl-
64844-48-0	1	0	0	1*H*-Indole, tetramethyl-
64844-49-1	1	0	0	1*H*-Indole, dimethylpropyl-
64844-50-4	1	0	0	1*H*-Indole, ethylpropyl-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
64844-51-5	1	0	0	9*H*-Carbazole, trimethyl-
64844-52-6	1	0	0	1*H*-Indole, methylphenyl-
64844-53-7	1	0	0	9*H*-Carbazole, tetramethyl-
64849-96-3	1	0	0	Pyridine, ethylphenyl-
64849-97-4	1	0	0	Phenanthrenamine
64849-98-5	1	0	0	Isoquinoline, propyl-
64849-99-6	1	0	0	Isoquinolinecarbonitrile
64850-00-6	1	0	0	Quinolinecarbonitrile
64850-01-7	1	0	0	[1,1′-Biphenyl]amine, *N*-methyl-
64859-47-8	1	0	0	Bipyridine, methyl- {four isomers detected in MSS}
64859-48-9	1	0	0	Bipyridine, ethyl-
64859-54-7	1	0	0	Benzocarbazole, methyl-
64859-55-8	1	0	0	Benzocarbazole, dimethyl-
64973-79-1	1	0	0	Isoquinoline, dihydro-
64990-23-4	1	0	0	Pyrenamine
65017-80-3	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-
34318-21-3				{4-keto-α-ionol, 4-oxo-α-ionol}
65017-84-7	0	1	0	5,8-Undecadien-2-one, 6,10-dimethyl-10-hydroxy- (*E,E*)-
133561-45-2				
65017-85-8	0	1	0	2-Nonen-4-one, 8-hydroxy-3-methyl-, (*E*)-
65028-58-2	0	1	0	Pectic acid, magnesium salt
65058-12-0	0	1	0	Hemicellulose C
65129-00-2	1	0	0	5*H*-Cyclopentapyrazine, 2-ethyl-
65307-84-8	1	0	0	Pyridine, propyl-
65307-85-9	1	0	0	Pyridine, pentyl-
65310-49-1	1	0	0	2-Cyclohexen-1-one, 2-hydroxy-3-propyl-
65312-74-5	1	0	0	Quinoline, methyltetrahydro-
65312-75-6	1	0	0	Isoquinoline, methyltetrahydro
65312-76-7	1	0	0	Quinoline, dihydroethyl-
65312-77-8	1	0	0	Isoquinoline, dihydroethyl-
65312-78-9	1	0	0	Quinoline, dihydromethyl-
65312-79-0	1	0	0	Isoquinoline, dihydromethyl-
65319-44-0	1	0	0	Naphthalene, dimethylethyl-
65319-49-5	1	0	0	9*H*-Fluorene, ethyl- {at least two isomers in MSS}
65319-51-9	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene, ethyl-
65331-00-2	1	0	0	2(3*H*)-Furanone, dihydro-4-(2-oxopropyl)-
65338-07-0	1	0	0	Naphthalene, dimethyl-1,2,3,4-tetrahydro- [2 CAS Nos.]
51855-29-9				{at least five isomers in MSS}
65357-69-9	1	0	0	Benzopyrene, methyl-
65375-17-9	1	0	0	Pyridine, propenyl-
65375-18-0	1	0	0	Pyridine, butenyl- {three isomers detected}
65416-14-0	0	1	0	Propanoic acid, 2-methyl-, 2-methyl-4-oxo-4*H*-pyran-3-yl ester
65416-59-3	0	1	0	1-Oxaspiro[4,5]dec-7-ene, 6-methylene-2,10,10-trimethyl- {vitispirane}
65436-85-3	1	0	0	2-Cyclopenten-1-one, propyl-
65436-86-4	1	0	0	1*H*-Inden-1-one, 2,3-dihydromethyl- {four isomers detected}
65445-62-7	1	1	1	3-Piperidinecarboxylic acid, 1-nitroso-
65452-01-9	1	0	0	2-Cyclopenten-1-one, methyl-
65462-39-7	1	0	0	**2-Cyclopenten-1-one, ethyl-**
65513-74-8	0	1	0	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-6-[1-(hydroxymethyl)ethenyl]-4,4a-dimethyl-, (1α,3β,4β,4aα,6α)-
65545-81-5	0	1	0	Benzeneacetaldehyde, α-(2-furanylmethylene)-, (*E*)-
65588-69-4	0	1	0	Naphtho[2,1-*b*]furan, dodecahydro-3a,6,6,9a-tetramethyl-, [3aR-(3aα,5aβ,9aα,9bβ)]- {ambroxide, ambroxyl}
6790-58-5				

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
65596-29-4	0	1	0	3,6-Dodecadienedioic acid, 10-hydroxy-4,9-dimethyl-
65620-50-0	0	1	0	1-Oxaspiro[4.5]decane, 6-hydroxy-2,6,10,10-tetramethyl- {6-hydroxydihydrotheaspirane}
65644-56-6	0	1	0	Propanoic acid, 2,3-dihydroxy-, calcium salt
65712-87-0	1	0	0	2*H*-Pyran-3(4*H*)-one, dihydro-6-methoxy-
65716-44-1	0	1	0	2,7-Octanedione, 3,3-dimethyl-
65716-45-2	0	1	0	2-Octanone, 7-hydroxy-3,3-dimethyl-, (±)-
65719-03-1	1	0	0	Pyridine, 3-(3,4-dihydro-2-methyl-2*H*-pyrrol-5-yl)-
65734-44-3	1	0	0	Pyridine, 3-(1,5-dimethyl-1*H*-pyrrol-2-yl)-
65745-66-6	1	0	0	Quinoline, 5-ethyl-
65777-08-4	1	0	0	Benzophenanthrene
65789-44-8	1	0	0	Acridine, 4-ethyl-
65820-56-6	0	1	0	Hexacosane, 3-methyl-
65820-58-8	1	1	1	Octacosane, 3-methyl-
66016-71-5	0	1	0	1,2-Cyclopentanedicarboxylic acid, 1-methyl-3-(1-methylethyl)-
66161-17-9	1	0	0	Pyrene, tetrahydro-
66164-30-5	1	0	0	Phenol, 3-ethenyl-4-methyl-
66214-27-5	1	1	1	Tritriacontane, 2-methyl-
66246-88-6	0	1	0	1,2,4-Triazole, 1-(2-(2,4-dichlorophenyl)pentyl)- {Penconazole®}
66274-27-9	1	0	0	Pentanoic acid, 5-hydroxy-4-oxo-, methyl ester
66288-40-2	1	0	0	Heneicosenoic acid, 19-methyl-
66288-41-3	1	0	0	Heneicosenoic acid, 20-methyl-
66288-42-4	1	1	1	Pyrazine, butenyl-
66288-51-5	1	0	0	1*H*-Inden-1-one, 2,3-dihydrotrimethyl- {three isomers detected}
66309-74-8	1	0	0	2(5*H*)-Furanone, 3,4-dimethyl-5-(1-propenyl)-
66309-75-9	1	0	0	2(5*H*)-Furanone, 5-ethenyl-
66309-76-0	1	0	0	1(3*H*)-Isobenzofuranone, 4,5,6,7-tetrahydro-
66309-77-1	1	0	0	Ethanone, 1-(4-ethyl-2,3-dimethylphenyl)-
66309-79-3	1	0	0	3-Cyclopentene-1,2-dione, 4-methyl-
66309-80-6	1	0	0	2-Cyclopenten-1-one, 2-methyl-5-methylene-
66309-82-8	1	0	0	2-Cyclopenten-1-one, 2,4,5-trimethyl-
66309-83-9	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-2,6-dimethyl-
66309-84-0	1	0	0	2-Pentanone, 5-hydroxy-4-methyl-
66309-85-1	1	1	1	5,9,13,17,21-Tricosapentaen-2-one, 6,10,14,18,22-pentamethyl-
66309-86-2	1	0	0	1*H*-Isoindole-1,3(2*H*)-dione, 4,5-dimethyl-
66309-87-3	1	0	0	1*H*-Pyrrole, 1-(2-methyl-1-cyclohexen-1-yl)-
66309-88-4	1	1	1	Tetratriacontane, 3-methyl-
66309-89-5	1	0	0	2,6,10,14,18,22,26,30-Dotriacontaoctaene, 2,6,10,14,18,22,26,30-octamethyl-, (all-*E*)-
66309-90-8	1	0	0	Naphthalene, 1,4-dimethyl-5-ethyl-
66309-91-9	1	0	0	Butanamide, 2,3-dimethyl-
66324-66-1	0	1	0	1-Naphthalenol, 1,2,3,4-tetrahydro-4,5,8-trimethyl-
66327-99-9	1	0	0	2,6,10,14,18,22,26,30,34-Hexatriacontanonaene, 2,6,10,14,18,22,26,30,34-nonamethyl-, (all-*E*)-
66328-00-5	1	0	0	2,6,10,14,18,22,26-Octacosaheptaene, 2,6,10,14,18,22,26-heptamethyl-, (all-*E*)-
66369-21-9	0	1	0	Glucuronoarabinoxylan
66434-99-9	0	1	0	3-Buten-2-one, 4-(5-methyl-2-furanyl)-, (*E*)-
66537-22-2	1	1	1	Glucometasaccharinic acid, γ-lactone
66576-73-6	0	1	0	Pentatriacontane, 2-methyl-
66586-93-4	1	0	0	Phenol, tetramethyl-
66607-70-3	0	1	0	3-Furanol, tetrahydro-5-[6-hydroxy-3-(1-methylethyl)-1-heptenyl]-5-methyl-
66611-15-2	1	0	0	Ethanone, 1-(3-benzofuranyl)-
66719-08-2	1	0	0	1*H*-Pyrazole, methyl-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
66735-69-***I***	1	0	0	3-Pentanone, 1-(methylthio)-
66841-25-6	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-, cyano(3-phenoxyphenyl)methyl ester {Tralomethrin®}
66890-73-1	0	1	0	2-Naphthalenol, decahydro-1-(3-hydroxy-3-methyl-1,4-pentadienyl)-2,5,5,8a-tetramethyl-, [1R-[1α(1*E*,3S*),2β,4aβ,8aα]]-
66890-76-4	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol,2,8,12-trimethyl-5-(1-methylethyl)-,[1S-(1R*,2S*,5R*,6*E*,8R*,10*E*,12S*)]-
66957-95-7	0	1	0	2,7-Octadiene-1,6-diol, 2,6-dimethyl-, [S-(*E*)]-
66966-02-7	0	1	0	2-Naphthalenol, decahydro-1-(3-hydroxy-3-methyl-1,4-pentadienyl)-2,5,5,8a-tetramethyl-, [1R-[1α(1*E*,3R*),2β,4aβ,8aα]]-
66966-04-9	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-diene-2,8-diol,2,8,12-trimethyl-5-(1-methylethyl)-,[1S-(1R*,2R*,5R*,6*E*,8R*,10*E*,12S*)]-
67028-20-0	1	0	0	Benz[*c*]acridine, 11-methyl-
67255-31-6	0	1	0	Phosphonic acid, 2-chloroethyl-, hydrazine salt {Hydrel®}
67360-38-7	1	0	0	7-Quinolinecarbonitrile
67375-30-8	1	1	1	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {α-Cypermethrin®}
67383-34-0	1	0	0	4(1*H*)-Pyrimidinone, 2,5-dimethyl- = 6-pyrimidinol, 2,5-dimethyl-
3059-71-0				
67401-25-6	0	1	0	2-Cyclohexen-1-one, 3-(2-butenyl)-2,4,4-trimethyl-, (*Z*)-
67493-77-0	0	1	0	Lanostane-3,7,11-triol, 3,7-diacetate, (3β,7β,11β)-
67494-22-8	0	1	0	Naphthalene, 1,2-dihydro-5-methyl-3-(1-methylethenyl)-
67494-23-9	0	1	0	1-Naphthalenol, 1,2,3,4-tetrahydro-8-methyl-2-(1-methylethenyl)-, (*Z*)-(±)
67517-48-0	1	0	0	Dibenzofuran, 1,2,3,4,8-pentachloro-
67526-84-5	1	0	0	Benzocarbazole
67528-84-1	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2-ol, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [2R-(2α,3β,4aα,6aβ,10aα,10bβ)]-
67537-80-8	1	0	0	Heptacosene
67557-56-6	1	0	0	Butanoic acid, 4-(methylnitrosoamino)-, methyl ester
67562-39-4	1	1	1	Dibenzofuran, 1,2,3,4,6,7,8-heptachloro-
67730-10-3	1	0	0	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine {Glu-P-2}
67730-11-4	1	0	0	Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 6-methyl- {Glu-P-1}
67771-72-6	1	0	0	1*H*-Pyrazole, dimethyl-
67775-07-9	1	0	0	Dibenzanthracene
414-29-9				
67845-38-9	0	1	0	Pyrazine, 2-ethyl-6-methoxy-
67880-95-9	0	1	0	Desaturase, fatty acid ω3-
67920-51-8	0	1	0	Pentanoic acid, 5-(acetylamino)-2-hydroxy-, (±)-
67952-65-2	0	1	0	Pyrazine, 3 (5 or 6)-methyl-2-methylthio-
67965-47-3	1	0	0	1,3-Benzenediol, ethenyl-
68006-83-7	1	0	0	1*H*-Pyrido[2,3-*b*]indol-2-amine, 3-methyl- {MeAαC}
68038-71-1	0	1	0	*Bacillus thuringiensis* {Dipel®}
68146-94-1	1	0	0	1,3-Benzenediol, propyl-
68175-07-5	1	0	0	1*H*-Imidazo[4,5-*b*]pyridine, 2-methyl-
68208-73-1	1	0	0	2-Hexanone, 6-hydroxy-5-methyl-
68245-76-1	1	1	1	Pyridine, 3-(1-ethyl-2-piperidinyl)-, (S)-
68258-35-5	0	1	0	Pyridine-2-^{13}C-3-^{14}C, 3-fluoro-5-(2-piperidinyl)-, (±)-, labeled with ^{13}C and ^{14}C
68295-84-1	0	1	0	β,β-Carotene, *neo*
68334-00-9	0	1	0	1,2,3-Propanetriol, trioctadecanoate {tristearin}
68359-37-5	0	1	0	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2,2-dichloroethenyl)-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester {Cyfluthrin®}
68420-60-0	0	1	0	2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-3-hydroxy-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)-
68510-02-1	0	1	0	1,2,3,4-Butanetetrol, 1-[5-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,5-deoxyfructosazine}
68510-03-2	0	1	0	1,2,3,4-Butanetetrol, 1-[6-(2,3,4-trihydroxybutyl)pyrazinyl]- {2,6-deoxyfructosazine}
68573-20-6	0	1	0	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-
68690-84-6	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-
68697-66-5	0	1	0	1-Butanone, 3-(methylthio)-1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
68742-28-9	1	0	0	1*H*-Indole, 5-ethyl-
68759-08-0	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [S-[R*,S*-(*E*)]]-
68831-78-7	0	1	0	β,β-Carotene-3,3′-diol, 5,6-epoxy-5,6-dihydro-, (3S,3′R,5R,6S,9-*cis*)-
68831-80-1	0	1	0	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [1*S*-[1α,4α(1*E*,3S*)]]-
68831-81-2	0	1	0	2-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, [1*S*-[1α,4α(1*E*,3R*)]]-
68858-66-2	0	1	0	Pyrophosphorylase
68860-42-4	1	1	1	1,4-Naphthalenedione, 2,3-dimethyl-6-(4,8,12-trimethyltridecyl)-, (R*,R*)-
68982-27-4	0	1	0	1-Naphthaleneacetaldehyde, decahydro-5,5,8a-trimethyl-2-oxo-, [1R-(1α,4aβ,8aα)]-
68982-28-5	0	1	0	Pentadecanal, 2-ethylidene-6,10,14-trimethyl-
68985-10-4	0	1	0	1-Naphthalenecarboxaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)-
68985-11-5	0	1	0	1-Naphthaleneacetaldehyde, 3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-, (4aS-*trans*)-
68985-12-6	0	1	0	1*H*-Naphtho[2,1-*b*]pyran-2(3*H*)-one, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-
68985-15-9	0	1	0	Oxacyclononadec-10-en-2-one, (*E*)-
68985-18-2	0	1	0	2-Nonen-4-one, 3-methyl-, (*E*)-
69010-30-6	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6,10-triene, 1,11-dimethyl-5-methylene-8-(1-methylethyl)-, [1R-(1R*,2*E*,6*E*,8S*,10*Z*,12S*)]-
69056-21-9	0	1	0	Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-, (*Z*)-
69135-98-4	1	0	0	4-Piperidinone, 2,6-dimethyl-, *trans*-
69453-35-6	1	0	0	Benzo[*a*]pyrene diol
69454-18-8	1	1	1	9-Octadecenoic acid (*Z*)-, pentadecyl ester
69521-46-6	0	1	0	Tetracosen-1-ol
69669-68-7	0	1	0	Phosphatase, glucose di-
69698-09-5	1	1	1	Pyridine, 3-(1-pyrrolidinyl)-
69671-26-7	0	1	0	Oxidase, ubiquinol
69730-90-1	0	1	0	1-Pyrrolidinecarboxylic acid, 2-(3-pyridinyl)-, ethyl ester, (S)-
69730-91-2	1	1	1	Pyrrolidine, 1-(1-oxobutyl)-2-(3-pyridinyl)-, (S)-
69730-92-3	0	1	0	Pyrrolidine, 1-[4-(dimethylamino)-1-oxobutyl]-2-(3-pyridinyl)-, (S)-
69745-71-7	1	0	0	1,2-Cyclopentanedione, 3-phenyl-
69772-40-3	0	1	0	Resinol: resinol, red
69806-50-4	0	1	0	Propanoic acid, 2-(4-(5-trifluoromethyl-2-pyridyloxy)phenoxy)-, butyl ester {Fluazifop-butyl®}
69845-49-4	1	0	0	1,2-Benzenediol, dimethyl-
69874-67-5	1	0	0	5-Cyclohexen1-one, 2-acetyl-3,3,5-trimethyl-
69975-94-6	1	0	0	Pentanenitrile, 2,4-dimethyl-
70021-47-5	0	1	0	Dibenzothiophene, dimethyl- {at least four isomers detected}
70106-56-8	0	1	0	3,5,9-Trioxa-4-phosphaheptacosan-1-aminium, 4-hydroxy-*N,N,N*-trimethyl-10-oxo-7-[(1-oxooctadecatrienyl)oxy]-, hydroxide, inner salt, 4-oxide, hexadehydro derivative, (R)-
70116-48-2	0	1	0	Ergost-8-en-3-ol, 4,14-dimethyl-, (3β,4α,5α,24ξ)-
70124-77-5	0	1	0	Benzeneacetic acid, 4-(difluoromethoxy)-α-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester {Flucythrinate®}
70185-59-0	0	1	0	1,4-Butanediamine, *N*-[3-amino)- (4-hydroxyphenyl)-1-oxo-2-propenyl]oxy- {*p*-coumaroylspermidine}
70199-60-9	1	0	0	Pyridine, 4-(methoxymethyl)-
70226-57-2	0	1	0	Starch, labeled with ^{14}C {starch-^{14}C}
70265-05-3	1	0	0	3-Pentenamide, 4-methyl-
70322-25-7	1	1	1	1,3,6,10,14,18,22,26,30,34-Hexatriacontadecaene, 3,7,11,15,19,23,27,31,35-nonamethyl- {solanesene}
71278-21-2				
70340-00-0	0	1	0	Pentanoic acid, 2-methylphenyl ester
70495-59-9	1	1	1	Octadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecanoate}
70495-60-2	1	1	1	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester
110115-39-4				{solanesyl octadecadienoate}
70587-92-7	1	0	0	Ethanone, 1-(hydroxyphenyl)-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
70648-26-9	1	0	0	Dibenzofuran, 1,2,3,4,7,8-hexachloro-
70687-51-3	0	1	0	5,7-Octadienoic acid, 7-methyl-4-(1-methylethyl)-, methyl ester
70688-47-0	1	0	0	Cyclohexene, 1,4-dimethyl-
70699-77-3	0	1	0	3-Morpholinepropanamide, 2-oxo-6-(1,2,3,4-tetrahydroxybutyl)-, [3S-[3α,6α(1R*,2S*,3S*)]]-
70875-03-5	0	1	0	6(2*H*)-Benzofuranone, 4,5,7,7a-tetrahydro-2-(1-hydroxyethyl)-4,4,7a-trimethyl-
70898-21-4	1	0	0	[2,3′-Bipyridin]-6′(1′*H*)-one, 3,4,5,6-tetrahydro-
70898-22-5	0	1	0	Cyclohexanecarboxylic acid, 3-[[3-[4-(β-*D*-glucopyranosyloxy)-3-hydroxyphenyl]-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-
70898-23-6	1	1	1	Decanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester, (all-*E*)- {solanesyl decanoate}
70898-24-7	0	1	0	Decanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-
70898-25-8	1	1	1	2,6(1*H*,3*H*)-Pyridinedione, 3,5-dimethyl-
70898-26-9	0	1	0	3-Hepten-2-ol, 5-ethyl-2,6-dimethyl-
70898-27-0	0	1	0	Lanostane-3,7-diol, (3β,7β)-
70898-29-2	0	1	0	2,7-Nonadienoic acid, (*E,Z*)-
70898-30-5	1	1	1	Octanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester, (all-*E*)- {solanesyl octanoate}
70898-31-6	0	1	0	Octanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-
70898-32-7	0	1	0	1*H*-Pyrrole-1-octanoic acid, 2-formyl-5-methyl-
70898-33-8	1	0	0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-
70898-34-9	0	1	0	Phosphorothioic acid, *O*,*O*-dimethyl S-[2-[[1-methyl-2-(methylamino)-2-oxoethyl]sulfonyl]ethyl] ester
70898-35-0	1	1	1	2*H*-Pyran-2-carboxaldehyde, 3,4-dihydro-6-hydroxy-3-oxo-
70898-36-1	0	1	0	3-Pyridinebutanol, δ-amino-
70898-37-2	0	1	0	3-Pyridinebutanal, γ-(methylamino)-
70901-63-2	0	1	0	1,6,10,14-Hexadecatetraene, 7,11,15-trimethyl-3-methylene-, (*E,E*)-
70906-15-9	0	1	0	*D*-Fructose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-
70919-26-5	1	0	0	2-Cyclopenten-1-one, 5-hydroxy-
70919-27-6	1	0	0	2-Cyclopenten-1-one, 5-hydroxy-3-methyl-
70941-91-2	0	1	0	Cyclohexene, 6-(3,7-dimethyl-1,3,5,7-octatetraenyl)-1,5,5-trimethyl-, (*E,E,E*)-
70954-04-0	0	1	0	*D*-Fructose, 1-[(1-carboxy-2-hydroxypropyl)amino]-1-deoxy-, [R-(R*,S*)]-
70969-36-7	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 4,8,14-trimethyl-11-(1-methylethyl)-
70969-38-9	0	1	0	2(1*H*)-Pyridinone, 5-(3,4-dihydro-2*H*-pyrrol-5-yl)-
70987-81-4	1	1	1	Ethanone, 1-(1,2,3-trimethyl-2-cyclopenten-2-yl)-
71010-46-3	0	1	0	β-Tabacenic acid
71010-47-4	0	1	0	γ-Tabacenic acid
71010-48-5	0	1	0	α-Tabacenic acid
71010-49-6	1	1	1	Phytadiene C
71030-52-9	0	1	0	Nonadiene
71050-53-8	0	1	0	2*H*-1-Benzopyran-2-one, 6-methoxy-7-(β-*D*-xylofuranosyloxy)-
71099-03-1	1	1	1	2,5-Pyrrolidinedione, 1,3,4-trimethyl-
71126-48-2	1	0	0	2(5*H*)-Furanone, 5-ethylidene-3-methyl-, (*Z*)-
71265-19-5	1	0	0	Benz[*c*]acridine, 6,9-dimethyl-
71265-20-8	1	0	0	Benzenamine, 3-ethyl-*N*-methyl-
71265-21-9	1	0	0	Benzo[*ghi*]fluoranthene, 1-methyl-
71265-22-0	1	0	0	Benzo[*ghi*]fluoranthene, 2-methyl-
71265-23-1	1	0	0	Benzo[*ghi*]fluoranthene, 3-methyl-
71265-24-2	1	0	0	Benzo[*ghi*]fluoranthene, 4-methyl- {7-methylbenzo[*ghi*]fluoranthene}
71265-25-3	1	0	0	11*H*-Benzo[*a*]fluorene, 11-methyl-
71265-26-4	1	0	0	Acenaphth[1,2-*a*]acenaphthylene, methyl-
71265-27-5	1	0	0	Benzenamine, ar-ethyl-ar-methyl-
71265-28-6	1	0	0	Benzenamine, ar,ar,ar,ar-tetramethyl-
71265-29-7	1	0	0	Anthracene, ethylmethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
71265-30-0	1	0	0	Anthracene, propyl-
71265-31-1	1	0	0	9,10-Anthracenedione, dimethyl-
71265-32-2	1	0	0	Benz[*a*]anthracene, ethylmethyl-
71265-33-3	1	0	0	Benz[*a*]anthracene, propyl-
71265-34-4	1	0	0	1*H*-Benz[*f*]indene, ethylmethyl-
71265-35-5	1	0	0	Benzo[*ghi*]fluoranthene, ethyl-
71265-36-6	1	0	0	Benzofuran, 2,3-dihydromethyl-
71265-37-7	1	0	0	Benzofuran, ethyldimethyl-
71265-38-8	1	0	0	Benzofuran, pentamethyl-
71265-39-9	1	0	0	1,1′-Binaphthalene, dimethyl-
71267-22-6	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-nitroso-, (S)- {NAT}
71608-13-4				
71277-81-1	1	0	0	1,1′-Binaphthalene, ethyl-
71277-82-2	1	0	0	2,2′-Binaphthalene, ethyl-
71277-83-3	1	0	0	1,1′-Biphenyl, ethylmethyl-
71277-84-4	1	0	0	1-Butanamine, methyl-
71277-85-5	1	0	0	9*H*-Carbazole, ethyl-
71277-86-6	1	0	0	Chrysene, ethyl-
71277-87-7	1	0	0	Chrysene, ethylmethyl-
71277-88-8	1	0	0	Chrysene, pentamethyl-
71277-89-9	1	0	0	Chrysene, propyl-
71277-90-2	1	0	0	Chrysene, tetramethyl-
71277-91-3	1	0	0	4*H*-Cyclopenta[*def*]phenanthrene, dimethyl-
71277-92-4	1	0	0	17*H*-Cyclopenta[*a*]phenanthrene, ethyl-
71277-93-5	1	0	0	17*H*-Cyclopenta[*a*]phenanthrene, methyl-
71277-94-6	1	0	0	Indeno[1,2,3,4-*defg*]chrysene, methyl- {indeno[3,2,1,7-*defg*]chrysene, methyl-; dibenzo[*b,mno*]fluoranthene, methyl-; naphtho[1,2,3,4-*ghi*]fluoranthene, methyl-}
71277-95-7	1	0	0	5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, methyl-
71277-96-8	1	0	0	Fluoranthene, ethylmethyl-
71277-97-9	1	0	0	Fluoranthene, hexamethyl-
71277-98-0	1	0	0	Fluoranthene, pentamethyl- {at least two isomers in MSS}
71277-99-1	1	0	0	Fluoranthene, tetramethyl-
71278-00-7	1	0	0	9*H*-Fluorene, dimethylethyl-
71278-01-8	1	0	0	9*H*-Fluorene, ethylmethyl- {at least two isomers in MSS}
71278-02-9	1	0	0	1*H*-Indene, 2,3-dihydroethyl-
71278-03-0	1	0	0	1*H*-Inden-1-one, 2,3-dihydrodimethyl- {six isomers detected}
71278-04-1	1	0	0	1*H*-Inden-1-one, 2,3-dihydro-ethyl-
71278-05-2	1	0	0	1*H*-Indene, diethyl-
71278-06-3	1	0	0	1*H*-Indene, dimethylethyl-
71278-07-4	1	0	0	1*H*-Indene, ethylpentamethyl-
71278-08-5	1	0	0	1*H*-Indene, hexamethyl-
71278-09-6	1	0	0	1*H*-Indene, pentamethyl-
71278-10-9	1	0	0	Ethanone, 1-(methyl-2-furanyl)-
71278-11-0	1	1	1	1-Butanone, 4-amino-1-(3-pyridinyl)- {poikiline}
71278-12-1	1	0	0	Phenol, 5-ethyl-2-methyl-4-nitro- {phenol, 3-ethyl-6-methyl-4-nitro-}
71278-13-2	1	0	0	2-Cyclopenten-1-one, 4-ethyl-2-methyl-
71278-14-3	1	0	0	Eicosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester
71278-15-4	1	1	1	Stigmasta-5,22-dien-3-ol, 9,12-octadecadienoate, [3β(9*Z*,12*Z*),22*E*]- {stigmasteryl linoleate}
71278-16-5	1	1	1	2-Furancarboxylic acid, 3-hydroxy-
71278-17-6	1	0	0	Heneicosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester
71278-18-7	1	0	0	Hentriacontanoic acid, hentriacontyl ester

