

# The Chemical Components Identified in Tobacco and Tobacco Smoke Prior to 1954: A Chronology of Classical Chemistry\*

by

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## SUMMARY

Because of the excellent fractionation and identification technologies developed during the early-1950s, the compositions of tobacco and tobacco smoke, both classified as highly complex mixtures, have been defined more completely than the composition of any other highly complex commercial product such as coffee. By year-end 1953, the many years of research by scientists using classical chemical techniques to define the composition of tobacco and its smoke provided meaningful information on the nature of over 300 tobacco components and fewer than 100 tobacco smoke components. Those involved in the pre-1954 research not only provided the cornerstone of our knowledge of the two compositions but also deserve the gratitude of their successors for the early information generated on tobacco and its smoke. This article is our tribute to those researchers who generated much meaningful knowledge on the composition of tobacco and tobacco smoke prior to 1954 despite the now known fractionation and analytical limitations of the so-called classical chemical techniques. It also notes the similarity of some of the early and more recent research results obtained on the chemical and biological properties of smoke condensate and several of its components from tobacco with those obtained by ROFFO in the 1930s on a destructive distillate of tobacco. [Beitr. Tabakforsch. Int. 23 (2009) 277–333]

## ZUSAMMENFASSUNG

Wegen der hervorragenden Technologien zur Fraktionierung und Identifizierung, die in den frühen 1950iger Jahren entwickelt wurden, wurden die Zusammensetzung von Tabak- und Tabakrauch, die beide als hochkomplexe Mischungen zu klassifizieren sind, umfassender beschrie-

ben als jedes andere komplexe, handelsübliche Gemisch, wie zum Beispiel Kaffee. Am Ende des Jahres 1953 lieferten die jahrelangen Forschungsarbeiten von Wissenschaftlern, die die Zusammensetzung des Tabaks und des Tabakrauchs mit klassischen chemischen Analysemethoden untersucht hatten, wichtige Informationen über die Eigenschaften von über 300 Tabakinhaltsstoffen und nahezu 100 Tabakrauchinhaltsstoffe. Die Wissenschaftler, die an der Forschung vor 1954 beteiligt waren, lieferten nicht nur den Grundstein unseres Wissens über beide Gemische, sondern sie verdienen auch den Dank ihrer Nachfolger für den frühen Kenntnisstand zur Zusammensetzung des Tabaks und des Tabakrauchs. Mit diesem Beitrag zollen wir jenen Wissenschaftlern Tribut, die bedeutende Kenntnisse über die chemische Zusammensetzung vor 1954 lieferten, trotz der heute bekannten damals existierenden Grenzen der sogenannten klassischen chemischen Methoden bei der Fraktionierung und Analyse. Diese Arbeit zeigt auch die Ähnlichkeit mancher früherer Ergebnisse zu den chemischen und biologischen Eigenschaften des Rauchkondensats und mehrerer Tabakinhaltsstoffe mit denen von ROFFO aus den 1930iger Jahren über ein gefährliches Destillat des Tabaks. [Beitr. Tabakforsch. Int. 23 (2009) 277–333]

## RESUME

La composition chimique du tabac et de la fumée de tabac, tous les deux classifiés comme des mélanges très complexes, a été étudiée de façon plus complète que la composition de chaque autre mélange complexe commerciale comme le café, à cause des technologies excellentes de fractionnement et de l'identification développées au début des années 1950. A la fin de l'année 1953, les nombreuses années de recherches effectuées par des

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chercheurs avec des techniques chimiques classiques pour analyser la composition chimique du tabac et de la fumée de tabac, ont fournit des informations compréhensibles sur plus de 300 composants de tabac et près de 100 composants de la fumée de tabac. Les chercheurs des années avant 1954 n'ont pas seulement fournit la base de nos connaissances sur la composition du tabac et de la fumée mais méritent également la reconnaissance de leurs successeurs pour leurs travaux précoce. Avec cet article nous exprimons notre estime aux chercheurs des années avant 1954, qui ont fournit beaucoup d'informations compréhensibles sur la composition du tabac et de la fumée de tabac, malgré les limitations analytiques des techniques chimiques dites classiques. La similarité de quelques résultats, sur les propriétés biologiques et chimiques du condensat de la fumée et plusieurs composants du tabac, obtenues par ROFFO dans les années 1930 sur un distillat nuisible du tabac, est également présentée. [Beitr. Tabakforsch. Int. 23 (2009) 277–333]

## INTRODUCTION

The compilation of the catalogue on the more than 8400 chemical components identified in tobacco and tobacco smoke provided an excellent assessment of the caliber of the research conducted since its escalation in the mid-1950s. The classical chemical analysis used before that date to isolate and characterize a component of a complex mixture was gradually augmented post-1953 by the inclusion of many different, new, and highly efficient separation and analytical technologies. Various types of chromatography coupled with various spectral technologies such as ultraviolet, infrared, nuclear magnetic resonance, and mass provided the means to identify more complex structures of components isolated in much lesser amounts than could be done by using the classical chemical approach. For example, inclusion of such technologies resulted in the increase of the number of identified chemical components in tobacco smoke from the fewer than 100 reported by KOSAK in 1954 (1) to the more than 5200 catalogued recently by RODGMAN and PERFETTI (2). The manifold scientific skills generated and employed during those more than 50 years of research obviously deserve great commendation.

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

In early tobacco research, nicotine and other related tobacco alkaloids were regarded as toxic constituents of tobacco and their presence in smoke was considered a health concern. Tobacco alkaloids were also important as raw materials for pesticides and as sources of raw material for the chemical industry. As a result, considerable effort was focused in the early years of tobacco research on

nicotine and related tobacco alkaloids. This work included the development of new analytical determinations for tobacco alkaloids and tests to measure its toxicity and dependence of nicotine for smokers. Work in the area of breeding new tobacco lines was focused on two directions. Efforts were directed at developing low nicotine or nicotine-free tobaccos for health reasons, and secondly in the direction of tobaccos extremely high in nicotine, as a raw material for pesticides, chemicals, and pharmaceuticals. During our cataloguing of the chemical components of tobacco and tobacco smoke, it became apparent that the chemical research conducted on them from early in the 1800s to September 1953, the date of submission of the KOSAK manuscript for publication, also deserved considerable commendation. Considerable skill in classical chemical methods was used to isolate and characterize the tobacco and smoke components known by late 1953. In this article, the results of that research are summarized in an attempt to illustrate that not only should they not be minimized or disregarded but also the investigators who generated such meaningful results deserve considerable credit.

One of the stimuli cited by KOSAK (1) for the generation of his 1954 catalogue of tobacco smoke components was the brief 1952 published report by GRAHAM *et al.* (3) on the induction of tumors in laboratory animals repeatedly painted with large doses of cigarette smoke tar, a report that was followed in early 1953 by a presentation at the American Association for Cancer Research (4) and then by a detailed publication in a peer-reviewed scientific journal in late 1953 (5). WYNDER *et al.* (5) described many of the early studies on the effects of exposure of laboratory animals to various tars, including those derived from tobacco by smoking or extraction [E. HOFFMANN *et al.* (6), HELWIG (7, 8), BOGEN and LOOMIS (9), COOPER *et al.* (10), CAMPBELL (11, 12), SCHÜRCH and WINTERSTEIN (13), TAKI (14), SUGIURA (15), FLORY (16, 17), and SHUBIK (18)]. An early study reported in 1911 by WACKER and SCHMINCKE (19) preceded the development and description of the procedure to induce cancer in laboratory animals by skin painting with coal tar in 1915–1918 by YAMAGIWA and ICHIKAWA (20, 21). As noted by WYNDER *et al.* (5), each of the tobacco tar studies conducted after The YAMAGIWA-ICHIKAWA reports suffered from one or more deficiencies such as a low number of daily or weekly paintings, low tar-painting dosage, inadequate smoking procedure for tar collection, and the like. However, seldom discussed is the fact that the WYNDER *et al.* study involved a cigarette smoking procedure (35-mL puff, 2-sec puff, 3 puff/min) different from the one in vogue since its elucidation (35-mL puff, 2-sec puff, 1 puff/min) by BRADFORD *et al.* in 1936 (22). Tripling the puff/min not only substantially increases the per cigarette tar yield but also drastically alters its composition, with substantial increases in several smoke components with known tumorigenicity to mouse skin, e.g., the polycyclic aromatic hydrocarbons (PAHs) benzo[a]pyrene (B[a]P) and dibenz[a,h]anthracene (DB[a,h]A). Other reports that triggered interest in the biological properties and chemical composition of cigarette smoke condensate (CSC) were the numerous publications between 1950 and 1953 on the epidemiology of lung cancer and cigarette smoking. They were presented in 1950 by WYNDER and GRAHAM (23), DOLL and HILL (24), LEVIN *et al.* (25),