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
71278-19-8	1	0	0	Heptadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester
71278-20-1	1	0	0	1-Hexadecene, 2,6,10-trimethyl-
71278-21-2	1	1	1	1,3,6,10,14,18,22,26,30,34-Hexatriacontadecaene, 3,7,11,15,19,23,27,31,35-nonamethyl- {solanesene}
70322-25-7				
71278-22-3	1	0	0	1,6,10,14,18,22,26,30,34-Hexatriacontanonaene, 7,11,15,19,23,27,31,35-octamethyl-3-methylene-
71278-23-4	1	1	1	Dodecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl
110053-53-7				dodecanoate}
71278-24-5	1	0	0	Dodecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl laurate}
72996-18-0				
71278-25-6	1	0	0	Fluoranthene, dihydromethyl-
71294-42-3	1	0	0	1,1′-Biphenyl, propyl-
71294-43-4	1	0	0	2,2′-Binaphthalene, dimethyl-
71369-76-1	1	0	0	2-Naphthalenol, tetrahydro-
71385-82-5	0	1	0	β-*D*-Fructofuranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-
71385-84-7	1	1	1	2(3*H*)-Furanone, dihydro-3-(2-oxopropyl)-
71387-71-8	1	0	0	2-Cyclopenten-1-one, 5-ethyl-2-hydroxy-3-methyl-
71526-64-2	1	0	0	Phenol, 2,6-dimethyl-4-ethenyl-
71532-24-6	1	0	0	Pyridine, 3-(3-butenyl)-
71607-54-0	1	0	0	Octene, methyl-
71607-56-2	1	0	0	Phenanthrene, dihydrobis(methylene)-
71607-57-3	1	1	1	Naphthalene, methyltetrahydro- {at least three isomers in MSS}
71607-59-5	1	0	0	Pyrrole, dihydromethyl-
71607-60-8	1	0	0	Naphthalene, dimethyl-2-phenyl-
71607-61-9	1	0	0	Naphthalene, methyl-2-phenyl-
71607-62-0	1	0	0	Naphtho[1,2-*b*]furan, dimethyl-
71607-63-1	1	0	0	3-Pyridinecarbonitrile, dimethyl-
71607-64-2	1	0	0	Benzene, octyl- [2 CAS Nos.] {phenyloctane}
2189-60-8				
71607-65-3	1	0	0	Phenanthrene, dimethylethyl-
71607-66-4	1	0	0	Phenanthrene, ethylmethyl-
71607-67-5	1	0	0	Phenanthrene, hexamethyl-
71607-68-6	1	0	0	Phenanthrene, pentamethyl-
71607-69-7	1	0	0	Phenanthrene, propyl-
71607-70-0	1	0	0	Phenanthrene, tetramethyl- {at least five isomers in MSS}
71607-71-1	1	0	0	Benzenediamine, *N*-methyl-
71607-72-2	1	0	0	Piperidine, (1-methylethyl)-
71607-73-3	1	1	1	Pyrazine, dimethylethyl-
71607-74-4	1	0	0	Pyrene, ethylmethyl-
71607-75-5	1	0	0	Pyrene, hexamethyl-
71607-76-6	1	0	0	Pyrene, pentamethyl- {at least three isomers in MSS}
71607-77-7	1	0	0	Pyridinamine, *N*-methyl-
71607-78-8	1	0	0	Pyrrolidine, diethyl-
71607-79-9	1	0	0	Pyrrolidine, dimethyl-
71607-80-2	1	0	0	Pyrrolidine, ethyl-
71607-81-3	1	0	0	Benzene, ethenylethyldimethyl-
77227-00-0				
71607-82-4	1	0	0	Benzene, ethenyltetramethyl-
77226-99-4				
71607-84-6	1	0	0	Cyclohexanone, ethenylmethyl-
71607-85-7	1	0	0	11*H*-Benzo[*a*]fluorene, trimethyl- {at least three isomers in MSS}
71607-87-9	1	1	1	Stigmasta-5,22-dien-3-ol, 9,12,15-octadecatrienoate, [3β(*Z,Z,Z*),22*E*]- {stigmasteryl linolenate}

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
71607-88-0 110053-62-8	1	1	1	Tetradecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl tetradecanoate}
71607-89-1	1	0	0	Naphthalene, 1,4-dimethyl-2-ethyl-
71607-90-4	1	0	0	Nonadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*-(*E*)]]-
71607-91-5	1	0	0	1,6-Octadiene, 4,7-dimethyl- {2,5-dimethyl-2,7-octadiene}
71607-92-6	1	0	0	2,5-Octadiene, 7-methyl-
71607-93-7 73037-55-5	1	1	1	9-Octadecenoic acid (*Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester {**solanesyl oleate**}
71607-94-8 11017-44-0	1	1	1	Hexadecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester {solanesyl hexadecanoate, solanesyl palmitate}
71607-95-9	1	0	0	2*H*-1,2-Oxazine, tetrahydro-3-(1-methylethyl)-6-(3-pyridinyl)-
71607-96-0	1	0	0	Pentadecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
71607-97-1	1	0	0	Phenol, 2-ethyl-3-nitro-
71607-98-2	1	0	0	Phenol, 4-ethyl-3-nitro-
71607-99-3	1	1	1	1-Propanamine, *N*-ethyl-2-methyl-*N*-nitroso-
71608-00-9	1	0	0	Pyrene, 1-octyl-
71608-01-0	0	1	0	3-Pyridinepentanoic acid, 1,6-dihydro-δ,6-dioxo-
71608-02-1	1	0	0	1,2-Benzenediol, 5-ethyl-3-nitro-
71608-03-2	1	0	0	1,3-Benzenediol, 4-methyl-6-nitro-
71608-04-3	1	0	0	Butanedioic acid, (hydroxymethylene)-
71608-06-5	1	0	0	Tricosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
71608-07-6	1	0	0	Tridecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
71608-08-7	1	0	0	Undecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester, [R-[R*,R*- (*E*)]]-
71608-10-1	1	0	0	Phenol, 3,6-dimethyl-2-nitro- {phenol, 2,5-dimethyl-6-nitro-}
71608-11-2	1	0	0	1,2-Cyclopentanedione, 3-ethyl-5-methyl- = 1,2-cyclopentanedione, 5-ethyl-3-methyl-
71608-12-3	1	0	0	1,2-Cyclopentanedione, 3-methyl-5-propyl-
71608-13-4 71267-22-6	1	1	1	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-nitroso-, (S)- {NAT}
71608-14-5	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]octadecyl hydrogen phosphate], disodium salt
71608-15-6	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]octadecyl hydrogen phosphate], disodium salt
71608-16-7	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]octadecyl hydrogen phosphate], disodium salt
71608-17-8	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-1-[(2-hydroxy-1-oxopentacosyl)amino]octadecyl hydrogen phosphate], disodium salt
71608-19-0	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxodocosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt
71608-20-3	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotricosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt
71608-21-4	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxotetracosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt
71608-22-5	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxopentacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt
71608-23-6	0	1	0	myo-Inositol, *O*-2-(acetylamino)-2-deoxy-α-*D*-glucopyranosyl-(1 → 4)-*O*-alpha-*D*-glucopyranuronosyl-(1 → 2)-, 1-[3,4-dihydroxy-2-[(2-hydroxy-1-oxohexacosyl)amino]-8-octadecenyl hydrogen phosphate], disodium salt
71626-11-4	0	1	0	*DL*-Alanine, *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)-, methyl ester {Benalaxyl®}
71630-68-7	1	0	0	Naphthalene, dimethyl-2-ethenyl-
71630-69-8	1	0	0	Dibenz[*j,mno*]aceanthrylene, methyl-
71630-70-1	1	0	0	Benzenediol, ethyl-nitro-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
71630-71-2	1	0	0	Pyrene, 1-tetradecyl-
71635-28-4	0	1	0	1-Piperidinecarboxaldehyde, 2-(3-pyridinyl)-, (S)-
71646-51-0	1	0	0	1*H*-Pyrrolecarbonitrile, methyl-
71697-04-6	1	0	0	Naphthalene, phenyl-, monomethyl derivative
71801-84-8	1	1	1	Tetradecanoic acid, 13-methyl-, hexadecyl ester
71899-42-8	0	1	0	5-Octadecyne
72074-11-4	0	1	0	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2-yl)-, [2S-[2α(*E*),3aα,5aβ,9aα,9bβ]]-
72227-00-0	1	1	1	Docosane, 3-methyl-
72227-01-1	1	1	1	Triacontane, 3-methyl-
72254-06-9	1	0	0	Indenopyrene
72312-07-3	0	1	0	Phenol, 4,5-dimethoxy-2-methyl-
72360-04-4	1	0	0	Acetic acid, 2-(5-methylfuranyl)-
72446-33-4	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4a,8,8-tetramethyl-4-(3-oxobutyl)-, (4aS-*trans*)-
72461-69-9	0	1	0	Pyridine, 3-[1-(1-methylethyl)-2-pyrrolidinyl]-, (S)-
72491-45-3	0	1	0	Cyclohexanone, 4-(2-butenylidene)-3,3,5-trimethyl-
72491-46-4	0	1	0	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-hydroxy-β-ionone}
72506-68-4	0	1	0	Synthase, 1-aminocyclopropanecarboxylate
72507-34-7	0	1	0	2(3*H*)-Furanone, dihydro-5-[1-methyl-4-(1-methylethyl)-7-oxo-2-octenyl]-
72611-71-3	1	0	0	Thiazole, 5-methyl-2-(2-methylpropyl)-
72686-97-6	0	1	0	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, (2α,3aα,5aβ,8β,9aS*)-
72692-68-3	1	0	0	1,2,3-Propanetriol, monoformate
72692-69-4	1	0	0	1*H*-Inden-1-one, 2,3-dihydro(methoxymethyl)-
72692-70-7	1	0	0	2,6-Piperidinedione, methyl-
72692-71-8	1	0	0	2-Cyclopenten-1-one, dimethyl-
72692-74-1	1	0	0	1*H*-Benzimidazole, dimethyl-
72692-75-2	1	0	0	1*H*-Benzimidazole, ethyl-
72692-76-3	0	1	0	2-Cyclopenten-1-one, 3,4-dimethyl-2-(1-methylethyl)-
72692-77-4	1	0	0	Quinoxaline, dimethyl-
72692-78-5	1	0	0	Quinoxaline, trimethyl-
72692-79-6	1	0	0	1*H*-Pyrrolecarboxylic acid, ethyl ester
72692-80-9	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, methyl- {at least four methyl isomers other than the 1- and 2-methyl- compounds}
72692-81-0	1	0	0	Pyrimidine, dimethyl-
72692-82-1	1	0	0	1*H*-Pyrrolemethanol
72692-83-2	1	0	0	2(1*H*)-Pyridinone, dimethyl-
72692-86-5	1	0	0	1*H*-Indenol, 2,3-dihydromethyl- [1*H*-Inden-4-ol, 2,3-dihydromethyl-]
72692-87-6	1	0	0	Indenone, 1,3(or 2,3)-dihydrodimethyl-
72692-88-7	1	0	0	Naphthalene, dihydrodimethyl- {at least four isomers in MSS}
72692-89-8	1	0	0	Pyrene, 1-hexyl-
72692-90-1	1	0	0	Benzoxazole, 2,4-dimethyl-
72692-91-2	1	0	0	Benzoxazole, 4,6-dimethyl-
72692-92-3	1	1	1	1,2-Cyclopentanedione, 3,3-dimethyl-
72692-94-5	1	0	0	2,6(1*H*,3*H*)-Pyridinedione, 5-methyl-
72692-95-6	1	0	0	2,6(1*H*,3*H*)-Pyridinedione, 4-methyl-
72692-96-7	1	0	0	3-Pyridinecarboxamide, 2,4-dimethyl-
72692-97-8	1	0	0	Pyridine, 3-(4-methylpentyl)-
72692-98-9	1	0	0	Pentitol, 2,3-dideoxy-3-methyl-
72692-99-0	1	0	0	Pyridine, 3-(1*H*-pyrrol-1-yl)-
50966-74-0				
72693-00-6	1	0	0	1*H*-Pyrido[2,3-*b*]indole, 1-butyl-
72693-01-7	1	0	0	1*H*-Pyrrole-2-acetaldehyde, α-oxo-
72693-02-8	1	0	0	2-Pyridinecarboxamide, 4,6-dimethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
72693-03-9	1	0	0	2,5-Pyrrolidinedione, 3-(1-methylethyl)-
72693-04-0	1	0	0	Pyridine, 3-methyl-2-(1-methylethyl)-
72693-05-1	1	1	1	15-Oxabicyclo[10.2.1]pentadeca-2,6-diene, 1-methyl-5,11-bis(methylene)-8-(1-methylethyl)-
72693-06-2	1	0	0	2-Butenamide, *N*,2-dimethyl-
1187-41-3				
72693-07-3	1	0	0	2(3*H*)-Furanone, dihydro-3,4-dimethyl-
72693-08-4	1	0	0	6-Oxabicyclo[3.2.1]octan-7-one, 8-hydroxy-1-methyl-
72693-09-5	1	0	0	1,2-Cyclopentanedione, 4-(1-methylethyl)-
72693-10-8	1	0	0	Formamide, *N*-(2-furanylmethyl)-
72693-11-9	0	1	0	2,5-Heptadienoic acid, 2,3-dimethyl-
72693-12-0	1	0	0	2-Heptanone, 6-hydroxy-
72693-13-1	1	0	0	2-Hexanone, 5,6-dihydroxy-
72693-14-2	1	0	0	1,4-Benzenediol, 2-ethyl-6-methyl-
72693-15-3	1	0	0	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-
72693-16-4	1	0	0	2,5-Furandione, 3-methyl-4-(phenylmethyl)-
72709-76-3	1	0	0	Ethanone, 1-(3-methyl-3*H*-pyrazol-4-yl)-
72747-21-8	0	1	0	2*H*-Furo[3,2-*c*]isobenzofuran-8-methanol, octahydro-2-methoxy-α,α,3a,5a-tetramethyl-, [2R-(2α,3aβ,5aα,8α,9aR*)]-
72762-00-6	1	0	0	2-Pyridinol {2(1*H*)-pyridinone}
142-08-5				
72777-88-9	0	1	0	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-
72843-02-8	1	0	0	Naphthalene, 1,2,3,4-tetrahydrotrimethyl- {at least three isomers in MSS}
72881-27-7	0	1	0	Decenoic acid {three isomers detected}
26446-27-5				
72902-81-9	1	0	0	2(3*H*)-Furanone, dihydro-3,3-dimethyl-4-hydroxy-
72906-87-7	0	1	0	Peroxidase, ascorbate
72918-21-9	1	0	0	Dibenzofuran, 1,2,3,7,8,9-hexachloro-
72962-43-7	0	1	0	β-homo-7-Oxaergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R,23R,24S)-
72996-18-0	1	0	0	Dodecanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl laurate}
71278-24-5				
73020-30-1	1	0	0	Benzofluoranthene, methyl-
73037-55-5	1	1	1	9-Octadecenoic acid (*Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatria contanonaenyl ester
71607-93-7				
73051-72-6	0	1	0	2-Benzofuranmethanol, 2,4,5,6,7,7a-hexahydro-6-hydroxy-α,4,4,7a-tetramethyl-
73051-73-7	0	1	0	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-
73120-40-8	1	0	0	2-Hexadecene, 2-methyl-
73360-07-3	0	1	0	Glycine, *N*-[2-(2-aminoethoxy)ethenyl]-
73467-76-2	1	0	0	Benzopyrene
73492-01-0	1	0	0	11*H*-Benzo[*c*]fluorine
73496-12-5	0	1	0	2,3-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl-1-(3-methyl-2,4-pentadienyl)-, [1S-[1α(*E*),2α,3β,4aβ,8aα]]-
73692-69-0	0	1	0	2*H*-Pyran-2-one, 3-hydroxy-6-methyl-
73757-28-5	0	1	0	2-Octenal, 2-propyl-
73850-01-8	1	0	0	2*H*-Pyran-2-one, hydroxyethyl-
73850-02-9	1	0	0	Phenol, trimethyl-
26998-80				
73850-03-0	1	0	0	Phenol, 3-ethenyl-methyl-
73850-04-1	1	0	0	Phenol, dimethyl-4-ethenyl-
73850-05-2	1	0	0	Phenol, ethenylmethyl-
73850-06-3	1	0	0	Phenol, 3-ethenyl-2,?,?-trimethyl-
73850-08-5	1	0	0	Phenol, (2-methylpropyl)-
73850-09-6	1	0	0	1*H*-Indenol, tetramethyl- [1*H*-Inden-4-ol, tetramethyl-]
73850-10-9	1	0	0	1*H*-Indenol, trimethyl- [1*H*-Inden-4-ol, trimethyl-]