MILLS and PORTER (26), and SCHREK *et al.* (27). These were followed in 1952 and 1953 by similar extensive studies conducted by DOLL and HILL (28), MCCONNELL *et al.* (29), KOULUMIES (30), LICKINT (31), and SADOWSKY *et al.* (32). It should be noted that the prospective method did not replace retrospective studies. Both approaches have their advantages and disadvantages. In the retrospective study, interviewers record the habits of smokers and controls; the prospective studies are better suited to survey larger groups of diseased and controls in terms of their environment, their behaviors, and specific diseases they contract.

Preceding these 1950–1953 epidemiological studies were several reported from 1912 to 1950 but, in their 1950 report, GRAHAM and WYNDE (23) described in general several of the deficiencies of the earlier epidemiological studies, e.g., small sample size, lack of a control population, statistical procedure, tumor definition. Among the earlier studies were reports and/or comments on respiratory tract cancer by ADLER (33) in 1912, by TYLCOTE (34) in 1927, by LICKINT (35) in 1935, by ARKIN and WAGNER (36) in 1936, by KENNAWAY and KENNAWAY (37, 38) in 1936 and 1947, by ROFFO (39) in 1937, by MÜLLER (40) in 1939, by OCHSNER and DEBAKEY (41, 42) in 1940 and 1941, and by SCHAIRER and SCHÖNINGER (43) in 1943.

The reports by OCHSNER and DEBAKEY subsequently led to an interesting situation in the content of several U.S. Surgeon Generals' reports on smoking and health. From the late 1930s through the late 1960s, OCHSNER, at that time one of the few eminent lung cancer surgeons in the U.S., authored or co-authored over 40 articles and three books in which it was repeatedly asserted that the major cause of lung cancer was cigarette smoking. Despite his number of publications between the late 1930s and late 1963, the 1964 Advisory Committee to the U.S. Surgeon General (44) and the 1979 (45) and 1982 (46) U.S. Surgeon Generals cited only one 1939 OCHSNER-authored publication (47) and one of his authored books, the 1954 edition (48) on the relationship between lung cancer and cigarette smoking. Was the limitation of the citations of OCHSNER's publications on cigarette smoking and lung cancer possibly due to either or both of the following situations?

- ▶ Despite the repeated assertion that the major cause of lung cancer was cigarette smoking, OCHSNER and his colleagues frequently included other comments in the same articles, e.g., a) The cause of the increasing incidence of cancer of the lung is not definite [see p. 212 in (42)], b) The etiology of bronchogenic carcinoma is unknown. (49), c) The etiological picture [for bronchogenic carcinoma] is obscure. It is probable that there are a number of etiological factors in the production of this disease (50).
- ▶ Despite the repeated assertion that the major cause of lung cancer was cigarette smoking, the data on patients undergoing lung resection in the Ochsner Clinic because of lung cancer were summarized in several OCHSNER *et al.* reports as follows: a) In 129 resected cases, no factor was found which might bear a significant relationship to the occurrence of the disease. Neither occupation nor smoking habits, which some reports, including our own, have stressed as of possible etiological significance seems of any special significance in this particular series (51). b) In the analysis

of 147 resected cases, no etiological factor was found to bear a significant relationship to the occurrence of the disease. Both occupation and smoking, which had been particularly emphasized by some observers as possible etiological factors and which we were inclined previously to consider more seriously, were found to have no special significance in this analysis (52).

## CHEMICAL COMPONENTS OF TOBACCO AND TOBACCO SMOKE IDENTIFIED PRIOR TO 1954

Many components were identified in tobacco and/or tobacco smoke prior to the issuance of the 1954 KOSAK report (1), the numerous epidemiological studies on tobacco smoking and respiratory cancer, and the 1953 report of tumor induction in laboratory animals by cigarette-tar painting (5). Most of the pre-1954 characterizations of such components were accomplished by the so-called "classical chemical procedures." The components are listed in Table 1 with the identification and confirmation listed chronologically. If more than one study on a specific component was reported in a given year, the investigators in that year are listed alphabetically.