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
73850-11-0	1	0	0	1*H*-Indenol, dimethyl- [1*H*-Inden-4-ol, dimethyl-]
73850-12-1	1	0	0	1*H*-Indenol, methyl- [1*H*-Inden-4-ol, methyl-]
73850-13-2	1	0	0	Phenol, ethenyltrimethyl-
73850-14-3	1	0	0	Phenol, dimethylethenyl-
73850-15-4	1	0	0	1,4-Naphthalenedione, tetramethyl-
73850-16-5	1	0	0	1,4-Naphthalenedione, trimethyl-
73850-17-6	1	0	0	1,4-Naphthalenedione, dimethyl-
73850-18-7	1	0	0	2-Naphthalenol, trimethyl-
73850-19-8	1	0	0	2-Naphthalenol, dimethyl-
73850-20-1	1	0	0	1*H*-Indenol, ethylmethyl- [1*H*-Inden-4-ol, ethylmethyl-]
73892-47-4	0	1	0	3-Buten-2-one, 4-[3-(acetyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-,[R-(*E*)]-
73904-44-6	0	1	0	Hydroxycinnamoyltransferase, shikimate
73952-98-4	1	0	0	Pyridine, 3-(dimethyl-1*H*-pyrrolyl)-
74051-80-2	0	1	0	2-Cyclohexen-1-one, 2-[1-(ethoximino)butyl]-5-[2-(ethylthio)-propyl]-3-hydroxy- {Sethoxydim®}
74173-71-0	1	0	0	Pyrrolidine, 1-(1-oxoheptyl)-2-(3-pyridinyl)-, (S)-
74233-03-7	1	0	0	Pyrazine, 2-methyl-6-phenyl-
74233-43-5	0	1	0	5,10-Undecadien-2-one, 6,10-dimethyl-9-hydroxy-
74392-36-2	1	1	1	2-Pentadecene, (*E*)-
74421-05-9	1	0	0	2,4-Heptadiene, 2,4-dimethyl-
74423-06-6	0	1	0	Cyclohexene, 2-(1,3-butadienyl)-1,3,3-trimethyl-, (*E*)- {megastigmatriene}
74430-25-4	1	1	1	Ethanone, 1-(methylfuranyl)-
74472-39-2	1	0	0	1,1′-Biphenyl, 2,3′,4,5′,6-pentachloro-
74630-29-8	0	1	0	1,5-Heptadiene, 3,3,5-trimethyl-
74635-33-9	0	1	0	Ergosta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-
74712-71-3	0	1	0	2*H*-1-Benzopyran-2-one, 7-[[6-*O*-(6-deoxy-α-*L*-mannopyranosyl)-β-*D*-glucopyranosyl]oxy]-6-methoxy-
75039-16-6	0	1	0	β-*D*-Glucopyranoside, 2-methyl-4-(1*H*-purin-6-ylamino)-2-butenyl-, mono(dihydrogen phosphate) (ester), (*E*)-
75081-82-2	0	1	0	Adenosine, *N*-[3-methyl-4-[(*O*-phosphono-β-*D*-glucopyranosyl)oxy]-2-butenyl]-, (*E*)-
75164-73-7	1	1	1	9-Octadecenoic acid (*Z*)-, tridecyl ester
75202-09-4	1	1	1	2-Pyrrolidinone, 1-methyl-5-(3-pyridinyl)-
75281-93-5	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol,4,8,14-trimethyl-11-(1-methylethyl)-,[1S-(1R*,4*E*,6S*,8S*,9*E*,11R*,14R*)]-
75281-99-1	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol,4,8,14-trimethyl-11-(1-methylethyl)-,[1S-(1R*,4*E*,6S*,8R*,9*E*,11R*,14R*)]-
75282-00-7	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol,4,8,14-trimethyl-11-(1-methylethyl)-,[1R-(1R*,4*E*,6R*,8S*,9*E*,11S*,14R*)]-
75581-03-2	1	0	0	2,6,10,14,18-Eicosapentaene, 2,6,10,14,18-pentamethyl-
75614-87-8	0	1	0	1*H*-Imidazole-4-ethanamine, α-methyl-
75696-56-9	1	1	1	Hexacosanoic acid, heptacosyl ester
75835-01-7	1	0	0	Pyridine, 4-methyl-2-(2-phenylethyl)-
75840-26-5	0	1	0	2(4*H*)-Benzofuranone, 5,6-dihydro-3,6-dimethyl-
76014-80-7	0	1	0	3-Pyridinebutanal, γ-oxo-
76014-81-8	1	1	1	3-Pyridinebutanol, δ-(methylnitrosoamino)- [2 CAS Nos.] {NNAL}
59578-66-4				{1-butanol, 4-(*N*-methylnitrosoamino)-1-(3-pyridinyl)-, 3-pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-}
76014-82-9	0	1	0	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)-, *N*-oxide
76015-10-6	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylpropyl)-
76162-60-2	1	0	0	9*H*-Pyrido[2,3-*b*]indole, 3-methyl-
76180-96-6	1	0	0	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3-methyl- {IQ}
76540-54-0	0	1	0	1,6,10,14-Hexadecatetraene-3,9-diol, 3,7,11,15-tetramethyl-
76540-55-1	0	1	0	2,6,10,15-Hexadecatetraene-1,14-diol, 2,6,10,14-tetramethyl-, [S-(*Z,E,E*)]-
76578-14-8	0	1	0	Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester {Quizalofop-Et®}
76602-27-2	1	0	0	Quinoline, tetramethyl-
76649-14-4	0	1	0	3-Octen-2-ol
76710-90-2	0	1	0	2(3*H*)-Furanone, dihydro-5-(2-pentenyl)-, (*Z*)-
76739-26-9	0	1	0	2(1*H*)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-3,4,4a,8,8-pentamethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
76774-50-0	1	0	0	Benz[*fg*]acenaphthylene
77046-64-1	1	1	1	Hentriacontene
77094-11-2	1	0	0	3*H*-Imidazo[4,5-*f*]quinolin-2-amine, 3,4-dimethyl- {MeIQ}
77208-25-4	1	0	0	1,3-Cyclopentadiene, dimethyl-
77220-32-7	1	0	0	Benzene, ethenyltrimethyl-
50976-21-1				
77220-33-8	1	0	0	Benzene, ethenylethylmethyl-
27138-10-9				
77226-99-4	1	0	0	Benzene, ethenyltetramethyl-
71607-82-4				
77227-00-0	1	0	0	Benzene, ethenylethyldimethyl-
71607-81-3				
77227-01-1	1	0	0	1*H*-Indene, ethylmethyl-
77242-77-4	1	0	0	1*H*-Indene, heptamethyl-
86901-30-6				
77242-78-5	1	0	0	Naphthalene, hexamethyl-
77242-81-0	1	0	0	1*H*-Benzo[*c*]fluorene, methyl-
77267-30-2	0	1	0	2(5*H*)-Furanone, 5-(2-pentenyl)-, (*Z*)-
77271-50-2	1	0	0	Benzofluorene, dimethyl- {at least three isomers in MSS}
77271-51-3	1	0	0	Benzofluorene, tetramethyl- {at least two isomers in MSS}
77271-52-4	1	0	0	Benzofluorene, trimethyl-
77271-81-0	1	0	0	Benzo[*c*]fluorene, methyl-
77272-02-7	0	1	0	Glucuronomannoarabinan
77288-93-8	0	1	0	2-Heptene-1,6-diol, 3-(1-methylethyl)-, (*E*)-
77288-94-9	0	1	0	Oxiranebutanol, 3-(1-hydroxyethyl)-α-methyl-δ-(1-methylethyl)-
77288-95-0	0	1	0	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [R-[R*,S*-(*E*)]]-
77288-96-1	0	1	0	6-Nonen-2-one, 8,9-dihydroxy-8-methyl-5-(1-methylethyl)-, [S-[R*,R*-(*E*)]]-
77288-97-2	0	1	0	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-, [2α(αS*,δR*),3α]-
77288-98-3	0	1	0	6-Decen-2-one, 8,10-dihydroxy-8-methyl-5-(1-methylethyl)-
77289-00-0	0	1	0	1,5-Hexanediol, 2-(1-methylethyl)-, [S-(R*,R*)]-
77327-07-2	1	0	0	Ergosta-3,5,7-triene, (24ξ)-
77341-24-3	0	1	0	Oxiranebutanol, 3-(1-hydroxy-1-methylethyl)-α-methyl-δ-(1-methylethyl)-
77411-76-8	0	1	0	3,5-Heptadien-2-ol, 2,6-dimethyl-
77417-07-3	1	0	0	1-Naphthalenecarbonitrile, 3-methyl-
77500-04-0	1	0	0	3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 3,8-dimethyl-
77699-19-5	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [R-[R*,R*-(*E*)]]-
77761-55-8	0	1	0	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)-3,5,5-trimethyl-
77829-17-5	0	1	0	Pyrrolidine, 1-(6-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-
77829-18-6	0	1	0	Pyrrolidine, 1-(7-hydroxy-1-oxooctyl)-2-(3-pyridinyl)-
77842-24-1	0	1	0	2-Cyclohexen-1-one, 4-(2,3-dihydroxybutylidene)-3,5,5-trimethyl- {isomer}
78075-83-9	1	0	0	1*H*-Pyrrole, 2-methyl-1-(phenylmethyl)-
78081-83-1	0	1	0	β-*D*-Glucopyranoside, 3-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-1-methyl-2-propenyl-
78094-66-3	1	0	0	2*H*-Pyran-2-one, tetrahydro-4,5-dimethyl-, *cis*-(±)-
78210-37-4	1	0	0	Pyridine, 3-(3,4-dihydro-3-methyl-2*H*-pyrrol-5-yl)-
78210-38-5	1	0	0	Pyridine, 3-(1,3-dimethyl-1*H*-pyrrol-2-yl)-
78210-39-6	1	0	0	Pyridine, 3-(3-ethyl-3,4-dihydro-2*H*-pyrrol-5-yl)-
78210-40-9	1	0	0	Pyridine, 2-(3-ethylphenyl)-
78210-41-0	1	0	0	Pyridine, 3-(4-ethylphenyl)-
78210-42-1	1	0	0	Pyridine, 3-methoxy-5-methyl-
78210-43-2	1	0	0	Pyridine, 3,3′-methylenebis-
78210-44-3	1	0	0	Pyridine, 3-(4-pyridinylmethyl)-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
78210-45-4	1	0	0	Pyridine, 3-[2,5-dihydro-1-[(5-methyl-2-furanyl)methyl]-1*H*-pyrrol-2-yl]-
78210-46-5	1	0	0	Pyridine, 3-[(5-methyl-2-furanyl)methyl]-
78210-47-6	1	0	0	Pyridine, 4-methyl-2-(3-methylbutyl)-
78210-48-7	1	0	0	Pyridine, 2-methyl-3-(1-propenyl)-
78210-49-8	1	0	0	Pyridine, 3-(2-methyl-1*H*-pyrrol-1-yl)-
78210-50-1	1	0	0	Pyridine, 3-(tetrahydro-2-furanyl)-
78210-51-2	1	0	0	Pyridine, 2-(1*H*-pyrrol-1-ylmethyl)-
78210-52-3	1	0	0	1*H*-Indole, 2,3-dihydro-3-(3-pyridinylmethyl)-
78210-53-4	1	0	0	1*H*-Pyrido[2,3-*b*]indole, 2-(2-methylpropyl)-
78210-54-5	1	0	0	1*H*-Pyrido[2,3-*b*]indole, 2-pentyl-
78210-55-6	1	0	0	9*H*-Pyrido[3,4-*b*]indole, 1-(1-propenyl)-
78210-56-7	1	1	1	Pyrazine, 3-butenyl- = pyrazine, 2-butenyl-
78210-57-8	1	0	0	Benzoxazole, 7-ethyl-
78210-58-9	1	0	0	Benzoxazole, 5,7-dimethyl-
78210-59-0	1	0	0	3-Pyridinecarboxamide, 4-ethyl-
78210-60-3	1	0	0	3-Pyridinecarboxamide, 6-ethyl-
78210-61-4	1	0	0	2-Pyridinecarboxamide, 6-ethyl-
78210-62-5	1	0	0	1*H*-Pyrrole-3-carboxaldehyde, 5-ethyl-
78210-63-6	1	0	0	2-Cyclopenten-1-one, 3-ethyl-4-hydroxy-
78210-64-7	1	0	0	2-Cyclopenten-1-one, 2-ethyl-5-methyl-
78210-65-8	1	0	0	2-Cyclopenten-1-one, 2-(2-furanyl)-
78210-66-9	1	0	0	Ethanone, 1-(2-methyl-1*H*-imidazol-4-yl)-
78210-67-0	1	0	0	Ethanone, 1-(5-propyl-1*H*-imidazol-4-yl)-
78210-68-1	1	0	0	2(1*H*)-Pyrazinone, 1-methyl-3-(1-methylethyl)-
78210-69-2	1	0	0	Ethanone, 1-(1,2-dihydro-2-methyl-3-pyridinyl)-
78210-70-5	1	0	0	1-Butanone, 2-methyl-1-(3-pyridinyl)-
78210-71-6	1	0	0	2*H*-Pyrrol-2-one, 3-ethyl-1,5-dihydro-5-methylene-
78210-72-7	1	0	0	2*H*-Pyrrol-2-one, 1,5-dihydro-1-methyl-5-(1-methylethylidene)-
78210-73-8	1	0	0	2,2′-Bipyridine, 4,5-dimethyl-
78210-74-9	1	0	0	2,3′-Bipyridine, 4-(2-propenyl)-
78210-75-0	1	0	0	2,3′-Bipyridine, 4-(2-butenyl)-
78210-76-1	1	0	0	2,3′-Bipyridine, 3-ethyl-
78210-77-2	1	0	0	2,3′-Bipyridine, 6-ethyl-
78210-78-3	1	0	0	2,3′-Bipyridine, 6-methyl-
78210-79-4	1	0	0	2,3′-Bipyridine, 5-(1-propenyl)-
78210-80-7	1	0	0	2,3′-Bipyridine, 5-propyl-
78210-81-8	1	0	0	2,3′-Bipyridine, 5-ethenyl-
78210-82-9	1	0	0	3,3′-Bipyridine, 5-methyl-
78210-83-0	1	0	0	3,3′-Bipyridine, 6-methyl-
78210-84-1	1	0	0	Pyridine, 3-[1-methyl-2-(1-methylethyl)-1*H*-imidazol-5-yl]- = imidazole, 1-methyl-2-(1-methylethyl)-5-(3-pyridinyl)-
78210-85-2	1	0	0	Pyridine, 3-[1-(2-furanylmethyl)-2-pyrrolidinyl]-, (S)-
78210-86-3	1	0	0	Pyridine, 3-[1-[(5-methyl-2-furanyl)methyl]-2-pyrrolidinyl]-, (S)-
78210-87-4	1	0	0	Pyridine, 3-[1-[2-(2-furanyl)ethyl]-2-pyrrolidinyl]-, (S)-
78210-88-5	1	0	0	Pyridine, 3-[1-(5-ethyl-2-furanyl)-1*H*-pyrrol-2-yl]-
78210-89-6	1	0	0	Pyridine, 3-[1-(5-propyl-2-furanyl)-1*H*-pyrrol-2-yl]-
78210-90-9	1	0	0	Pyridine, 3-(2-butenyl)-
78210-91-0	1	0	0	Pyridine, 4-(1-butenyl)-
78249-81-7	1	0	0	Pyridine, 3-(3,4-dihydro-2*H*-pyrrol-5-yl)-, monomethyl derivative
78249-82-8	1	0	0	Quinoline, methyl-1,2,3,4-tetrahydro- {several isomers present in MSS}
78249-83-9	1	0	0	Quinoline, methyl-5,6,7,8-tetrahydro-
78249-84-0	1	0	0	Quinoline, ethyl-5,6,7,8-tetrahydro-
78249-85-1	1	0	0	1*H*-Pyrrolo[2,3-*b*]pyridine, ethyl-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
78249-86-2	1	0	0	Ethanone, 1-(dimethylpyridinyl)-
78249-87-3	1	0	0	Ethanone, 1-(methylpyridinyl)- {two isomers}
78249-88-4	1	0	0	1*H*-Pyrrole-1-carboxaldehyde, 1-methyl-
78310-61-9	1	0	0	Bipyridine, dimethyl- {two isomers detected}
78310-62-0	1	0	0	Bipyridine, phenyl-
78328-47-9	1	0	0	Benzo[*c*]phenanthrene, methyl-
78504-05-9	1	0	0	Pyrrolidine, 1-(2-furanoyl)-
78509-52-1	1	1	1	Hexadecanoic acid, octacosyl ester
78538-74-6	1	0	0	9*H*-Pyrido[3,4-*b*]indole-3-carboxamide, *N*-methyl-
78579-58-5	1	1	1	1-Butanamine, 3-methyl-*N*-propyl-
78692-70-3	0	1	0	Pentatriacontane, 3-methyl-
78830-91-8	0	1	0	3-Cyclohexen-1-ol, 1-(3-hydroxy-1-butenyl)-6,6-dimethyl-2-methylene-
78914-62-2	1	0	0	1-Pyrrolidinecarboxaldehyde, 2-methyl-, (R)-
78919-13-8	1	0	0	Cyclohexadienedione {quinone}
78986-08-0	0	1	0	Butanoic acid, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-2-cyclohexen-1-yl ester
79082-92-1	0	1	0	β-*D*-Fructofuranose, 2,6-bis(dihydrogen phosphate)
79147-47-0	1	0	0	9*H*-Fluoren-9-one, methyl- {two isomers detected}
79407-66-2	0	1	0	2-Propenal, 3-(2,4-dihydroxyphenyl)-
79637-61-9	1	0	0	Cyclopentane, propenyl-
79734-43-3	0	1	0	2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)-, (*E*)- {3-oxo-α-ionone}
79755-53-6	1	0	0	Phenol, 3-(1-propenyl)-
79886-47-8	0	1	0	β-*D*-Fructopyranose, 1-deoxy-1-[2-(3-pyridinyl)-1-pyrrolidinyl]-, (S)-
79886-54-7	0	1	0	1,2-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl-, [1R-(1α,2β,4aβ,8aα)]-
79897-80-6	1	1	1	Stigmasta-3,5-diene, (24ξ)-
79925-80-7	0	1	0	3-Buten-2-ol, 4-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)-
79951-97-6	0	1	0	1,2-Naphthalenediol, decahydro-2,5,5,8a-tetramethyl- {11-nor-8-drimanol}
80111-68-8	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethylcyclohexenyl)- [3 CAS Nos.] {damascone}
23770-92-3				
35044-68-9				
80126-41-6	0	1	0	2,7,11-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1S-(1R*,2*E*,4R*,7*E*,11*E*)]-
80252-34-2	1	1	1	Tetradecanoic acid, hexacosyl ester
80252-38-6	1	1	1	Hexadecanoic acid, dotriacontyl ester
80252-40-0	1	1	1	Octacosanoic acid, tetracosyl ester
80436-91-5	1	0	0	2(5*H*)-Furanone, 3-acetyl-
80449-01-0	0	1	0	Isomerase, deoxyribonucleate topo-
80455-52-3	1	0	0	Cyclopentaphenanthrene {at least two isomers in MSS}
80466-34-8	0	1	0	2,4-Hexadienal
80508-24-3	1	0	0	2-Buten-1-one, 1-(3-pyridinyl)-
80638-48-8	1	1	1	Benzenepropanal, 4-hydroxy-3-methoxy-
80652-16-0	1	0	0	Phenol, ethyl-methoxy-
80657-57-4	1	0	0	Propanoic acid, 3-hydroxy-2-methyl-
80700-46-5	1	0	0	Pyridoindole, *N*-methyl-
80722-28-7	0	1	0	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-
80736-41-0	0	1	0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3α,5α,22R, 23R,24S)-
80744-25-8	0	1	0	2(3*H*)-Furanone, dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-
80756-16-7	1	1	1	Octacosanoic acid, hexadecyl ester
80797-69-9	0	1	0	2(3*H*)-Furanone, dihydro-5-(3-methyl-1-butenyl)-
80802-00-2	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-
80866-95-1	1	0	0	Pyridine, 3-(1*H*-pyrrol-1-ylmethyl)-
80904-75-2	1	0	0	2(5*H*)-Furanone, 4-(hydroxymethyl)-
80933-75-1	0	1	0	1-Propanone, 1-[2-(3,4,5,6-tetrahydropyridinyl)]-

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
80934-44-7	1	1	1	Benzenediol, methyl-
80935-98-4	1	0	0	Pyrazine, 2,5-dimethyl-3-ethenyl-
81345-07-5	1	0	0	3,8,12,14-Pentadecatetraen-2-one, 8,12-dimethyl-5-(1-methylethyl)-, (*E,E,E*)-
81345-08-6	1	0	0	3,8,12,14-Pentadecatetraen-2-one, 8,12-dimethyl-5-(1-methylethyl)-, (*E,Z,E*)-
81531-12-6	1	1	1	Stigmasta-3,5,22-triene, (22*E*,24ξ)-
81540-27-4	1	1	1	3-Buten-2-one, 4-(2-furanyl)-3-methyl-
81777-89-1	0	1	0	3-Isoxazolidinone 2-([2-chlorophenyl)methyl]-4,4-dimethyl- {Clomazone®}
81901-03-3	0	1	0	3,5,9-Trioxa-4-phosphaheptacosadien-1-aminium, 4-hydroxy-*N,N,N*-trimethyl-10-oxo-7-[(1-oxooctadecadienyl)oxy]-, hydroxide, inner salt, 4-oxide
82000-05-3	1	0	0	2-Cyclopenten-1-one, trimethyl-
82003-46-1	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7*E*,9R*,12R*,13*E*)]-
82147-26-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-propyl-
82326-40-7	1	0	0	1*H*-Benzimidazole, 2-(2-naphthalenylmethyl)-
82395-89-9	0	1	0	2(4*H*)-Benzofuranone, 6-(β-*D*-glucopyranosyloxy)-5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (6S-*Z*)-
82451-46-5	0	1	0	2-Naphthalenol, decahydro-4a,8,8-trimethyl-3-methylene-4-(3-methyl-2,4-pentadienyl)-, [2S-[2α,4α(*E*),4aα,8aβ]]-
82458-63-7	0	1	0	2-Naphthalenol, decahydro-4a,8,8-trimethyl-3-methylene-4-(3-methylene-4-pentenyl)-, [2S-(2α,4α,4aα,8aβ)]-
82546-67-6	1	0	0	Propanoic acid, 3-(ethoxycarbonyl)-3-(1-cyclohexenenyl)-
82560-54-1	0	1	0	β-Alanine, *N*-(((((2,3-dihydro-2,2-dimethyl-7-benzofuranyl)oxy)carbonyl)methylamino)thio)-*N*-(1-methylethyl)-, ethyl ester {Benfuracarb®}
82612-14-4	0	1	0	1,2-Cyclohexanediol, 4-[1-(acetyloxy)-1-methylethyl]-1-methyl-, (1α,2β,4α)-(±)-
82657-04-3	0	1	0	Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-trifluoro-1-propenyl]-2,2-dimethyl-, (2-methyl[1,1′-biphenyl]-3-yl) methyl ester, (1R,3R)-rel- {Bifenthrin®, Biphenthrin®}
82796-87-0	1	0	0	*D*-Xylonic acid, δ-lactone
82806-40-4	1	1	1	Butenamine
82826-13-9	0	1	0	2-Propenoic acid, 3-(2-furanyl)-2-methyl-, ethyl ester
83174-26-9	1	0	0	2,5-Furandione, 3-propyl-
83177-17-7	0	1	0	3*H*-Pyrido[3,4-*b*]indol-7-ol, 1,2-dihydro- {1,2-dihydro-1-demethylharmalol}
83534-39-8	0	1	0	Glycosidase
83704-32-9	1	0	0	Dibenzofuran, 2,3,4,8-tetrachloro-
83841-47-8	0	1	0	2-Butenal, 4-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-2-methyl-, [1R-[1α(*E*),2β,4aβ,8aα]]-
84302-42-1	1	0	0	4*H*-Pyran-4-one, 2,3-dihydro-
84367-90-8	1	1	1	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1S-(1R*,2*E*,5R*,6*E*,8R*,11*E*)]-
84367-92-0	0	1	0	2,6,11-Cyclotetradecatriene-1,5-diol, 1,5,11-trimethyl-8-(1-methylethyl)-, [1R-(1R*,2*E*,5S*,6*E*,8S*,11*E*)]-
84461-48-3	1	1	1	Hexadecanoic acid, tetratriacontyl ester
84499-92-3	0	1	0	1*H*-Pyrrole-1-acetic acid, 2-(ethoxymethyl)-5-formyl-
84625-54-7	1	0	0	Pyridine, 4-methyl-2-pentyl-
84808-91-9	1	0	0	Hexacosene
85213-22-5	0	1	0	Ethanone, 1-(2,5-dihydro-1*H*-pyrrol-2-yl)- {2-acetylpyrroline}
85248-56-2	0	1	0	1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-, (S)- {8,9-dehydrotheaspirone}
85352-99-4	0	1	0	3-Pyridinemethanol, α-[3-(methylnitrosoamino)propyl]-, 1-oxide
85373-77-9	1	0	0	4*H*-Pyran-3-carboxylic acid, 5,6-dihydro-2,6-dimethyl-, methyl ester
85502-23-4	0	1	0	Propanal, 3-(nitrosomethylamino)-
85528-07-0	1	0	0	Phenol, dimethylethyl-
85564-78-9	1	0	0	2(3*H*)-Furanone, dihydro-3,4,5-trimethyl-
85792-05-8	1	0	0	Dotriacontene
85949-43-5 23726-92-3	1	1	1	2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*Z*)- [2 CAS Nos.] {β-damascone}
85960-81-2	1	0	0	Phenol, 4-(1-propen-1-yl)-, (*Z*)-
86154-08-7	0	1	0	4*H*-Cyclopenta[3′,4′]cycloocta[1′,2′:1,5]cyclopent[1,2-*b*]oxiren-4-one, 1,2,2a,7,7a,8,9,10,10a,10b-decahydro-2a,6,10a-trimethyl-8-(1-methylethyl)-, (2aα,3aR*,7aβ,8β,10aβ,10bβ)-
86687-05-0	1	0	0	1,3-Dioxane, 5-hydroxy-
86709-50-4	1	1	1	Stigmasta-3,5,24(28)-triene

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
86900-39-2	0	1	0	Pyrrolidine, 1-ethyl-2-(3-pyridinyl)- {*N*′-ethylnornicotine}
86901-30-6	1	0	0	1*H*-Indene, heptamethyl-
77242-77-4				
87116-68-5	1	0	0	Thiazole, 4-ethyl-5-methyl-2-(1-methylethyl)-
87323-67-9	1	0	0	Benzoic acid, hydroxy-methoxy-
87387-80-2	0	1	0	2,6,12-Cyclotetradecatrien-1-ol, 3,7,13-trimethyl-10-(1-methylethenyl)-
87513-63-1	0	1	0	Benzoic acid, 3-hydroxy-6-methoxy-, methyl ester
87554-04-9	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8*E*,12S*,13*Z*)]-
87562-12-7	0	1	0	2-Buten-1-one, 1-[3-(formyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, (*E*)-
87563-33-5	0	1	0	2-Penten-1-ol, 3-methyl-5-(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [1S-[1α(*E*),4aβ,8aα]]-
87584-34-7	0	1	0	2-Buten-1-ol, 3-(dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-*b*]furan-2-yl)-, [2R-[2α(*E*),3aβ,5aα,9aβ,9bα]]-
87585-55-5	0	1	0	2-Penten-1-ol, 3-methyl-5-(3,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-, [4aS-[1(*E*),4aα,8aβ]]-
87734-68-7	0	1	0	Ergostan-6-one, 3,22,23-trihydroxy-, (3α,5α,22R,23R,24S)-
87797-88-4	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,7,8-tetramethyl-, (R)-
87797-89-5	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,6-tetramethyl-, (R)-
88070-43-3	1	0	0	Pyrimidine, 5-hydroxy-4-phenyl-
88111-63-1	1	0	0	Pyridine, 3-(1-methylethoxy)-
88125-11-5	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one,1a,2,3,4,7a,7b-hexahydro-1a,5,7b-trimethyl-,[1aS-(1aα,2β,4aβ,7aα,7bα)]-
88125-12-6	0	1	0	2,3-Naphthalenedione, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (4aS-*cis*)-
88381-44-6	0	1	0	4-Thiazolidinecarboxylic acid, 3-nitroso- {*N*-nitrosothioproline}
88437-32-5	0	1	0	Cyclohexanol, 4-(2-hydroxy-1-methylethylidene)-1-methyl-, 1-acetate
88476-94-2	0	1	0	Glycine, *N*-(1-nitroso-*L*-prolyl)-
88663-71-2	0	1	0	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*E*)-
88663-72-3	0	1	0	1,4-Cyclohexanediol, 1-(1-hydroxy-1-methylethyl)-4-methyl-, 4-acetate, (*Z*)-
88663-73-4	0	1	0	1-Cyclohexene-1-methanol, 4-(acetyloxy)-α,α,4-trimethyl-
88813-63-2	1	0	0	Benzoquinoline, methyl-
88848-60-6	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 6-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-glucopyranosyl)oxy]octahydro-1a,5,7b-trimethyl-, [1aS-(1aα,2β,4aβ,5α,6β,7aα,7bα)]-
88848-61-7	0	1	0	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl 2-*O*-β-*D*-glucopyranosyl-, [1S-(1α,2β,3α,7β)]-
89126-45-4	1	0	0	Azafluoranthene
89126-46-5	1	0	0	Azapyrene
89145-04-0	0	1	0	1*H*-Pyrrolecarboxaldehyde
89194-80-9	0	1	0	myo-Inositol, *O*-*D*-glucopyranosyl-
89288-59-5	0	1	0	4,13-Cyclotetradecadiene-1,3-diol,8-hydroperoxy-1,5-dimethyl-9-methylene-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,8R*,12R*,13*E*)]-
89288-60-8	0	1	0	4,7,13-Cyclotetradecatriene-1,3-diol,9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,7*E*,9R*,12R*,13*E*)]-
89362-05-0	0	1	0	4,13-Cyclotetradecadiene-1,3-diol,8-hydroperoxy-1,5-dimethyl-9-methylene-12-(1-methylethyl)-,[1R-(1R*,3R*,4*E*,8S*,12S*,13*E*)]-
89362-06-1	0	1	0	4,7,13-Cyclotetradecatriene-1,3-diol,9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,7*E*,9S*,12R*,13*E*)]-
89362-07-2	0	1	0	4,7,13-Cyclotetradecatriene-1,3-diol,9-hydroperoxy-1,5,9-trimethyl-12-(1-methylethyl)-,[1R-(1R*,3R*,4*E*,7*E*,9S*,12S*,13*E*)]-
89362-08-3	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-
89362-09-4	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,8S*,12S*,13*E*)]-
89362-10-7	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7*E*,9R*,12R*,13*E*)]-
89362-11-8	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7*E*,9R*,12R*,13*E*)]-
89364-27-2	1	0	0	3(2*H*)-Furanone, dihydro-4-methyl-
89647-62-1	0	1	0	19-Norlanosta-5,23-diene-2,11,22-trione, 25-(acetyloxy)-3,16,20-trihydroxy-9-methyl-, (3β,9β,10α,16α,23*E*)-
90026-55-4	1	1	1	2(3*H*)-Furanone, dihydro-4,5-dimethyl-, (4R-*Z*)-
90357-58-7	1	1	1	Acetic acid, hydroxy-, propyl ester
90534-46-6	1	0	0	Phenol, 2-ethyl-6-methoxy-
90660-18-7	0	1	0	4,9-Cyclotetradecadien-1-one, 6,8-dihydroxy-4,8-dimethyl-14-methylene-11-(1-methylethyl)-
90803-60-4	0	1	0	M-1nkh
91048-13-4	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)butylidene]-3,5,5-trimethyl-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
91163-46-1	0	1	0	5,9-Cyclotetradecadiene-1,4,8-triol, 4,8-dimethyl-14-methylene-11-(1-methylethyl)-, [1S-(1R*,4R*,5*E*,8S*,9*E*,11R*)]-
91200-13-4	0	1	0	4,13-Cyclotetradecadiene-1,3,8-triol, 1,5-dimethyl-9-methylene-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,8S*,12R*,13*E*)]-
91200-14-5	0	1	0	4,7,13-Cyclotetradecatriene-1,3,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7*E*,9R*,12R*,13*E*)]-
91238-45-8	1	1	1	4-Pentene-2,3-dione
91429-66-2	1	0	0	Pyridine, 3-(1-ethyl-2-pyrrolidinyl)- {ethylnicotine}
91465-08-6	1	1	1	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester {λ-Cyhalothrin®}
91491-09-7	1	0	0	1*H*-Imidazole, propyl-
91491-14-4	1	0	0	3-Pyridinol, methyl-
91538-84-0	1	0	0	Dibenzofuran, 1,2,3,4,7,9-hexachloro-
91599-03-0	0	1	0	1-Butanol, 4-[(7-β-*D*-glucopyranosyl-7*H*-purin-6-yl)amino]-2-methyl-
91907-45-8	0	1	0	Pyrrolidine, 1-propyl-2-(3-pyridinyl)- {*N*′-propylnornicotine}
91914-04-4	1	0	0	2-Pyridinol, 3-methyl- {2(1*H*)-pyridinone, 3-methyl-}
1003-56-1				
91914-05-5	1	0	0	2-Pyridinol, 4-methyl- {2(1*H*)-pyridinone, 4-methyl-}
91914-06-6	1	0	0	2-Pyridinol, 5-methyl- {2(1*H*)-pyridinone, 5-methyl-}
1003-68-5				
92751-21-8	0	1	0	Ergostan-6-one, 3,22,23-trihydroxy-, (3β,5α,22R,23R,24S)-
93451-46-8	1	1	1	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [1S-(1α,3β,4α,5α)]-
327-97-9				[2CAS Nos.] {chlorogenic acid, 3-*O*-caffeoylquinic acid}
93526-86-4	1	0	0	Phenol, 2-methoxy-trimethyl-
93976-08-0	1	1	1	Octadecenoic acid, hexacosyl ester, (*Z*)-
93976-09-1	1	1	1	Octadecenoic acid, tetracosyl ester, (*Z*)-
93976-10-4	1	1	1	Octadecenoic acid, docosyl ester, (*Z*)-
94185-89-4	0	1	0	Cyclase, farnesyl pyrophosphate
94390-73-5	1	0	0	Ethanone, 1-[2-methyl-5-(1-methylethyl)-2,5-cyclohexadien-1-yl]-
94414-19-4	0	1	0	Urs-12-en-28-oic acid, 3,23-dihydroxy-, (3β,4α)-
94434-40-9	1	0	0	2-Nonadecene, (*E*)-
94618-71-0	1	0	0	2,4-Cyclopentadien-1-one, 2-methyl-
94632-81-2	1	1	1	Hexadecanoic acid, pentacosyl ester
94632-82-3	1	1	1	Hexadecanoic acid, heptacosyl ester
94806-37-8	1	0	0	1,5-Hexadien-3-ol, 5-methyl-
95334-70-6	0	1	0	2,6,10-Cyclotetradecatriene-1,5,9-triol, 1,5,9-trimethyl-12-(1-methylethyl)-
95360-16-0	0	1	0	4,9-Pentadecadienal, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4*E*,6R*,8S*,9*E*,11S*)]-
95415-29-5	1	1	1	Octacosanoic acid, octadecyl ester
95896-78-9	1	0	0	3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 3,4,8-trimethyl-
95907-02-1	1	0	0	2-Pyridinol, 3,4-dimethyl- {2(1*H*)-pyridinone, 3,4-dimethyl-}
36330-90-2				
96168-15-9	1	0	0	2*H*-Pyran-2-one, tetrahydro-4-methyl-6-(3,7,11-trimethyldodecyl)-
96443-01-5	1	0	0	Cholest-4-en-3-ol, 4-methyl- (3α)
96552-69-1	1	0	0	Piperidine, 1-(1-oxooctyl)-2-(3-pyridinyl)-, (S)-
96552-70-4	1	0	0	[2,3′-Bipyridine]-1(2*H*)-carboxylic acid, 3,6-dihydro-, methyl ester, (S)-
96552-71-5	1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxohexyl)-, (S)- {*N*′-hexanoylanatabine}
96552-72-6	1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-1-(1-oxooctyl)-, (S)- {*N*′-octanoylanatabine}
96552-73-7	1	0	0	Pyrrolidine, 1-(4-methyl-1-oxohexyl)-2-(3-pyridinyl)-
96574-02-6	1	0	0	Pyrrolidine, 1-(6-methyl-1-oxoheptyl)-2-(3-pyridinyl)-, (S)-
96937-33-6	1	0	0	Benzenepropanoic acid, 3,4-dihydroxy-ar-methyl-
96937-34-7	1	0	0	Benzenepropanoic acid, 2,5-dihydroxy-ar-methyl-
96937-35-8	1	0	0	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methyl-
96937-36-9	1	0	0	Benzenepropanoic acid, ar,ar-dihydroxy-ar-methoxy-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
96937-37-0	1	0	0	Benzeneacetic acid, ar,α-dihydroxy-ar-ethyl-
96937-38-1	1	0	0	Benzenepropanoic acid, 2,3-dihydroxy-ar-methyl-
96937-39-2	1	0	0	Benzoic acid, 3,4-dihydroxy-dimethyl-
96937-40-5	1	0	0	Benzoic acid, 3,4-dihydroxy-methyl-
96937-41-6	1	0	0	Benzeneacetic acid, 3,4-dihydroxy-ar-methyl-
96937-42-7	1	0	0	Benzeneacetic acid, ar,ar-dihydroxy-ar,ar-dimethyl-
96937-43-8	1	0	0	Benzoic acid, ethyl-hydroxy-
96937-44-9	1	0	0	Benzoic acid, dimethyl-hydroxy-
96937-45-0	1	0	0	Benzoic acid, 4-hydroxymethyl-
96937-46-1	1	0	0	Benzoic acid, dihydroxy-dimethyl-
96937-47-2	1	0	0	Benzoic acid, dihydroxyethyl-
96937-48-3	1	0	0	Benzeneacetic acid, ar,ar-dihydroxy-ar-methyl-
96937-49-4	1	0	0	Benzoic acid, 2,5-dihydroxy-methyl-
96937-51-8	1	0	0	Octanoic acid, oxo-
96937-52-9	1	0	0	Pentanoic acid, hydroxymethyl-
96937-53-0	1	0	0	Pentanoic acid, oxo-
96937-54-1	1	0	0	Pentanoic acid, methyl-oxo-
96961-47-6	1	0	0	Benzenepropanoic acid, 3,4-dihydroxy-2,5,6-trimethyl-
97089-70-8	0	1	0	Peroxidase, glutathione [2 CAS Nos.]
9013-66-5				
97122-27-5	1	0	0	Benzaldehyde, hydroxy-3-methyl-
97145-16-9	0	1	0	Octadecadienoic acid, 1-[[[(2-aminoethoxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl ester, (all-*Z*)-
97162-77-1	0	1	0	Demethylase, nicotine
97170-14-4	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-
97170-15-5	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl, (all-*Z*)-
97190-07-3	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy)hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monooctadecadienoate monooctadecatrienoate, (all-*Z*)-
97190-08-4	0	1	0	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecadienoate, (all-*Z*)-
97190-09-5	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy)hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecatrienoate, (*Z,Z,Z*)-
97190-10-8	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy)hydroxyphosphinyl]oxy]-*N,N,N*-trimethyl-, hydroxide, inner salt, monohexadecanoate monooctadecadienoate, (*Z,Z*)-
97190-11-9	0	1	0	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) hexadecanoate
97190-12-0	0	1	0	Ethanaminium, 2-[[(2,3-dihydroxypropoxy)hydroxyphosphinyl]oxy]-*N,N,N*- trimethyl-, hydroxide, inner salt, monooctadecadienoate
97190-13-1	0	1	0	Octadecadienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) octadecanoate, (*Z,Z*)-
97210-24-7	0	1	0	Octadecadienoic acid, monoester with 1,2,3-propanetriol 1,1′-(hydrogen phosphate) mono-3-hexadecenoate, [R-[R*,S*-(*E*)]]-
97229-62-4	0	1	0	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1-(2-aminoethyl hydrogen phosphate) 2(or 3)-hexadecanoate, (*Z,Z,Z*)-
97229-63-5	0	1	0	Octadecatrienoic acid, ester with 1,2,3-propanetriol 1,1′-(hydrogen phosphate) 2(or 3)-(3-hexadecenoate), [R-(R*,S*)]-
97232-94-5	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecadienyl)oxy]propyl *O-D*-galactosyl-, (all-*Z*)-
97233-43-7	0	1	0	*D*-Galactoside, 2,3-bis[(1-oxooctadecatrienyl)oxy]propyl *O-D*-galactosyl-, (all-*Z*)-
97234-09-8	0	1	0	*D*-Galactoside, [(1-oxohexadecatrienyl)oxy][(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-
97234-10-1	0	1	0	*D*-Galactoside, [(1-oxohexadecyl)oxy][(1-oxooctadecatrienyl)oxy]propyl, (*Z,Z,Z*)-
97259-93-3	0	1	0	Heptanoic acid, dimethyl-
97275-71-3	0	1	0	*D*-Galactoside, 2,3-dihydroxypropyl, 2′(or 3′)-hexadecanoate 3′(or 2′)-octadecadienoate, (*Z,Z*)-
97276-55-6	0	1	0	*D*-Galactoside, [(1-oxooctadecadienyl)oxy][(1-oxooctadecatrienyl)oxy]propyl, (all-*Z*)-
97281-47-5	0	1	0	Lecithins
97542-81-9	1	0	0	1*H*-Indole, ethyl-
97614-61-4	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(3-methylpentanoate)
98064-73-4	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-dien-6-one, 8-hydroxy-4,8,14-trimethyl-11-(1-methylethyl)-, [1S-(1R*,4*E*,8R*,9*E*,11R*)]
98064-74-5	0	1	0	2,5,11-Cyclotetradecatrien-1-one, 7,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-, [7S-(2*E*,5*E*,7R*,10R*,11*E*,13R*)]-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
98064-75-6	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-6,10-dien-3-one,5-hydroxy-1,5,11-trimethyl-8-(1-methylethyl)-,[1R-(1R*,5S*,6*E*,8S*,10*E*)]-
98064-76-7	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one,5-hydroxy-1,5-dimethyl-11-methylene-8-(1-methylethyl)-,[1R-(1R*,5S*,6*E*,8S*,1)]-
98064-77-8	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one,5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-,[1R-(1R*,5S*,6*E*,8S*,11R*)]-
98114-50-2	1	0	0	Benzenepropanoic acid, 2,6-dihydroxy-
98166-23-5	1	1	1	2*H*-Pyran-3(6*H*)-one
98167-33-0	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-en-3-one,5,11-dihydroxy-1,5,11-trimethyl-8-(1-methylethyl)-,[1R-(1R*,5S*,6*E*,8S*,11S*,12S*)]-
98188-02-4	0	1	0	Heptanoic acid, 7-(2-furanyl)-, methyl ester
98791-40-3	1	0	0	1*H*-Cyclopent[*d*]acenaphthylene, 2,7-dihydro-
98791-41-4	1	0	0	1*H*-Indeno[1,7-*ab*]fluorene
98791-42-5	1	0	0	1*H*-Indeno[1,7-*ab*]fluorene 2,11-dihydro-
98791-43-6	1	0	0	Dicyclopenta[*cd,jk*]pyrene
98791-44-7	1	0	0	Dicyclopenta[*cd,jk*]pyrene, 1,2-dihydro-
98791-45-8	1	0	0	Dicyclopenta[*cd,jk*]pyrene, 1,2,3,4-tetrahydro-
98886-44-3	0	1	0	Phosphonodithioic acid, *O*-ethyl *S*-(1-methylpropyl) (2-oxo-3-thiazolidinyl)- {Fosthiazate®}
98910-85-1	0	1	0	3-Buten-2-one, 4-(4-oxo-2,6,6-trimethyl-1-cyclohexen-1-yl)- {4-oxo-β-ionone}
98913-58-7	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 3-methylpentanoate
99431-70-6	0	1	0	9,12-Octadecadienoic acid (*Z,Z*)-, monoester with 1,2,3-propanetriol dihexadecanoate
26836-30-6				{dipalmitolinolein}
99499-89-5	0	1	0	β-*D*-Glucopyranoside, 1,2,3,4,5,6,7,8-octahydro-3-hydroxy-1-methyl-7-(1-methylethenyl)-2-naphthalenyl *O*-6-deoxy-α-*L*-mannopyranosyl-(1 → 4)-*O*-β-*D*-glucopyranosyl-(1 → 4)-, [1S-(1α,2β,3α,7β)]-
99694-82-3	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl)-, [2R-[2α(S*),8β,8aα]]-
99881-86-4	0	1	0	2*H*-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-
100017-41-2	0	1	0	Cholest-9(11)-en-3-ol, 14-methyl-, (3β,5α)-
100092-00-0	0	1	0	Galactoxyloglucan {amyloid}
100210-90-0	1	0	0	1,3-Hexadecadiene, 2,6,10,14-tetramethyl-
30917-33-0				
100404-00-0				
2140-82-1	1	1	1	1-Pentadecene, 2,6,10,14-tetramethyl- [3 CAS Nos.] {norphytene}
60976-73-0				
101159-07-3	0	1	0	1,4,7,10-Cyclotetradecatetraene, 1,7,11-trimethyl-4-(1-methylethenyl)-
101159-08-4	1	1	1	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)- {cembrene}
101159-09-5	1	1	1	3-Nonene-2,8-dione, 5-(1-methylethyl)-, [S-(*E*)]- [2 CAS Nos.] {oxysolanone}
60619-46-7				
35953-21-0				
101330-76-1	0	1	0	2,6,10,14,18,22,26,30,34-Hexatriacontanonaen-1-ol, 3,7,11,15,19,23,27,31,35-nonamethyl-, labeled with ^{14}C, (*Z,Z,Z*)- {solanesol-^{14}C}
101540-79-8	0	1	0	Pyridine, 3-(1-methyl-2-pyrrolinyl)-6-methyl-
101758-45-6	0	1	0	2-Pentene-1,4-diol, 5-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl)-3-methyl-, [1α(3*E*,4S*),2β,4a
102056-77-9	1	1	1	Butane, 2-methyl- {methylbutane}
78-78-4				
102488-04-0	0	1	0	2-Octanone, 3,3-dimethyl-7-hydroxy-
102488-05-1	0	1	0	1,5-Hexanediol, 2-(1-methylethyl)-
102488-06-2	0	1	0	2-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-, (*E*)
102488-07-3	1	1	1	2-Cyclohexen-1-one, 4-(3-hydroxybutylidene)-3,5,5-trimethyl-, (*E*)
102488-08-4	0	1	0	3-Cyclohexen-1-one, 4-(1-butenyl)-3,5,5-trimethyl-, (*E*)
102488-09-5	1	1	1	2-Buten-1-one, 1-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-
				{3-hydroxy-β-damascone}
102488-10-8	0	1	0	2,2′-Bifuran, 2,3,4,5-tetrahydro-2,5′-dimethyl-5-(1-methylethenyl)-
102491-96-3	1	1	1	Stigmasta-3,5,22-triene, (22*E*)-
102518-80-9	0	1	0	7-Oxabicyclo[2.2.1]heptan-2-ol, 1-(3-hydroxy-1-butenyl)-2,6,6-trimethyl-[1 R[1AL]]
102518-81-0	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-
52812-41-6				