Examination of the data in Table 1 reveals the many investigators who contributed much meaningful information on tobacco and/or smoke composition prior to year-end 1953. They include the following: BRÜCKNER, BURKHARD, EULENBERG, FRANKENBURG, GABELYA, GARNER, GOTTSCHO, KIRIYANOV, KISSLING, KOBEL, LEHMANN, MOLINARI, NEUBERG, PFYL, PONTAG, PREISS, PYRIKI, ROFFO, SCHÖLLER, SHMUK, SPÄTH, THOMS, VOHL, and WENUSCH. Each of them deserves much tribute for their contributions. Several of them continued to contribute to our knowledge of the composition of tobacco and/or tobacco smoke after 1953, e.g., FRANKENBURG, GARNER, GOTTSCHO, and PYRIKI.

Compared to the fewer than 100 tobacco smoke components listed by KOSAK (1), Table 1 contains 325 chemical components identified and studied in tobacco prior to the publication of the KOSAK article. Included in 383 entries in Table 1 (as they were in the KOSAK tabulation) are several components originally assumed to be individual alkaloid-related components but subsequently were found to be known compounds or mixtures of known compounds, e.g., anodmine, gudham, lathrein, lohitam, obelin, poikiline,  $\alpha$ -socratine,  $\beta$ -socratine, and  $\gamma$ -socratine (53, 54, 55, 56, 57). They were not included in the count of the 325 identified tobacco components. The eventual characterization of anodmine, gudham, lathrein, lohitam, obelin, and the three socratines was described in 1955 by KUFFNER *et al.* (58). Their characterization of these supposedly alkaloid-related components was summarized by JOHNSTONE and PLIMMER (59) in their 1959 review of tobacco and tobacco smoke composition. They wrote in 1959:

The constitution of these bases remained unknown until recently when investigators having access to original specimens were able to elucidate the identities of some of them by application of modern analytical techniques.  $\gamma$ -socratine was found to be identical with *l*-nornicotine, and a crude mixture of  $\alpha$ - and  $\beta$ -socratine (the only sample available), was shown to consist mainly of nicotyrine and 2,3'-dipyridyl with small quantities of nicotinic acid, nornicotine, and possibly anatabine (58).