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
102518-82-1	0	1	0	Ethanone, 1-[5-methyl-2-(1-methylethyl)-6,8-dioxabicyclo[3.2.1]oct-7-yl]-, (exo,exo)-(±)-
57934-85-7				
102608-53-7	0	1	0	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-
102673-27-8	0	1	0	4,9-Pentadecadienal, 6-(acetyloxy)-8-hydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-, [6R-(4*E*,6R*,8R*,9*E*,11S*)]-
102734-47-4	0	1	0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-
102734-49-6	0	1	0	4,9-Pentadecadienoic acid, 6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo- {isomer}
102734-50-9	0	1	0	4,9-Pentadecadienoic acid,6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-,methylester,[6R-(4*E*,6R*,8S*,9*E*,11S*)]-
102734-51-0	0	1	0	4,9-Pentadecadienoic acid,6,8-dihydroxy-4,8-dimethyl-11-(1-methylethyl)-14-oxo-,methylester,[6R-(4*E*,6R*,8R*,9*E*,11S*)]-
102734-52-1	0	1	0	2(3*H*)-Furanone,dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-,[5S-[5R*(1*E*,4R*,5*E*,7R*)]]-
102734-53-2	0	1	0	2(3*H*)-Furanone,dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-,[5S-[5R*(1*E*,4S*,5*E*,7R*)]]-
102734-54-3	0	1	0	2(3*H*)-Furanone,dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-,[5R-[5R*(1*E*,4S*,5*E*,7S*)]]-
102734-55-4	0	1	0	2(3*H*)-Furanone,dihydro-5-[4-hydroxy-4-methyl-7-(1-methylethyl)-10-oxo-1,5-undecadienyl]-5-methyl-,[5R-[5R*(1*E*,4R*,5*E*,7S*)]]-
102734-57-6	0	1	0	5,10-Cyclotetradecadiene-1,2,7,9-tetrol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,2R*,5*E*,7S*,9R*,10*E*,12R*)]-
102851-06-9	0	1	0	Valine, *N*-(2-chloro-4-(trifluoromethyl)phenyl)-, cyano(3-phenoxyphenyl)methyl ester {Fluvalinate®}
102977-86-6	0	1	0	2(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,8-dimethyl-7-(1-methylethenyl)-
102977-87-7	0	1	0	2-Naphthaleneethanol, 3,4-dihydro-1,5,6-trimethyl-
102977-88-8	0	1	0	15-Oxabicyclo[10.2.1]pentadeca-2,6-dien-5-ol, 5-methyl-11-methylene-8-(1-methylethyl)-
103002-58-0	0	1	0	1*H*-Pyrrole-3-carboxaldehyde, 4,5-dihydro-2-methyl-
103469-25-6	0	1	0	Deoxyribonucleic acid (tobacco clone PROB12 protein TL messenger RNA complementary)
104077-06-7	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-3-[(1-oxo-9-octadecenyl)oxy]propyl ester, (*Z,Z,Z*)-
104077-07-8	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]propyl ester, (all-*Z*)-
104077-08-9	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 2-hydroxy-3-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]propylester,(all-*Z*)-
104077-09-0	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-2- [(1-oxo-9-octadecenyl)oxy]ethyl ester, (*Z,Z,Z*)-
104077-10-3	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-
104077-11-4	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-
104077-12-5	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-1,2-ethanediyl ester, (all-*Z*)-
104077-13-6	0	1	0	9-Octadecenoic acid, 18-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]-, 1-(hydroxymethyl)-2-[[1-oxo-18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-9-octadecenyl]oxy]ethyl ester, (all-*Z*)-
104100-34-7	0	1	0	9-Octadecenoic acid, 18-[(1-oxo-9-octadecenyl)oxy]-, 2-hydroxy-1,3-propanediyl ester, (all-*Z*)-
104100-35-8	0	1	0	9-Octadecenoic acid,18-[[1-oxo-18-[(1-oxo-9-octadecenyl)oxy]-9-octadecenyl]oxy]-,2-hydroxy-1,3-propanediylester,(all-*Z*)-
104153-60-8	0	1	0	1,2,3-Cyclohexanetriol, 1-methyl-4-(1-methylethyl)-
104669-35-4	0	1	0	6-Hepten-2-one, 5-(1-methylethyl)-7-(tetrahydro-4-hydroxy-2-methyl-2-furanyl)-
104932-26-5	1	1	1	Triacontanoic acid, eicosyl ester
105300-09-2	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one,1a-[(β-*D*-glucopyranosyloxy)methyl]octahydro-5,7b-dimethyl-[1aR-(1aa,2b,4ab,5a,7aa,7ba)]-
105300-10-5	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 5-[(β-*D*-glucopyranosyloxy)methyl]octahydro-1a, 7b-dimethyl-, [1aS-(1aα,2β,4aβ,5α,7aα,7bα)]-
105650-23-5	1	0	0	1*H*-Imidazo[4,5-*b*]pyridin-2-amine, 1-methyl-6-phenyl- {PhIP}
105728-84-5	0	1	0	4-Heptenoic acid, 6-hydroxy-
105827-78-9	0	1	0	1*H*-Imidazol-2-amine, ((6-chloro-3-pyridinyl)methyl)-4,5-dihydro-*N*-nitro- {Admire®}
106033-38-9	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(3-methylpentanoate), [2(S),3(S),4(S)]-
106398-69-0	1	0	0	Pyrrole, butyl-
106777-19-9	0	1	0	*D*-Ribonic acid, 2-C-[(phosphonooxy)methyl]-
106799-60-4	0	1	0	Benzaldehyde, hydroxymethoxy-
107389-81-1	0	1	0	Galactoglucomannan
107544-21-8	0	1	0	Desaturase, phytoene
108281-08-9	0	1	0	Synthase, mannopine
108657-23-4	1	1	1	Hexacosanoic acid, docosyl ester

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
109682-81-7	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-(1-methylethyl)-
109682-85-1	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-5-propyl-
109682-87-3	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl-
109682-88-4	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-4-methyl-3-propyl-
109682-89-5	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-4-propyl-
109682-90-8	1	0	0	2-Cyclopenten-1-one, 3,5-dimethyl-4-ethyl-2-hydroxy-
109682-91-9	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(3-methylbutyl)-
109682-92-0	1	0	0	2-Cyclopenten-1-one, 2-hydroxy-3-(2-methylbutyl)-
110053-51-5 2503-46-0	1	1	1	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-
110053-52-6	1	0	0	Phenanthrene, dimethylene-
110053-53-7 71278-23-4	1	1	1	Dodecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl dodecanoate}
110053-55-9 126165-82-0 64091-91-4 121268-99-3	1	1	1	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}
110053-56-0	1	0	0	2,6,10,14,18,22,26,30-Dotriacontaoctaene, 3,7,11,15,19,23,27-heptamethyl-
110053-57-1	1	0	0	2-Propanol, 1,1-bis(2-hydroxypropoxy)-
110053-58-2	1	0	0	1-Propanol, 2,2-bis(1-hydroxypropoxy)-
110053-62-8	1	1	1	Tetradecanoic acid, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl tetradecanoate}
71607-88-0 110053-63-9	1	0	0	3,8-Dioxabicyclo[3.3.0]octan-2-one, 6-hydroxy-
110053-64-0	1	0	0	1,3-Cyclohexanecarbolactone, 2-hydroxy-3-methyl-
110053-65-1 503-48-0	1	1	1	2*H*-Pyran-2-one, tetrahydro-4-hydroxy-4-methyl-
110081-38-4	1	0	0	Benzo[*a*]pyrene, 3,4-dihydro-
110115-39-4 70495-60-2	1	1	1	9,12-Octadecadienoic acid (*Z,Z*)-, 3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl ester {solanesyl octadecadienoate}
110171-22-7	1	0	0	2(3*H*)-Furanone, dihydro-4,5-dimethyl-, (4R-*E*)-
110187-42-3	0	1	0	Glucose, labeled with ^{13}C {Glucose-^{13}C}
110484-93-0	1	0	0	Furan, 2,2′-methylenebis[5-ethyl-
110484-94-1	1	0	0	Furan, 2-[1-(5-ethyl-2-furanyl)ethyl]-5-methyl-
110488-70-5	0	1	0	Morpholine, 3-(3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-oxo-2-propenyl)- {Dimethomorph®, Acrobat®}
110746-39-9	1	0	0	2-Nonadecene, 2-methyl-
111924-41-5	0	1	0	1,2,8-Phenanthrenetriol, tetradecahydro-8,10a-dimethyl-4-methylene-5-(1-methylethyl)-
112019-00-8	0	1	0	1,2-Cyclohexanediol, 2-(3-hydroxy-1-butenyl)-1,3,3-trimethyl-, [1R-[1α,2α,2(1*E*,3S*)]]-
112468-46-9	1	1	1	2*H*-Pyran-2,5(6*H*)-dione
112523-81-6	0	1	0	Ethanone, 1-[2,3,3a,4,6a,7,8,9,9a,9b-decahydro-5,9a-dimethyl-7-(1-methylethyl)-1*H*-cyclopent[*a*]azulen-3-yl]-, [3R-(3α,3aα,6aβ,7β,9aα,9bβ)]-
114393-99-6	0	1	0	1,3-Naphthalenediol, 1,2,3,4,4a,5,6,7-octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, 3-acetate, [1R-(1α,3β,4.
115600-67-4	1	0	0	2*H*-Pyrrol-2-one, 4-ethyl-1,5-dihydro-
115742-70-6	0	1	0	Cryptogein
115788-20-0	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-5-hydroxy-8,8a-dimethyl-2-naphthalenyl)-, [2R-[2α(R*),5α,8.
115788-21-1	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-3-hydroxy-8,8a-dimethyl-2-naphthalenyl)-, [2S-[2α(S*),3α,8β,8aα]]-
115849-75-7	0	1	0	Pyrrolidine, 1-(1-oxododecyl)-2-(3-pyridinyl)-, (S)-
115849-79-1	0	1	0	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-
115849-80-4	0	1	0	Pyrrolidine, 1-(3-hydroxy-1-oxododecyl)-2-(3-pyridinyl)-
115849-82-6	0	1	0	Pyrrolidine, 1-(3-hydroxy-10-methyl-1-oxododecyl)-2-(3-pyridinyl)-
115849-83-7	0	1	0	Pyrrolidine, 1-(3-hydroxy-1-oxotridecyl)-2-(3-pyridinyl)-
115849-84-8	0	1	0	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
115849-85-9	0	1	0	Pyrrolidine, 1-(3-hydroxy-1-oxotetradecyl)-2-(3-pyridinyl)-
115888-33-0	0	1	0	1,2-Propanediol, 2-(1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl)-, [2S-[2α(S*),8α,8aβ]]-
116348-80-2	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3S*,4*E*,8*E*,12S*,13*E*)]-
116353-95-8	0	1	0	Pyrrolidine, 1-(3-hydroxy-12-methyl-1-oxotetradecyl)-2-(3-pyridinyl)-
116502-44-4	1	0	0	Hexane, 2,4-dimethyl-
589-43-5				
117063-83-9	1	1	1	Heptacosanoic acid, eicosyl ester
117065-21-1	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,7,8-tetramethyl-, (±)-
117065-22-2	0	1	0	2-Naphthalenemethanol, 1,2,3,4-tetrahydro-α,α,5,6-tetramethyl-, (±)-
117210-48-7	0	1	0	6-Hepten-2-one, 7-[tetrahydro-2-methyl-5-(1-methylethyl)-2-furanyl]-
117210-49-8	0	1	0	Ethanone, 1-(1,4,4a,5,6,7,8,8a-octahydro-4a,8,8-trimethyl-2-naphthalenyl)-, (4aR-*trans*)-
117210-50-1	0	1	0	Ethanone, 1-(3a,4,5,6,7,7a-hexahydro-3a,7,7-trimethyl-1*H*-inden-2-yl)-, (3aR-*trans*)-
117210-51-2	0	1	0	2-Tridecanone, 4,8,12-trimethyl-
117210-52-3	0	1	0	1(2*H*)-Naphthalenone, 3,4-dihydro-5-methyl-3-(1-methylethenyl)-
117210-53-4	0	1	0	2,7-Dioxabicyclo[2.2.1]heptane, 1,3-dimethyl-3-(4-methyl-3-pentenyl)-, endo-
117210-54-5	0	1	0	2,7-Dioxabicyclo[2.2.1]heptane-3-butanol, α,α,1,3-tetramethyl-
117232-64-1	0	1	0	5,10-Dodecadien-2-one, 9-hydroxy-6,11-dimethyl-
117277-96-0	0	1	0	Glucanase, preproendo-1,3-β-
117277-97-1	0	1	0	Glucanase, proendo-1,3-β-
117305-90-5	0	1	0	2,7-Dioxabicyclo[2.2.1]heptane, 1,3-dimethyl-3-(4-methyl-3-pentenyl)-, exo-
117332-54-4	0	1	0	Spiro[4.5]dec-6-en-8-one,2-[1-(hydroxymethyl)ethenyl]-6-methyl- {spirovetivan B}
117407-01-9	0	1	0	Spiro[4.5]dec-6-en-8-one, 9-hydroxy-6,10-dimethyl-2-(1-methylethenyl)- {spirovetivan A}
117472-47-6	0	1	0	1(4*H*)-Naphthalenone, 5,6,7,8-tetrahydro-8-methyl-5-(1-methylethenyl)-
117642-93-0	0	1	0	Pyrrolidine, 1-(10-methyl-1-oxododecyl)-2-(3-pyridinyl)-
117642-94-1	0	1	0	Pyrrolidine, 1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-, (S)-
117769-21-8	0	1	0	5(4*H*)-Benzofuranone, 2,7a-dihydro-2-(1-hydroxyethyl)-4,4-dimethyl-
117769-22-9	0	1	0	2,3-Naphthalenedione, 4,4a,5,6,7,8-hexahydro-1,4a-dimethyl-7-(1-methylethenyl)-
119613-98-8	0	1	0	5,10-Cyclotetradecadien-1-one, 7,9-dihydroxy-7,11-dimethyl-4-(1-methylethyl)-, [4S-(4R*,5*E*,7R*,9S*,10*E*)]-
119613-99-9	0	1	0	15-Oxabicyclo[12.1.0]pentadec-9-en-5-one, 11,13-dihydroxy-1,11-dimethyl-8-(1-methylethyl)-, [1S-(1R*,8R*,9*E*,11R*, 13S*,14S*)]-
119864-28-7	0	1	0	2,7,10-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1R-(1R*,2*E*,4S*,7*E*,10*E*)]-
119944-62-6	0	1	0	2,7,10-Cyclotetradecatrien-1-ol, 1,7,11-trimethyl-4-(1-methylethyl)-, [1S-(1R*,2*E*,4R*,7*E*,10*E*)]-
119973-28-3	1	0	0	Chol-3-ene, 23-methyl-, (5α)-
119973-29-4	1	0	0	26,27-Dinorergosta-3,5-diene
119973-30-7	1	0	0	26,27-Dinorergost-3-ene, (5α)-
119973-31-8	1	0	0	26,27-Dinorergosta-3,5,22-triene, (22*E*)-
120042-32-2	0	1	0	Pyrrolidine, 1-(3-hydroxy-1-oxohexadecyl)-2-(3-pyridinyl)-
120042-33-3	0	1	0	Pyrrolidine, 1-(3-hydroxy-14-methyl-1-oxopentadecyl)-2-(3-pyridinyl)-
120042-34-4	0	1	0	Pyrrolidine, 1-(3-hydroxy-1-oxopentadecyl)-2-(3-pyridinyl)-
120042-35-5	0	1	0	Pyrrolidine, 1-(1-oxotridecyl)-2-(3-pyridinyl)-, (S)-
120042-36-6	0	1	0	Pyrrolidine, 1-(11-methyl-1-oxododecyl)-2-(3-pyridinyl)-, (S)-
120042-32-2	0	1	0	Pyrrolidine, 1-(3-hydroxy-1-oxohexadecyl)-2-(3-pyridinyl)-
120056-06-6	0	1	0	Ethanone, 1-[3-(decahydro-2-hydroxy-2,5,5,8a-tetramethyl-1-naphthalenyl) oxiranyl]-, [1S-[1α(2S*,3R*),2β,4a
120056-15-7	1	0	0	Stigmasta-7,24(28)-dien-3-ol, 4-methyl-, (3β,5α)-
120293-52-9	0	1	0	1*H*-Imidazo[4,5-*c*]pyridine-4-propanoic acid, 4,6-dicarboxy-4,5,6,7-tetrahydro-, (4R-*cis*)-
120376-92-3	0	1	0	Pyrrolidine, 1-(10-methyl-1-oxoundecyl)-2-(3-pyridinyl)-
120376-93-4	0	1	0	Pyrrolidine, 1-(12-methyl-1-oxotridecyl)-2-(3-pyridinyl)-
120550-69-8	1	0	0	Phenol, 2-ethenyl-6-methoxy-
120550-70-1	1	0	0	Phenol, 4-ethyl-2-methoxy-6-methyl-
120550-71-2	1	0	0	Phenol, 4-ethyl-2-methoxy-5-methyl-

(*continued*)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
120598-69-8	0	1	0	Hydroxycinnamoyltransferase, putrescine
120904-94-1	0	1	0	Ubiquitin, poly-
121197-11-3	1	1	1	2*H*-Pyran-3(4*H*)-one, dihydro-4-(hydroxymethyl)-
121197-12-4	1	1	1	5-Hexen-3-one, 4,5-dihydroxy-
121197-14-6	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dipropyl-
121197-15-7	1	1	1	2,4-Pyrrolidinedione, 5-propyl-3-propylidene-
121197-16-8	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-propyl-
121197-17-9	1	1	1	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-(2-methylpropylidene)-
121197-18-0	1	1	1	2,4-Pyrrolidinedione, 3-butylidene-5-propyl-
121197-19-1	1	1	1	2,4-Pyrrolidinedione, 3-(2-methylpropylidene)-5-propyl-
121197-20-4	1	1	1	2,4-Pyrrolidinedione, 5-butyl-3-propylidene-
121197-21-5	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-(2-methylpropyl)-3-propyl-
121197-22-6	1	1	1	2,4-Pyrrolidinedione, 5-(2-methylpropyl)-3-propylidene-
121197-23-7	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-dibutyl-
121197-24-8	1	0	0	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-(2-methylpropyl)-
121197-25-9	1	1	1	2,4-Pyrrolidinedione, 3-butyl-5-propylidene-
121197-26-0	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 3-butyl-5-(2-methylpropyl)-
121197-27-1	1	0	0	2*H*-Pyrrole-2,4(3*H*)-dione, 3,5-bis(2-methylpropyl)-
121197-28-2	1	1	1	2,4-Pyrrolidinedione, 3-butylidene-5-(2-methylpropyl)-
121198-47-8	1	1	1	Pyranone, dimethyl-
121198-50-3	1	1	1	Ethanone, 1-(tetrahydrofuranyl)-
121198-51-4	0	1	0	Naphthalenol, 6,8-dimethyl-
121198-52-5	0	1	0	Naphthalenol, 7,8-dimethyl-
121213-25-0	1	1	1	Furan, 2,3-dihydro-2-methoxy-
121213-26-1	1	1	1	2*H*-Pyrrole-2,4(3*H*)-dione, 5-butyl-3-propyl-
121214-18-4	1	0	0	Naphthalene, tetrahydrotrimethyl- {at least three isomers in MSS}
121268-99-3	1	1	1	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK}
126165-82-0				{1-Butanone, 4-[(nitrosomethyl)amino]-1-(3-pyridinyl)-}
64091-91-4				[4 CAS Nos.]
110053-55-9				
121269-00-9	0	1	0	2-Heptanone, 6-(5-methyl-2-furanyl)-
121269-01-0	0	1	0	2-Naphthalenemethanol, 3,4-dihydro-1,5,6-trimethyl-
121269-03-2	0	1	0	3-Cyclohexen-1-ol, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-, (*E*)-
121468-15-3	0	1	0	Ergostan-6-one, 2,3,22,23-tetrahydroxy-, (2α,3β,5α,22R,23R,24S)-
121850-61-1	0	1	0	Benzenepropanamide, *N*-[3-[[4-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]amino]butyl]amino]propyl]-3,4-dihydroxy-
121877-07-4	1	1	1	Tridecanoic acid, 11-methyl-, heptadecyl ester
121877-08-5	1	1	1	Tetradecanoic acid, 12-methyl-, hexadecyl ester
121877-09-6	1	1	1	Tridecanoic acid, 12-methyl-, octadecyl ester
121877-10-9	1	1	1	Dodecanoic acid, 11-methyl-, eicosyl ester
121877-11-0	1	1	1	Tridecanoic acid, 12-methyl-, nonadecyl ester
121877-12-1	1	1	1	Tetradecanoic acid, 13-methyl-, octadecyl ester
121877-13-2	1	1	1	Pentadecanoic acid, 14-methyl-, heptadecyl ester
121877-14-3	1	1	1	Tridecanoic acid, 12-methyl-, heptadecyl ester
121877-15-4	1	1	1	Dodecanoic acid, 10-methyl-, eicosyl ester
121877-16-5	1	1	1	Tridecanoic acid, 11-methyl-, nonadecyl ester
121877-17-6	1	1	1	Tetradecanoic acid, 12-methyl-, octadecyl ester
121877-18-7	1	1	1	Pentadecanoic acid, 13-methyl-, heptadecyl ester
121877-19-8	1	1	1	Tridecanoic acid, 12-methyl-, eicosyl ester
121877-20-1	1	1	1	Pentadecanoic acid, 14-methyl-, octadecyl ester
121877-21-2	1	1	1	Tetradecanoic acid, 13-methyl-, eicosyl ester
121877-22-3	1	1	1	Tridecanoic acid, 12-methyl-, heneicosyl ester
121877-23-4	1	1	1	Tetradecanoic acid, 12-methyl-, eicosyl ester

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
121877-24-5	1	1	1	Tridecanoic acid, 11-methyl-, heneicosyl ester
121877-25-6	1	1	1	Tridecanoic acid, 12-methyl-, docosyl ester
121877-26-7	1	1	1	Tetradecanoic acid, 13-methyl-, heneicosyl ester
121877-27-8	1	1	1	Pentadecanoic acid, 14-methyl-, eicosyl ester
121877-28-9	1	1	1	Tetradecanoic acid, 12-methyl-, heneicosyl ester
121877-29-0	1	1	1	Tetradecanoic acid, 13-methyl-, docosyl ester
121877-30-3	1	1	1	Tetradecanoic acid, 12-methyl-, docosyl ester
121877-31-4	1	1	1	Pentadecanoic acid, 14-methyl-, docosyl ester
121877-32-5	1	1	1	Tetradecanoic acid, 13-methyl-, tricosyl ester
121877-33-6	1	1	1	Hexadecanoic acid, 14-methyl-, heneicosyl ester
121877-34-7	1	1	1	Tetradecanoic acid, 12-methyl-, tricosyl ester
121877-35-8	1	1	1	Tetradecanoic acid, 13-methyl-, tetracosyl ester
121877-36-9	1	1	1	Heptadecanoic acid, 16-methyl-, heneicosyl ester
121877-37-0	1	1	1	Nonadecanoic acid, 18-methyl-, nonadecyl ester
121877-38-1	1	1	1	Pentadecanoic acid, 14-methyl-, tricosyl ester
121877-39-2	1	1	1	Hexadecanoic acid, 15-methyl-, docosyl ester
121877-40-5	1	1	1	Tetradecanoic acid, 12-methyl-, tetracosyl ester
121877-41-6	1	1	1	Hexadecanoic acid, 14-methyl-, docosyl ester
121877-42-7	1	1	1	Heptadecanoic acid, 15-methyl-, heneicosyl ester
121877-43-8	1	1	1	Pentadecanoic acid, 13-methyl-, tricosyl ester
121877-44-9	1	1	1	Pentadecanoic acid, tetracosyl ester
121877-45-0	1	1	1	Tetradecanoic acid, pentacosyl ester
121877-46-1	1	1	1	Heptadecanoic acid, 16-methyl-, docosyl ester
121877-47-2	1	1	1	Pentadecanoic acid, 14-methyl-, tetracosyl ester
121877-48-3	1	1	1	Tetradecanoic acid, 12-methyl-, pentacosyl ester
121877-49-4	1	1	1	Tetradecanoic acid, 13-methyl-, hexacosyl ester
121877-50-7	1	1	1	Heptadecanoic acid, 16-methyl-, tricosyl ester
121877-51-8	1	1	1	Nonadecanoic acid, 18-methyl-, heneicosyl ester
121877-52-9	1	1	1	Heptadecanoic acid, 15-methyl-, tricosyl ester
121877-53-0	1	1	1	Octadecanoic acid, 16-methyl-, docosyl ester
121877-54-1	1	1	1	Nonadecanoic acid, 17-methyl-, heneicosyl ester
121877-55-2	1	1	1	Pentadecanoic acid, 13-methyl-, pentacosyl ester
121877-56-3	1	1	1	Tetradecanoic acid, 12-methyl-, hexacosyl ester
121877-57-4	1	1	1	Tridecanoic acid, 11-methyl-, heptacosyl ester
121877-58-5	1	1	1	Hexadecanoic acid, 14-methyl-, hexacosyl ester
121877-59-6	1	1	1	Nonadecanoic acid, 17-methyl-, tricosyl ester
121877-60-9	1	1	1	Eicosanoic acid, 18-methyl-, docosyl ester
121877-61-0	1	1	1	Heneicosanoic acid, 19-methyl-, heneicosyl ester
121877-62-1	1	1	1	Docosanoic acid, 20-methyl-, eicosyl ester
121877-63-2	1	1	1	Tricosanoic acid, 21-methyl-, nonadecyl ester
121877-64-3	1	1	1	Heptadecanoic acid, hexacosyl ester
121877-65-4	1	1	1	Octadecanoic acid, pentacosyl ester
121877-66-5	1	1	1	Nonadecanoic acid, tetracosyl ester
121877-67-6	1	1	1	Hexadecanoic acid, 14-methyl-, heptacosyl ester
121877-68-7	1	1	1	Heptadecanoic acid, 15-methyl-, hexacosyl ester
121877-69-8	1	1	1	Nonadecanoic acid, 17-methyl-, tetracosyl ester
121877-70-1	1	1	1	Heneicosanoic acid, 19-methyl-, docosyl ester
121877-71-2	1	1	1	Docosanoic acid, 20-methyl-, heneicosyl ester
121877-72-3	1	1	1	Tricosanoic acid, 21-methyl-, eicosyl ester
121877-73-4	1	1	1	Tricosanoic acid, 21-methyl-, heneicosyl ester
121877-74-5	1	1	1	Hexadecanoic acid, 14-methyl-, octacosyl ester
121877-75-6	1	1	1	Octadecanoic acid, 16-methyl-, hexacosyl ester

(*continued*)

(continued)

Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
121877-76-7	1	1	1	Docosanoic acid, 20-methyl-, docosyl ester
121877-77-8	1	1	1	Tetracosanoic acid, 22-methyl-eicosyl ester
121877-78-9	1	1	1	Octadecanoic acid, heptacosyl ester
121877-79-0	1	1	1	Eicosanoic acid, pentacosyl ester
121877-80-3	1	1	1	Pentacosanoic acid, eicosyl ester
121877-81-4	1	1	1	Heptadecanoic acid, 15-methyl-, octacosyl ester
121877-82-5	1	1	1	Tricosanoic acid, 21-methyl-, docosyl ester
121877-83-6	1	1	1	Hexacosanoic acid, eicosyl ester
121877-85-8	1	1	1	Pentacosanoic acid, 23-methyl-, heneicosyl ester
121877-86-9	1	1	1	Octadecanoic acid, nonacosyl ester
121877-87-0	1	1	1	Eicosanoic acid, heptacosyl ester
121877-88-1	1	1	1	Pentacosanoic acid, docosyl ester
121877-89-2	1	1	1	Hexacosanoic acid, heneicosyl ester
121877-90-5	1	1	1	Hexacosanoic acid, 24-methyl-, heneicosyl ester
121877-91-6	1	1	1	Octacosanoic acid, eicosyl ester
121877-92-7	1	1	1	Hexacosanoic acid, 24-methyl-, docosyl ester
121877-93-8	1	1	1	Heptacosanoic acid, 25-methyl-, heneicosyl ester
121877-94-9	1	1	1	Nonacosanoic acid, eicosyl ester
121877-95-0	1	1	1	Octacosanoic acid, heneicosyl ester
121877-96-1	1	1	1	Heptacosanoic acid, docosyl ester
121877-97-2	1	1	1	Hexacosanoic acid, tricosyl ester
121877-98-3	1	1	1	Tricosanoic acid, hexacosyl ester
121877-99-4	1	1	1	Docosanoic acid, heptacosyl ester
121878-00-0	1	1	1	Heneicosanoic acid, octacosyl ester
121878-01-1	1	1	1	Heptacosanoic acid, 25-methyl-, docosyl ester
121878-02-2	1	1	1	Octacosanoic acid, docosyl ester
121878-03-3	1	1	1	Tetracosanoic acid, hexacosyl ester
121878-04-4	1	1	1	Octacosanoic acid, 26-methyl-, docosyl ester
121878-05-5	1	1	1	Nonacosanoic acid, docosyl ester
121878-06-6	1	1	1	Dotriacontanoic acid, eicosyl ester
121878-07-7	1	1	1	Triacontanoic acid, docosyl ester
121916-90-3	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3R*,4*E*,8*E*,12S*,13*E*)]-
121927-14-8	0	1	0	15-Oxabicyclo[10.2.1]pentadec-6-ene-2,3,5-triol,1,5-dimethyl-11-methylene-8-(1-methylethyl)-,[1R-(1R*,2S*,3R*,5S*,6*E*,8*)]-
121927-15-9	0	1	0	13,14-Dioxabicyclo[10.2.2]hexadec-6-ene-2,3,5-triol,1,5-dimethyl-11-methylene-8-(1-methylethyl)-,[1R-(1R*,2S*,3R*,5S*)]-
122319-88-4	0	1	0	Phosphatase, 2-carboxyarabinitol 1-
122620-36-4	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-, (1R*,3R*,4*E*,8*E*,12S*,13*E*)-(±)-
122836-35-5	0	1	0	1*H*-1,2,4-Triazol-1-yl)phenyl)methane-sulfonamide, *N*-(2,4-dichloro-5-(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo- {Methanesulfonamide, *N*-(2,4-dichloro-5(4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl) phenyl)-; {Sulfentrazone®}
122855-83-8	0	1	0	5,10,12-Tridecatrien-2-one, 6,12-dimethyl-9-(1-methylethyl)-
122881-64-5	0	1	0	3-Nonen-8-one, 1,2-dihydroxy-2-methyl-5-(1-methylethyl)-
123617-80-1	1	0	0	Acetic acid, 2-furanyl-
123676-95-9	0	1	0	Pyridine, 3-[1-[(hydroxy-1-oxooctyl)oxy]-2-pyrrolidinyl]-
123695-64-7	1	0	0	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy-6-(1-methylethyl)-, exo-
123695-65-8	1	0	0	5,7-Nonadien-2-one, 8-hydroxy-5-(1-methylethyl)-, (*E,Z*)-
123695-66-9	1	0	0	Ethanone, 1-[6-hydroxy-6-methyl-3-(1-methylethyl)-2-cyclohexen-1-yl]-
123716-12-1	1	0	0	Cyclohexanone, 4-(1-methylethyl)-3-(2-oxopropyl)-
123743-84-0	1	1	1	3-Pyridinebutanoic acid, γ-(methylnitrosoamino)- {iso-NNAC}
133201-36-2				
123844-48-4	1	0	0	Phenol, 5,6-dimethyl-2-methoxy-
124051-99-6	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-[[2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,6-dihydroxy-3-oxo-4-benzofuranyl]oxy]-2,3-dihydro-3,5-dihydroxy-
124052-00-2	0	1	0	4*H*-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-2,3-dihydro-2,3,5,7-tetrahydroxy-