**Table 1. Chronology from 1800 to late 1953 of identified items in tobacco, tobacco smoke, and tobacco distillate**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
75-07-0	Acetaldehyde	1908 Brasch and Neuberg (64) 1909 Brasch (65) 1931 Neuberg and Burkard (66) 1933 Pfyl (67) 1954 Kosak (1)	1926 Neuberg and Kobel (68) 1931 Neuberg and Burkard (66) 1936 Dixon <i>et al.</i> (69)
	Acetate	1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1954 Kosak (1)	
64-19-7	Acetic acid	1843 Zeise (74) ( <b>D</b> r) 1871 Vohl and Eulenberg (75, 76) 1892 Abeles and Paschkis (77) 1929 Gabelya and Kipriyanov (78) ( <b>D</b> r) 1931 Neuberg and Burkard (66) 1937 Bradford <i>et al.</i> (79) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1950 Peterson (80) 1951 Garner (81) 1952 James and Martin (82) 1954 Kosak (1)	1871 Vohl and Eulenberg (75) 1884 Takayama (83) 1909 Garner (84) 1924 Shmuk (85) 1929 Balabucha-Popzova (86) 1929 Shmuk (87) 1931 Yamafuji (88) 1935 Koenig (89) 1936 Dixon <i>et al.</i> (69) 1941 Sabetay <i>et al.</i> (90) 1951 Garner (81)
	Acids, aliphatic	1931 Neuberg and Burkard (66) 1937 Wenusch and Schöller (91) 1940 Haag (92) 1954 Kosak (1)	1930 Shmuk and Piatnicki (93) 1931 Yamafuji (88) 1953 Wada and Kobashi (94) 1943 Venkataraao <i>et al.</i> (95)
	Acids, amino-		1951 Roberts and Wood (96) 1952 Frankenburg and Gottscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99) 1914 Garner <i>et al.</i> (100) 1931 Vickery and Pucher (101) 1933 Pucher and Vickery (102) 1951 Garner (81)
	Acids, non-volatile		
	Acids, phenolic	1939 Roffo (8, 9, 10, 11) ( <b>D</b> ) 1954 Kosak (1)	
7440-34-8	Actinium		1937 Drobkov (103)
56-41-7	L- $\alpha$ -Alanine		1952 Frankenburg and Gottscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99) 1953 Ross (104)
107-95-9	$\beta$ -Alanine		1901 Pictet and Rotschy (108, 109) 1908 Pictet and Court (110) 1931 Ehrenstein (111) 1938 Marion (112) 1939 Späth and Kuffner (113) 1941 Jackson (114) 1948 Frankenburg (115) 1952 Badgett <i>et al.</i> (116) 1953 Tso and Jeffrey (117) 1932 Eisenmenger (119) 1938 McMurtrey and Robinson (120) 1938 Morgan and Street (121) 1944 LeCompte (122) 1951 Garner (81)
7429-90-5	Aluminum	1952 Bailey (118)	
	Amines, aliphatic		
7664-41-7	Ammonia	1929 Gabelya and Kipriyanov (78) ( <b>D</b> r) 1857 Vogel (123, 124) 1858 Vogel (125) 1871 Vohl and Eulenberg (75, 76) 1879 Périgord (126) 1880 LeBon (127) 1899 Thoms (128) 1900 Thoms (129) 1902 Pontag (130) 1903 Pontag (131) 1908 Biederbeck (132) 1908 Lee (133) 1908 Lehmann (134) 1909 Lehmann (135)	1885 Müller-Thurgen (153) 1894 Behrens (154) 1908 Pictet and Court (110) 1914 Garner <i>et al.</i> (100) 1928 Shmuk (140) 1929 Gabelya and Kipriyanov (78) 1930 Smirnov and Izvoshtshikov (55) 1936 Dixon <i>et al.</i> (69) 1936 Preiss (156) 1937 Fromm (157) 1939 Gaertner (158) 1939 Shmuk (165) 1948 Pyriki (166)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
7664-41-7	Ammonia (cont.)	1910 Toth and Krampera (136) 1911 Vaubel (137) 1912 Anonymous (138, 139) 1928 Shmuk (140) 1929 Bogen (141) 1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1929 Koperina (142) 1931 Gavrilov and Koperina (143) 1931 Haley <i>et al.</i> (144) 1931 Shmuk and Kolesnik (105) 1932 Barta and Toole (145, 146) 1932 McNally (147) 1933 Pfyl (148) 1934 Barta (149) 1936 Bogen (150) 1936 Preiss (151, 152, 156) 1937 Bradford <i>et al.</i> (79) 1939 Dittmar (162, 163, 164) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939 Shmuk (165) 1948 Pyriki (166) 1950 Peterson (80) 1951 Garner (81) 1952 Larsen (167) 1954 Kosak (1) 1936 Cuvelier (168)	1950 Molinari (159) 1951 Garner (81) 1952 Hough <i>et al.</i> (160) 1952 Jensen (161)  1936 Späth and Zajic (169) 1913 Oosthuizen and Shedd (170) 1937 Matsumina (171) 1942 Ward (172) 1946 Garner (173) 1951 Garner (81) 1951 Nakai and Inaba (174) 1953 Barrett <i>et al.</i> (175) 1939 Henry (176) 1935 Wenusch and Schöller (55, 56)
9000-92-4	Ammonium salts Ammoresinol Amylase		