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
124052-01-3	0	1	0	2*H*-1-Benzopyran-3,4-dione, 2-(3,4-dihydroxyphenyl)-2,5,7-trihydroxy-
124052-02-4	0	1	0	3(2*H*)-Benzofuranone, 2-(3,4-dihydroxyphenyl)-2,4,6-trihydroxy-
124354-88-7	0	1	0	Octen-4-one, 2,6-dimethyl-, monoepoxy derivative
124713-05-9	0	1	0	9,19-Cyclolanost-5-en-3-ol, 24-methylene-, (3β)-
124749-69-5	1	0	0	Bicyclo[3.3.1]nonan-3-one, 1-hydroxy-6-(1-methylethyl)-, endo-
124757-79-5	0	1	0	Deoxyribonucleic acid (tobacco clone E22 protein PR 5 gene)
125239-87-4	1	0	0	Nitrate, peroxy-
125537-95-3	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 4-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα, 2β,4β,4aβ,5α,7aα,7bα)]-
125537-96-4	0	1	0	7*H*-2,4a-Methano-1*H*-cyclobuta[*de*]naphthalen-7-one, 3-(β-*D*-glucopyranosyloxy)octahydro-1a,5,7b-trimethyl-, [1aS-(1aα, 2β,3β,4aβ,5α,7aα,7bα)]-
125572-76-1	1	1	1	2,6,11,13-Tetradecatetraenal, 3,7,13-trimethyl-10-(1-methylethyl)-
126165-82-0 121268-99-3 64091-91-4 110053-55-9	1	1	1	1-Butanone, 4-(methylnitrosoamino)-1-(3-pyridinyl)- {NNK} {1-Butanone, 4-[(nitrosomethyl)amino]-1-(3-pyridinyl)-} [4 CAS Nos.]
126454-22-6	1	0	0	2,3′-Bipyridine, 1,2,3,6-tetrahydro-, (R)- {*d*-anatabine}
126458-49-9	0	1	0	4*H*-Cyclopenta[3′,4′]cycloocta[1′,2′:1,5]cyclopent[1,2-*b*]oxiren-4-one, 1,2,2a,5,6,8,9,10,10a,10b-decahydro-2,6,10a-trimethyl-8-(1-methylethyl)-, [2aS-(2aα,3aS*,6β,8β,10aβ,10bβ)]-
127353-53-1	1	0	0	Docosanoic acid, 3,7,11,15-tetramethyl-2-hexadecenyl ester {phytyl docosanoate}
128284-58-2	0	1	0	Deoxyribonucleic acid (tobacco clone lambda CHN17 chitinase basic isoenzyme gene)
128285-01-8	0	1	0	Ribonucleic acid (tobacco clone lambda CHN17 chitinase basic isoenzyme-specifying messenger)
128285-05-2	0	1	0	Chitinase (tobacco clone lambda CHN17 basic isoenzyme precursor reduced)
128285-06-3	0	1	0	Chitinase (tobacco clone lambda CHN17 basic isoenzyme reduced)
128475-00-3	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme signal peptide)
128475-01-4	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme signal peptide) 26-*L*-threonine-28-*L*-glutamic acid
128512-15-2	0	1	0	Deoxyribonucleic acid (tobacco clone pBSGlu39.1 endo-1,3-β-glucanase isoenzyme gene coding region)
128512-16-3	0	1	0	Deoxyribonucleic acid (tobacco clone pBSGlu39.3 endo-1,3-β-glucanase isoenzyme gene coding region)
128512-17-4	0	1	0	Deoxyribonucleic acid, (tobacco clone pBSGlu39.1 endo-1,3-β-glucanase isoenzyme gene coding region plus 5′- and 3′-flanking region fragment)
128512-18-5	0	1	0	Deoxyribonucleic acid, (tobacco clone pBSGlu39.3endo-1,3-β-glucanase isoenzyme gene coding region plus 5′- and 3′-flanking region fragment)
128512-19-6	0	1	0	Deoxyribonucleic acid (tobacco clone pGL31 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)
128512-20-9	0	1	0	Deoxyribonucleic acid (tobacco clone pGL36 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)
128512-21-0	0	1	0	Deoxyribonucleic acid (tobacco clone pGL43 endo-1,3-β-glucanase isoenzyme messenger RNA complementary)
128512-22-1	0	1	0	Deoxyribonucleic acid, (tobacco clone pGL31 endo-1,3-β- glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)
128512-23-2	0	1	0	Deoxyribonucleic acid, (tobacco clone pGL36 endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)
128512-24-3	0	1	0	Deoxyribonucleic acid, (tobacco clone pGL43 endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)
128512-25-4	0	1	0	Deoxyribonucleic acid (tobacco endo-1,3-β-glucanase isoenzyme messenger RNA complementary)
128512-26-5	0	1	0	Deoxyribonucleic acid, (tobacco endo-1,3-β-glucanase isoenzyme messenger RNA complementary plus 5′- and 3′-flanking region fragment)
128512-83-4	0	1	0	Glucanase, endo-1,3-β-(tobacco clone pGL31 isoenzyme)
128512-84-5	0	1	0	Glucanase, endo-1,3-β- (tobacco clone pGL36 isoenzyme)
128512-85-6	0	1	0	Glucanase, endo-1,3-β- (tobacco clone pGL43 isoenzyme)
128512-86-7	0	1	0	Glucanase, endo-1,3-β- (tobacco isoenzyme)
128512-87-8	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGlu39.1 isoenzyme protein moiety)
128512-88-9	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pBSGluc39.3 isoenzyme protein moiety)
128512-89-0	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pGL31 isoenzyme protein moiety)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	S T	Component
128512-90-3	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pGL36 isoenzyme protein moiety)
128512-91-4	0	1	0	Glucanase, preproendo-1,3-β- (tobacco clone pGL43 isoenzyme protein moiety)
128512-92-5	0	1	0	Glucanase, preproendo-1,3-β- (tobacco isoenzyme protein moiety)
128909-19-3	0	1	0	Hydroxycinnamoyltransferase, tyramine
129074-11-9	1	0	0	Pentacosanol
129742-47-8	0	1	0	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-, [R-(*E*)]-
129742-48-9	0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-, (*E*)-(+)-
129777-21-5	0	1	0	2,6-Nonadienal, 2-methyl-5-(1-methylethyl)-8-oxo-, (*E,E*)-(+)-
129777-22-6	0	1	0	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-, (*E*)-
129777-23-7	0	1	0	4-Decenoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-oxo-, [R-[R*,S*-(*E*)]]-
129777-24-8	0	1	0	3,7-Tridecadiene-2,12-dione, 6-hydroxy-6-methyl-9-(1-methylethyl)-
129970-88-3	0	1	0	5,9-Undecadienal, 6,10-dimethyl-2-methylene-
129990-04-1	0	1	0	Saponin B, from tobacco
130061-32-4	0	1	0	Deoxyribonucleic acid (*Nicotiana sylvestris* clone NySS4 ribulose diphosphate carboxylase small subunit gene)
131201-61-1	0	1	0	Carboxylase, ribulose diphosphate (*N. sylvestris* clone NySS4 small subunit precursor reduced)
131524-02-2	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2,5-dimethyl-
131524-03-3	1	0	0	4*H*-Pyran-4-one, 5-hydroxy-2,3-dimethyl-
131524-04-4	1	0	0	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5-methyl-
131524-05-5	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2,5,6-trimethyl-
131524-06-6	1	0	0	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-methyl-
131524-07-7	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylethyl)-
131524-08-8	1	0	0	4*H*-Pyran-4-one, 2-ethyl-3-hydroxy-5,6-dimethyl-
131524-09-9	1	0	0	4*H*-Pyran-4-one, 2,6-diethyl-3-hydroxy-
131524-10-2	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-methyl-6-propyl-
131524-11-3	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(2-methylbutyl)-
131524-12-4	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-(3-methylbutyl)-
131524-13-5	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-2-pentyl-
131524-14-6	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(1-methylpropyl)-
131524-15-7	1	0	0	4*H*-Pyran-4-one, 3-hydroxy-6-methyl-2-(2-methylpropyl)-
131524-16-8	1	0	0	4*H*-Pyran-4-one, 2-butyl-3-hydroxy-6-methyl-
131524-17-9	1	1	1	4*H*-Pyran-4-one, 6-ethyl-3-hydroxy-2-propyl-
131553-15-6	0	1	0	Deoxyribonucleic acid (*Nicotiana tabacum* samsun chitinase isoenzyme messenger RNA complementary)
131553-16-7	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun 16.5 kilodalton protein messenger RNA complementary)
131553-54-3	0	1	0	Osmotin (*N. tabacum* samsun reduced)
131554-01-3	0	1	0	Chitinase (*N. tabacum* samsun isoenzyme reduced)
131754-88-6	0	1	0	Synthase, nicotine
131860-33-8	0	1	0	Benzeneacetic acid, methyl (α*E*)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)- {Azoxystrobin®}
132966-16-6	0	1	0	Protein (tobacco 27.4 kilodalton RNA-binding)
132966-19-9	0	1	0	Protein (tobacco 27.4 kilodalton RNA-binding precursor reduced)
133007-80-4	0	1	0	2-Butanone, 4-(6-ethenyl-2,2,6-trimethylcyclohexyl)-
133201-36-2	1	1	1	3-Pyridinebutanoic acid, γ-(methylnitrosoamino)- {iso-NNAC}
123743-84-0				
133201-38-4	1	1	1	β-Alanine, *N*-(nitrosomethyl)-
133201-39-5	1	1	1	Butanoic acid, 4-(methylnitrosoamino)- = butanoic acid, 4-[(nitrosomethyl)amino]- [2 CAS Nos.] {NMBA}
61445-55-4				
133304-85-5	1	0	0	2-Cyclohexen-1-one, 3,4-dimethyl-2-hydroxy-
133480-20-3	0	1	0	Naphthalenone, hexahydro-8-methyl-(1-methylethenyl)-
133561-45-2	0	1	0	5,8-Undecadien-2-one, 6,10-dimethyl-10-hydroxy- (*E,E*)-
65017-84-7				
133561-46-3	0	1	0	3-Hepten-2-one, 5-ethyl-5-hydroxy-6-methyl-
133561-47-4	0	1	0	2(3*H*)-Furanone, dihydro-5-(1-methylethyl)-5-(3-oxo-1-butenyl)-
133561-48-5	0	1	0	5-Undecene-2,10-dione, 4-hydroxy-4-methyl-7-(1-methylethyl)-

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
133561-49-6	0	1	0	Cyclohexanone, 3,3,5-trimethyl-4-(3-oxobutyl)-
133829-71-7	1	0	0	1*H*-Pyrrole-2-carbonitrile, methyl- {two isomers}
134632-85-2	0	1	0	Phosphatase, adenosine tri- (*Petunia hybrida* strain 3704 mitochondria subunit 9)
135295-09-9	1	0	0	Phenol, 2-ethenyl-6-methyl-
136448-99-2	0	1	0	β-*D*-Glucopyranoside, 2-[5-(acetyloxy)-1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthalenyl]-2-hydroxypropyl-, 2,3,4,6-tetraacetate, [2R-[2α(S*),5α,8β,8aα]]-
137801-72-0	0	1	0	Protein (tobacco chloroplast clone pTB24 gene psbK)
138261-41-3	1	1	1	Imidazolidinimine, 1-((6-chloro-3-pyridinyl)methyl)-*N*-nitro- {Imidacloprid®}
139636-55-8	0	1	0	Adenosine, 2′-deoxyadenylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxyadenylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxycytidylyl-(3′→5′)-thymidylyl-(3′→5′)-2′-deoxyguanylyl-(3′→5′)-2′-deoxy-
139637-37-9	0	1	0	Deoxyribonucleic acid, d(A-T-G-T-T-C-T-C-T-C-T-T-T-T-A-A-T-G-G-T-G-G-T-T-C-T-T-T-A-G)
139681-65-5	0	1	0	*L*-Leucine,*N*-[*N*-[*N*-[*N*-[*N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-phenylalanyl)-*L*-seryl]-*L*-leucyl]-*L*-leucyl]-*L*-methionyl]-*L*-valyl]-*L*-valyl]-
139681-66-6	0	1	0	*L*-Isoleucine, *N*-[*N*-[*N*-(*N*-*L*-methionyl-*L*-valyl)-*L*-phenylalanyl]-*L*-leucyl]-
139837-73-3	0	1	0	Deoxyribonucleic acid, (tobacco clone NtDAHPS-1 phospho-2-keto-3-deoxyheptonate aldolase messenger RNA complementary plus 5′- and 3′-flanking region fragment)
139854-77-6	0	1	0	GenBank X60057
139857-64-0	0	1	0	GenBank X61750
139860-37-0	0	1	0	Deoxyribonucleic acid (*Nicotiana plumbaginifolia* clone NeIF-4A2 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′-and 3′-flanking region fragment)
139867-08-6	0	1	0	GenBank X64398
139869-01-5	0	1	0	GenBank X64399
139872-57-4	0	1	0	Deoxyribonucleic acid (tobacco clone.lambda.5A gene RB7)
139872-58-5	0	1	0	Deoxyribonucleic acid (tobacco clone.lambda.5A gene RB7 plus 5′- and 3′-flanking region fragment)
139872-63-2	0	1	0	Ribonucleic acid (tobacco clone.lambda.5A gene RB7 protein-specifying 1524-nucleotide messenger)
139872-64-3	0	1	0	Ribonucleic acid (tobacco clone.lambda.5A gene RB7 protein-specifying 1549-nucleotide messenger)
139874-82-1	0	1	0	Protein (tobacco clone.lambda.5A gene RB7 reduced)
139874-83-2	0	1	0	Protein (tobacco clone.lambda.18C gene RB7 reduced)
140095-89-2	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A3 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′-and 3′-flanking region fragment)
140104-46-7	0	1	0	GenBank X62395
140110-39-0	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun clone NeIF-5A3 protein formation initiation factor eIF 5A isoform gene plus 5′- and 3′-flanking region fragment)
140114-22-3	0	1	0	Deoxyribonucleic acid (tobacco thioredoxin messenger RNA complementary plus 5′- and 3′-flanking region fragment)
140352-16-5	0	1	0	GenBank X61113
140352-17-6	0	1	0	GenBank X61114
140360-04-9	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-5A2 protein formation initiation factor eIF 5A isoform messenger RNA complementary plus 5′- and 3′-flanking region fragment)
140360-05-0	0	1	0	GenBank X62339
140812-74-4	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* gene pma1 plus 5′- and 3′-flanking region fragment)
140830-68-8	0	1	0	GenBank X64423
141002-75-7	0	1	0	Deoxyribonucleic acid (tobacco clone pVK5 osmotin messenger RNA complementary)
141004-11-7	0	1	0	Deoxyribonucleic acid (tobacco ribosome protein L 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
141005-27-8	0	1	0	GenBank X62368
141093-08-5	0	1	0	Osmotin (*N. tabacum* samsun clone pMOG404 reduced)
141093-09-6	0	1	0	1-226-Osmotin (*N. tabacum* samsun clone pMOG404 reduced)
141093-81-4	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun clone pMOG404 osmotin messenger RNA complementary)
141093-82-5	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun clone pMOG404 osmotin messenger RNA complementary plus 5′- and 3′-flanking region fragment)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
141093-84-7	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun clone pMOG4041-226-osmotin-specifying plus 5′- and 3′-flanking region fragment)
141164-36-5	0	1	0	GenBank X65118
141164-37-6	0	1	0	GenBank X65117
141374-52-9	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone pSOD3 copper–zinc superoxide dismutase messenger RNA complementary plus 5′- and 3′-flanking region fragment)
141683-31-0	0	1	0	GenBank M94135
141712-74-5	0	1	0	Deoxyribonucleic acid (*Arabidopsis thaliana* strain Heynhold glycerol phosphate acyltransferase messenger RNA complementary)
141712-75-6	0	1	0	Deoxyribonucleic acid (*A. thaliana* strain Heynhold glycerol phosphate acyltransferase messenger RNA complementary plus 5′- and 3′-flanking region fragment)
141733-40-6	0	1	0	Acyltransferase, glycerol phosphate (*A. thaliana* clone BX3.6/BB2.6 reduced)
142193-19-9	0	1	0	Parasiticein (*Phytophthora parasitica* reduced)
142193-29-1	0	1	0	Parasiticein
142235-82-3	0	1	0	4*H*-1-Benzopyran-4-one, 3-[(2-*O*-β-*D*-glucopyranosyl-β-*D*-galactopyranosyl)oxy]-7-(β-*D*-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-
142583-50-4	0	1	0	Osmotin (tobacco clone pVK5 precursor reduced)
142583-51-5	0	1	0	Osmotin (tobacco clone pVK5 reduced)
142693-30-9	0	1	0	GenBank M84650
142750-40-1	0	1	0	4,10(1*H*,5*H*)-Cyclopentacycloundecenedione, 2,3,3a,6,7,11,12,12a-octahydro-1,3,12-trihydroxy-3,8,12-trimethyl-5-(1-methylethyl)-, (1R*,3S*,3aR*,5S*,8Z,12R*,12aR*)-(–)-
142750-43-4	0	1	0	Cyclopentacycloundecene, tetradecahydro-1,4,8-trimethyl-11-(1-methylethyl)-
142785-07-7	0	1	0	*L*-Serine, *L*-alanyl-*L*-prolyl-*L*-isoleucyl-*L*-prolylglycyl-*L*-valyl-*L*-methionyl-*L*-prolyl-*L*-isoleucylglycyl-*L*-asparaginyl-*L*-tyrosyl-*L*-valyl-
142914-45-2	0	1	0	GenBank Z12623
142914-46-3	0	1	0	GenBank Z12619
142965-21-7	0	1	0	GenBank X63078
142978-88-9	0	1	0	Protein L 27 (tobacco chloroplast clone L27-1 ribosome precursor reduced)
142978-89-0	0	1	0	Protein L 27 (tobacco chloroplast clone L27-1 ribosome reduced)
142978-98-1	0	1	0	Deoxyribonucleic acid (tobacco chloroplast clone L27-1 ribosome protein L 27 messenger RNA complementary)
142978-99-2	0	1	0	Deoxyribonucleic acid (tobacco chloroplast clone L27-1 ribosome protein L 27 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
143341-50-8	0	1	0	GenBank X67158
143341-52-0	0	1	0	Deoxyribonucleic acid (tobacco 1-109-extensin-like protein precursor-specifying)
143341-53-1	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 171-amino acid C-terminal fragment-specifying plus 3′-flanking region fragment)
143341-54-2	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 264-amino acid C-terminal fragment-specifying plus 3′-flanking region fragment)
143341-55-3	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 107-amino acid fragment-specifying)
143341-56-4	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 81-amino acid fragment-specifying)
143341-57-5	0	1	0	Deoxyribonucleic acid (tobacco extensin-like protein 393-amino acid C-terminal fragment-specifying plus 3′-flanking region fragment)
143341-58-6	0	1	0	Deoxyribonucleic acid (tobacco clone pMG15 extensin-like protein messenger RNA complementary plus 5′- and 3′-flanking region fragment)
143348-77-0	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone pSOD3 copper–zinc superoxide dismutase messenger RNA complementary)
143352-40-3	0	1	0	Dismutase, superoxide (*N. plumbaginifolia* clone pSOD3 copper–zinc protein moiety reduced)
143513-68-2	0	1	0	Deoxyribonucleic acid (tobacco strain NK326 gene oee2-A plus 5′- and 3′-flanking region fragment)
143513-69-3	0	1	0	Deoxyribonucleic acid (tobacco strain NK326 gene oee2-A)
143513-70-6	0	1	0	Protein OEE 2 (tobacco strain NK326 precursor reduced)
143514-64-1	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-5A2 protein formation initiation factor eIF 5A isoform messenger RNA complementary)
143514-65-2	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun clone NeIF-5A3 protein formation initiation factor eIF 5A isoform gene)
143514-66-3	0	1	0	Protein formation initiation factor eIF 5A (*N. plumbaginifolia* clone NeIF-5A1 isoform C-terminal fragment reduced)
143514-67-4	0	1	0	Protein formation initiation factor eIF 5A (*N. plumbaginifolia* clone NeIF-5A2 isoform reduced)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
143514-68-5	0	1	0	Protein formation initiation factor eIF 5A (*N. tabacum* samsun clone NeIF-5A3 isoform reduced)
143638-31-7	0	1	0	Osmotin (*N. tabacum* samsun clone pTOL1 precursor reduced)
143638-32-8	0	1	0	Osmotin (*N. tabacum* samsun clone pTOL1 reduced)
143638-33-9	0	1	0	Deoxyribonucleic acid (*N. tabacum* samsun clone pTOL1 osmotin messenger RNA complementary)
143787-54-6	0	1	0	GenBank L02124
144031-18-5	0	1	0	GenBank X66145
144324-42-5	0	1	0	Synthase, 5-enolpyruvoylshikimate 3-phosphate (petunia clone pMON9531/pMON9556 reduced) 101-*L*-alanine-
144324-43-6	0	1	0	Synthase, 5-enolpyruvoylshikimate 3-phosphate (petunia clone pMON9531/pMON9556 reduced) 101-*L*-alanine-192-*L*-threonine-
144419-45-4	0	1	0	Protein (*A. thaliana* clone G9.1 gene A9 11.6 kilodalton reduced)
144680-37-5	0	1	0	GenBank M74103
144680-39-7	0	1	0	GenBank M74102
144997-81-9	0	1	0	Deoxyribonucleic acid (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa protein D 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
144997-82-0	0	1	0	Deoxyribonucleic acid (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa protein D 2 messenger RNA complementary)
144997-83-1	0	1	0	Protein D 2 (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa precursor)
144997-84-2	0	1	0	Protein D 2 (*N. sylvestris* clone yaDC12/yaDC17 gene psaDa)
145090-31-9	0	1	0	Nonadecanoic acid, 18-methyl-, 2-(acetyloxy)-1-(hydroxymethyl)ethyl ester
145090-32-0	0	1	0	Proteinase inhibitor, PI-1
145093-14-7	0	1	0	Deoxyribonucleic acid (tobacco clone EPSPS-1 5-enolpyruvoylshikimate 3-phosphate synthase messenger RNA complementary plus 5′- and 3′-flanking region fragment)
145137-42-4	0	1	0	Deoxyribonucleic acid (tobacco clone NtDAHPS-1 phospho-2-keto-3-deoxyheptonate aldolase messenger RNA complementary)
145137-43-5	0	1	0	Aldolase, phospho-2-keto-3-deoxyheptonate (tobacco clone NtDAHPS-1 precursor reduced)
145735-56-4	0	1	0	Deoxyribonucleic acid (tobacco clone pcGS2-17 glutamine synthetase isoenzyme 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
145767-36-8	0	1	0	GenBank M87838
145767-40-4	0	1	0	GenBank M87839
145895-79-0	0	1	0	Protein (tobacco flower-associated reduced)
145905-43-7	0	1	0	GenBank X63607
145917-24-4	0	1	0	2-Propen-1-one, 1,3-di-3-pyridinyl-, (*E*)-
146150-24-5	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A2 protein formation initiation factor eIF 4A messenger RNA complementary)
146150-25-6	0	1	0	Protein formation initiation factor eIF 4A (*N. plumbaginifolia* clone NeIF-4A2 isoform reduced)
146150-26-7	0	1	0	Deoxyribonucleic acid (*N. plumbaginifolia* clone NeIF-4A3 protein formation initiation factor eIF 4A messenger RNA complementary)
146440-48-4	0	1	0	*L*-Serine, *L*-methionyl-*L*-alanyl-*L*-lysyl-*L*-alanyl-*L*-leucyl-*L*-valyl-*L*-leucyl-*L*-phenylalanyl-*L*-glutaminyl-*L*-leucyl-*L*-seryl-*L*-valyl-*L*-leucyl-*L*-leucyl-*L*-leucyl-*L*-seryl-*L*-seryl-*L*-phenylalanyl-*L*-threonyl-*L*-valyl-*L*-valyl-*L*-leucyl-
146480-37-7	0	1	0	Glucosyltransferase, uridine diphosphoglucose-salicylate 3-
156859-11-9				
146506-80-1	1	0	0	Benzo[*g*]chrysene, methyl-
146564-66-1	0	1	0	4,9,13-Cyclotetradecatriene-1,3,8-triol, 3,9,13-trimethyl-6-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,6S*,8R*,9*E*,13*E*)]-
146564-67-2	0	1	0	4,8,13-Cyclotetradecatriene-1,3-diol,9-(hydroxymethyl)-1,5-dimethyl-12-(1-methylethyl)-,[1S-(1R*,3S*,4*E*,8*Z*,12R*,13*E*)]-
146591-93-7	0	1	0	Protein (tobacco clone PRP3g12 gene PRP3 pistil-specific proline-rich precursor)
146609-95-2	0	1	0	4,9,13-Cyclotetradecatriene-1,3,8-triol, 3,9,13-trimethyl-6-(1-methylethyl)-, [1R-(1R*,3S*,4*E*,6S*,8R*,9*E*,13*E*)]-
146689-29-4	0	1	0	Adenosine, 2′-deoxycytidylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxyguanylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxycytidylyl-(5′→3′)-2′-deoxyguanylyl-(5′→3′)-2′-deoxy-
147427-29-0	0	1	0	*L*-Proline, 1-[1-[1-(1-*L*-seryl-*L*-prolyl)-*L*-prolyl]-*L*-prolyl]-
147445-75-8	0	1	0	Protein (tobacco clone pMG15 extensin-like precursor reduced)
147533-09-3	0	1	0	Deoxyribonucleic acid (*Nicotiana alata* clone NaPRP3g12 proline-rich protein PRP 3 gene plus 5′- and 3′-flanking region fragment)
147626-92-4	0	1	0	Deoxyribonucleic acid (tobacco clone pcGS2-17 glutamine synthetase isoenzyme 2 messenger RNA complementary)

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Chemical Abstract Number Sequence for Identified Chemical Components in Tobacco, Tobacco Smoke, and Tobacco Substitute Smoke

CAS No.	S	T	ST	Component
147626-93-5	0	1	0	Synthetase, glutamine (tobacco clone pcGS2-17 isoenzyme 2 subunit precursor reduced)
147688-58-2	0	1	0	Morpholine, 2,2-dimethyl-
147904-32-3	0	1	0	GenBank X65982
148037-15-4	0	1	0	Deoxyribonucleic acid (*A. thaliana* thioredoxin h messenger RNA complementary plus 5′- and 3′-flanking region fragment)
148348-37-2	0	1	0	Chitinase (*N. tabacum* xanthi clone pBSCL226 isoenzyme III precursor reduced)
148544-79-0	0	1	0	GenBank Z16403
148544-80-3	0	1	0	GenBank Z16404
148757-17-9	0	1	0	GenBank X71015
148757-18-0	0	1	0	Deoxyribonucleic acid (tobacco clone G27.1/G27.2 gene Npg1 plus 5′- and 3′-flanking region fragment)
149021-93-2	1	0	0	Benz[*e*]acephenanthrylene, 10-methyl-
149241-78-1	0	1	0	GenBank L14953
149309-58-0	0	1	0	Deoxyribonucleic acid (tobacco thioredoxin h2 gene plus 5′- and 3′-flanking region fragment)
149312-89-0	0	1	0	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-, [6S-(2*E*,6R*,7*E*,9R*,11S*,12*E*)]-
149312-90-3	0	1	0	2,6,11-Cyclotetradecatrien-1-one, 5,13-dihydroxy-3,7,13-trimethyl-10-(1-methylethyl)-, [5S-(2*E*,5R*,6*E*,10R*,11*E*,13R*)]-
149331-19-1	0	1	0	Cyclononane, 1,1,4,4,7,7-hexamethyl-
149403-67-8	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7S*,8*E*,12R*)]-
149403-68-9	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1S-(1R*,3S*,4*E*,7R*,8*E*,12R*)]-
149403-69-0	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7R*,8*E*,12S*)]-
149403-70-3	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7S*,8*E*,12S*)]-
149403-71-4	0	1	0	4,8,13-Cyclotetradecatriene-1,3,7-triol, 1,5,9-trimethyl-12-(1-methylethyl)-, [1R-(1R*,3R*,4*E*,7S*,8*Z*,12S*)]-
149403-72-5	0	1	0	2,7,12-Cyclotetradecatrien-1-one, 9,11-dihydroxy-3,9,13-trimethyl-6-(1-methylethyl)-, [6S-(2*E*,6R*,7*E*,9S*,11S*,12*E*)]-
149956-84-3	0	1	0	Thioredoxin h2 (tobacco)
150001-42-6	0	1	0	Deoxyribonucleic acid (tobacco clone TSC81 ribosome protein L 17 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
150405-75-7	0	1	0	6,8-Nonadien-2-ol, 8-methyl-5-(3-methylbutyl)-
150405-76-8	0	1	0	1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-
150405-77-9	0	1	0	2,6,11,13-Tetradecatetraen-1-ol, 3,7,13-trimethyl-10-(1-methylethyl)-
150462-98-9	0	1	0	Heptadecanoic acid, 16-methyl-, 3-(acetyloxy)-2-hydroxypropyl ester
150462-99-0	0	1	0	Heptadecanoic acid, 16-methyl-, 2-(acetyloxy)-1-(hydroxymethyl)ethyl ester
150472-46-1	0	1	0	GenBank L13439
150472-47-2	0	1	0	GenBank L13440
150472-48-3	0	1	0	GenBank L13441
150472-49-4	0	1	0	GenBank L13442
150472-50-7	0	1	0	GenBank L13443
150474-40-1	0	1	0	Proteinase inhibitor, prepro-TIMPb (*N. tabacum* samsun reduced)
150474-41-2	0	1	0	Proteinase inhibitor, prepro-TIMPa (*N. tabacum* samsun reduced)
150474-42-3	0	1	0	Proteinase inhibitor, pro-TIMPb (*N. tabacum* samsun reduced)
150474-43-4	0	1	0	Proteinase inhibitor, TIMPb (*N. tabacum* samsun reduced)
150474-44-5	0	1	0	Proteinase inhibitor, pro-TIMPa (*N. tabacum* samsun reduced)
150474-45-6	0	1	0	Proteinase inhibitor, TIMPa (*N. tabacum* samsun reduced)
150498-11-6	0	1	0	Trypsin inhibitor, TTI (tobacco isoform 1 reduced)
150643-41-7	0	1	0	Nonadecanoic acid, 18-methyl-, ester with 1,2,3-propanetriol monoacetate mono(16-methylheptadecanoate)
150656-38-5	0	1	0	Kinase (phosphorylating), protein (tobacco BY-2 cell isoenzyme ZmPK1 reduced)
150669-53-7	0	1	0	2(5*H*)-Furanone, 4-(4-methyl-1-pentyl)-
150669-54-8	0	1	0	2(5*H*)-Furanone, 5-methyl-5-(1-methylethyl)-
150669-55-9	0	1	0	2(5*H*)-Furanone, 5,5-dimethyl-4-ethyl-
150669-57-1	0	1	0	2(5*H*)-Furanone, 4-methyl-5-(3-oxobutyl)
150669-60-6	1	1	1	2*H*-Pyran-2-one, 4-(1-methylethyl)-
151468-68-7	0	1	0	GenBank X69971
151876-45-8	0	1	0	Deoxyribonucleic acid (tobacco clone OMT3.4 catechol methyltransferase isoenzyme II messenger RNA complementary plus 5′- and 3′-flanking region fragment)
152060-37-2	0	1	0	Oxygenase, benzoate 2-mono-

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CAS No.	S	T	ST	Component
152186-01-1	0	1	0	Ethanone, 1-[2,3,3a,4,6a,7,8,9,9a,9b-decahydro-5,9a-dimethyl-7-(1-methylethyl)-1*H*-cyclopent[*a*]azulen-3-yl]-, (3α,3aα,6aβ,7β,9aα,9bβ)-(±)-
152209-53-5	0	1	0	15-Oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol, 11-(1-hydroxy-1-methylethyl)-4,8,14-trimethyl-, [1S-(1R*,4*E*,6S*,8R*,9*E*,11S*,14R*)]-
152209-54-6	0	1	0	3-Hepten-2-one, 5-(1-methylethyl)-7-[2-methyl-3-(3-methyl-5-oxo-3-hexenyl)oxiranyl]-, [2S-[2α(3*E*,5R*),3β(*E*)]]-
152209-55-7	0	1	0	6,11-Pentadecadien-2-one, 8,10,15-trihydroxy-8,12-dimethyl-5-(1-methylethyl)-, [5S-(5R*,6*E*,8R*,10S*,11*E*)]-
152209-56-8	0	1	0	6,10-Undecadien-2-one, 8-hydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-2-methyl-2-furanyl)-
152288-82-9	0	1	0	Methyltransferase, catechol (tobacco clone OMT3.4 isoenzyme II reduced)
152347-16-5	0	1	0	GenBank D16206
152347-17-6	0	1	0	GenBank D16204
152347-18-7	0	1	0	GenBank D16205
152415-56-0	0	1	0	Polygalacturonase (tobacco clone G27.1/G27.2 gene Npg1 precursor reduced)
152619-15-3	0	1	0	Deoxyribonucleic acid (tobacco chitinase acidic isoenzyme III messenger RNA complementary plus 5′- and 3′-flanking region fragment)
152619-16-4	0	1	0	Deoxyribonucleic acid (tobacco chitinase basic isoenzyme III messenger RNA complementary plus 5′- and 3′-flanking region fragment)
152619-17-5	0	1	0	Chitinase (tobacco basic isoenzyme III precursor reduced)
152651-57-5	0	1	0	GenBank Z14082
152651-58-6	0	1	0	GenBank Z14081
152651-59-7	0	1	0	GenBank Z14080
152651-60-0	0	1	0	GenBank Z14079
152651-61-1	0	1	0	GenBank Z14085
152720-16-6	0	1	0	3-Pyridinebutanoic acid, γ-(methylnitroamino)-
152745-97-6	0	1	0	Protein L 17 (tobacco clone TSC81 ribosome reduced)
152789-83-8	0	1	0	Deoxyribonucleic acid, d(C-A-T-C-A-C-G-T-G-A-G-A-T-A-A-G-A-G-C-C-G-C-C-A), double-stranded complementary
152789-84-9	0	1	0	Deoxyribonucleic acid, d(T-A-A-A-G-T-C-A-A-A-G-A-A-T-T-T-C-A-A-T-G-T-C-A-C-A), double-stranded complementary
154063-13-5	0	1	0	α-*D*-Glucopyranoside, β-*D*-fructofuranosyl-, 6-acetate 2,3,4-tris(2-methylbutanoate)
155077-18-2	0	1	0	Protein (tobacco gene MST1 hydrogen ion-monosaccharide-cotransporting reduced)
155317-10-5	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A13 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155317-11-6	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A14 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155317-12-7	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A15 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155317-13-8	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A6 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155317-14-9	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A7 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155317-15-0	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A9 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155317-25-2	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone NeIF-4A11 protein formation initiation factor eIF 4A messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155663-09-5	0	1	0	Deoxyribonucleic acid (tobacco clone cpb20-52 antifungal protein CPB 20 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
155663-10-8	0	1	0	Protein CPB 20, prepro- (tobacco clone cpb20-52 antifungal reduced)
155663-11-9	0	1	0	Protein CPB 20, pro- (tobacco clone cpb20-52 antifungal reduced)
155663-12-0	0	1	0	Protein CPB 20 (tobacco clone cpb20-52 antifungal reduced)
155663-13-1	0	1	0	Protein CPB 20, pro- (tobacco clone cpb20-44 antifungal reduced)
155663-14-2	0	1	0	Protein CPB 20 (tobacco clone cpb20-44 antifungal reduced)
155728-85-1	0	1	0	2-Butanol, 1-(4-bromophenoxy)-3-[(phenylmethyl)amino]-, (R*,R*)-
156553-68-3	0	1	0	Deoxyribonucleic acid (tobacco clone 59 gene chi-V chitinase plus 5′- and 3′-flanking region fragment)

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CAS No.	S	T	ST	Component
156553-69-4	0	1	0	Deoxyribonucleic acid (tobacco clone cA-3 gene chi-V chitinase messenger RNA complementary plus 5′- and 3′-flanking region fragment)
156859-11-9	0	1	0	Glucosyltransferase, uridine diphosphoglucose-salicylate 3-
146480-37-7				
158815-70-4	0	1	0	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-
158815-71-5	0	1	0	2(3*H*)-Furanone, dihydro-3-hydroxy-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1*E*,3S*)]]-
158815-72-6	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)-
158815-73-7	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)-
158815-74-8	0	1	0	2(3*H*)-Furanone, dihydro-5-(3-ethyl-4-methyl-1-pentenyl)-3-hydroxy-5-methyl-
158928-82-6	0	1	0	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 1 fragment)
158928-83-7	0	1	0	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 2 fragment)
158928-84-8	0	1	0	Deoxyribonucleic acid (tobacco clone pTGF220 gene NFL1 exon 3 fragment)
158928-85-9	0	1	0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 1 fragment)
158928-86-0	0	1	0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 2 fragment)
158928-87-1	0	1	0	Deoxyribonucleic acid (tobacco clone lambda T-FLO 4 gene NFL2 exon 3 fragment)
159169-57-0	0	1	0	Stigmasta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3β,4α,5α)-
159169-58-1	0	1	0	Stigmasta-8,14,24(28)-trien-3-ol, 4-methyl-, (3β,4α,5α)-
159520-75-9	0	1	0	Chitinase (tobacco clone 59 gene chi-V precursor reduced)
159813-37-3	0	1	0	2-Cyclohexen-1-one, 4-[3-(β-*D*-glucopyranosyloxy)-1-butenyl]-3,5,5-trimethyl-, [4R-[4R*(1*E*,3S*)]]-
159844-35-6	0	1	0	Deoxyribonucleic acid (*A. thaliana* clone TAY029 gene UbcAt3 ubiquitin-carrier enzyme E 2 messenger RNA complementary plus 5′- and 3′-flanking region fragment)
159844-36-7	0	1	0	Enzyme E 2 (*A. thaliana* clone TAY029 gene UbcAt3 ubiquitin-carrier)
159965-67-0	0	1	0	Desaturase, fatty acid ω3- (tobacco clone Ntfad3)
159965-71-6	0	1	0	Polyubiquitin (*N. tabacum* clone Ubi.U4 gene Ubi.U4)
160074-66-8	0	1	0	Deoxyribonucleic acid (*N. tabacum* clone Ubi.U4 gene Ubi.U4 polyubiquitin plus 5′- and 3′-flanking region fragment)
160075-53-6	0	1	0	Deoxyribonucleic acid (*N. tabacum* cv. SR1 leaf clone Ntfad3 ω-3 fatty acid desaturase mRNA complementary plus 5′- and 3′-flanking region fragment)
160082-04-2	0	1	0	Protein LTP (tobacco)
160115-51-5	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*E*)-(+)-
160115-52-6	0	1	0	2-Butanone, 4-[3,6-dihydro-6-hydroxy-6-methyl-3-(1-methylethyl)-1,2-dioxin-3-yl]-, (*Z*)-(−)-
160115-53-7	0	1	0	4,9-Decadienoic acid, 3-hydroxy-3-methyl-6-(1-methylethyl)-9-(tetrahydro-5-oxo-2-furanyl)-, methyl ester
160115-54-8	0	1	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5β(1*E*,3S*)]]-
160115-55-9	0	1	0	6-Hepten-2-one, 7-[4-(acetyloxy)tetrahydro-5-hydroxy-2-methyl-2-furanyl]-5-(1-methylethyl)-
160115-56-0	0	1	0	6-Undecen-2-one,10-(acetyloxy)-8,11-dihydroxy-8-methyl-5-(1-methylethyl)-11-(tetrahydro-5-hydroxy-2-methyl-2-furanyl)-
160224-93-1	0	1	0	2(3*H*)-Furanone, 3-(acetyloxy)dihydro-5-methyl-5-[3-(1-methylethyl)-6-oxo-1-heptenyl]-, [3R-[3α,5α(1*E*,3S*)]]-
160550-77-6	0	1	0	2-Buten-1-one, 1-[4-(β-*D*-glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexen-1-yl]-, [R-(*E*)]-
160550-79-8	0	1	0	2-Buten-1-one, 1-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, [R-(*E*)]-
160936-44-7	0	1	0	Deoxyribonucleic acid (tobacco leaf curl virus coat protein gene)
160936-45-8	0	1	0	Protein (tobacco leaf curl virus coat)
162188-91-2	1	0	0	1,4-Dioxaspiro[4.5]decan-8-one, 7-(acetyloxy)-7,9,9-trimethyl-, (±)-
162188-92-3	0	1	0	Acetic acid, bromo-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro[4.5]dec-7-yl ester, (±)-
162188-93-4	0	1	0	Acetic acid, (diethoxyphosphinyl)-, 7,9,9-trimethyl-8-oxo-1,4-dioxaspiro[4.5]dec-7-yl ester, (±)-
162188-94-5	0	1	0	Spiro[benzofuran-6(2*H*),2′-[1,3]dioxolan]-2-one, 4,5,7,7a-tetrahydro-4,4,7a-trimethyl-, (±)-
162572-19-2	0	1	0	Protein (tobacco clone pTGF220 gene NFL1)
162572-20-5	0	1	0	Protein (tobacco clone lambda T-FLO 4 gene NFL2)
162572-22-7	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A9)
162572-23-8	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A11)
162572-24-9	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A7)
162572-25-0	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A15)
162572-26-1	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A6)
162572-27-2	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A13)
162572-28-3	0	1	0	Protein formation initiation factor eIF 4A (*N. tabacum* clone NeIF-4A14)
378750-46-0	1	1	1	Europium, isotope of mass 152