120-12-7	Anabaseine Anodmin = mixture of basic components of tobacco and its smoke (58)	1935 Wenusch and Schöller (55, 56) 1936 Wenusch and Schöller (177) 1954 Kosak (1) 1939 Roffo (70, 71, 72, 73, 178) ( <b>D</b> ) 1953 Cooper and Lindsey (179) 1954 Kosak (1)	1935 Wenusch and Schöller (55, 56)
7440-36-0	Antimony	1934 Heffer <i>et al.</i> (180)	
147-81-9	Arabinose	1929 Gabelya and Kipriyanov (181)	
7004-12-8	Arginine	1933 Vickery <i>et al.</i> (182) 1935 Vickery <i>et al.</i> (183) 1951 Garner (81) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)	
7440-38-2	Arsenic	1922 Leitch and Kennaway (184) 1927 Remington (185) 1932 McNally (147) 1934 Gross and Nelson (186) 1935 Bastedo (187) 1945 Thomas and Collier (188) 1947 Griffon and Delga (189) 1950 Daff and Kennaway (190, 191) 1951 Daff <i>et al.</i> (192) 1952 Goulden <i>et al.</i> (193) 1953 Monnet and Dupont (194) 1954 Kosak (1)	1905 Boening (195) 1922 Leitch and Kennaway (184) 1927 Remington (185) 1928 Popp (196, 197) 1934 Carey <i>et al.</i> (198) 1935 McMurtrey (199) 1938 McMurtrey (200) 1939 Barksdale (201) 1940 Barksdale (202) 1941 McMurtrey (203) 1942 Vucetic and Carratala (204) 1944 Vincent (205) 1947 Griffon and Delga (189) 1950 Daff and Kennaway (190, 191) 1951 Daff <i>et al.</i> (192) 1951 Garner (81) 1951 Oliver (206) 1952 Bunce (207) 1953 Monnet and Dupont (194) 1953 Wolff <i>et al.</i> (208)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
1327-53-3	Arsenic oxide ( $\text{As}_2\text{O}_3$ )	1927 Remington (185) 1932 McNally (147) 1934 Gross and Nelson (186) 1935 Bastedo (187) 1945 Thomas and Collier (188) 1947 Griffon and Delga (189) 1950 Daff and Kennaway (190, 191) 1951 Daff <i>et al.</i> (192) 1952 Goulden <i>et al.</i> (193) 1953 Monnet and Dupont (194) 1954 Kosak (1)	1905 Boening (195) 1927 Remington (185) 1928 Popp (196, 197) 1934 Carey <i>et al.</i> (198) 1935 McMurtrey (199) 1938 McMurtrey (200) 1940 Barksdale (202) 1941 McMurtrey (203) 1942 Vucetich and Carratala (204) 1947 Griffon and Delga (189) 1950 Daff and Kennaway (190, 191) 1951 Daff <i>et al.</i> (192) 1951 Garner (81) 1953 Monnet and Dupont (194) 1901 Marlatt (209) 1908 Marlatt (210) 1947 Maton (211) 1951 Lona and Porzio-Giovanola (212) 1951 Tombesi (213) 1894 Behrens (154) 1937 Vickery <i>et al.</i> (214) 1951 Garner (81) 1952 Frankenburg and Gottscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99) 1952 Frankenburg and Gottscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
	Arsenical insecticides		
50-81-7	Ascorbic acid		
7006-34-0	Asparagine		
56-84-8	Aspartic acid		
275-51-4	Azulene	1947 Ikeda (215) 1954 Kosak (1)	
7440-39-3	Barium		1913 McHargue (216) 1913 Traetta-Mosca (217) 1916 Artis and Maxwell (218) 1916 Knight (219) 1921 Headden (220) 1931 Yamafuji (88) 1934 Nito and Kitamura (221)
	Bases	1940 Haag (92)	
100-52-7	Benzaldehyde	1931 Neuberg and Burkard (66) 1954 Kosak (1)	
	Benzenamine, alkyl-	{coridine}	1871 Vohl and Eulenberg (75)
	Benzenamine, alkyl-	{rubidine}	1871 Vohl and Eulenberg (75)
	Benzenamine, alkyl-	{viridine}	1871 Vohl and Eulenberg (75)
	Benzenamine, 4-(1,1-dimethylethyl)-	{parvoline}	1871 Vohl and Eulenberg (75)
53-19-0	Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]-	{ <i>o,p'</i> -DDD; <i>o,p'</i> -TDE}	1951 Vinzant (60)
4329-12-8	Benzene, 1-chloro-3-[2,2-dichloro-1-(4-chlorophenyl)ethyl]-	{ <i>m,p'</i> -DDD}	1951 Vinzant (60)
789-02-6	Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]-	{ <i>o,p'</i> -DDT}	1951 Vinzant (60)
50-29-3	Benzene, 1,1'-(2,2,2-trichloroethylidene)bis[4-chloro-	{ <i>p,p'</i> -DDT}	1951 Vinzant (60)
100-21-0	1,4-Benzenedicarboxylic acid	{terephthalic acid}	1946 Frankenburg (222)
120-80-9	1,2-Benzenediol	{catechol}	1935 Koenig (89)
123-31-9	1,4-Benzenediol	{hydroquinone}	1952 Volgunov (225)
100-51-6	Benzenemethanol	{benzyl alcohol}	1939 Wenusch (226)
65-85-0	Benzoic acid	1931 Neuberg and Burkard (66)	
	{benzenecarboxylic acid}	1939 Wenusch (226) 1940 Haag (92) 1954 Kosak (1)	

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
99-50-3	Benzoic acid, 3,4-dihydroxy- {protocatechuic acid}		1929 Shmuk (87)
149-91-7	Benzoic acid, 3,4,5-trihydroxy- {gallic acid}		1929 Shmuk (87)
59-02-9	2H-1-Benzopyran-6-ol, 3,4- dihydro-2,5,7,8-tetramethyl-2- (4,8,12-trimethyltridecyl)- { $\alpha$ -tocopherol}		1945 Riemenschneider <i>et al.</i> (227)
92-61-5	2H-1-Benzopyran-2-one, 7- hydroxy-6-methoxy- {scopoletin}		1948 Best (228) 1953 Johanson (229)
21637-25-2	4H-1-Benzopyran-4-one, 2-(3,4- dihydroxyphenyl)-3-( $\beta$ -D- glucofuranosyloxy)-5,7-dihydroxy- {isoquercitrin}		1935 Kurilo (230) 1937 Kurilo (231) 1950 Howard <i>et al.</i> (232)
117-39-5	4H-1-Benzopyran-4-one, 2-(3,4- dihydroxyphenyl)-3,5,7-trihydroxy- {quercitin}		1935 Kurilo (230) 1936 Neuberg and Kobel (233) 1950 Howard <i>et al.</i> (232)
153-18-4	4H-1-Benzopyran-4-one, 3-[6-O- (6-deoxy- $\alpha$ -L-mannopyranosyl)- $\beta$ - D-glucopyranosyl]oxy]-2-(3,4- dihydroxyphenyl)-5,7-dihydroxy- {rutin}		1931 Hasegawa (234) 1935 Kobel and Neuberg (235) 1935 Neuberg and Kobel (236) 1936 Neuberg and Kobel (233, 237) 1944 Couch and Krewson (238, 239) 1944 Griffith <i>et al.</i> (240) 1947 Couch (241) 1949 Badgett <i>et al.</i> (242) 1951 Garner (81) 1951 Nio and Wada (243) 1953 Wada (244)
480-10-4	4H-1-Benzopyran-4-one, 3-( $\beta$ -D- glucopyranosyloxy)-5,7- dihydroxy-2-(4-hydroxyphenyl)- {kaempferol glycoside}		1953 Wada (244)
50-32-8	Benzo[a]pyrene	1937 Roffo (245) ( <b>D</b> ) 1939 Roffo (70, 71, 72, 73, 178, 246) ( <b>D</b> ) 1941 Roffo (247) ( <b>D</b> ) 1942 Roffo (248) ( <b>D</b> ) 1954 Kosak (1)	1937 Roffo (245) ( <b>D</b> ) 1939 Roffo (70, 71, 72, 73, 178, 246) ( <b>D</b> ) 1941 Roffo (247) ( <b>D</b> ) 1942 Roffo (248) ( <b>D</b> ) 1954 Kosak (1)
8001-35-2	Bicyclo[2.2.1]heptane, 2,2- dimethyl-3-methylene-, polychlorinated {Toxaphene®}		1951 Vinzant (60)
507-70-0	Bicyclo[2.2.1]heptan-2-ol, 1,7,7- trimethyl-, <i>endo</i> - {borneol}		1941 Sabetay <i>et al.</i> (90)
366-18-7	2,2'-Bipyridine		1901 Pictet and Rotschy (108) 1928 Shmuk (140)
581-50-0	2,3'-Bipyridine		1928 Shmuk (140) 1936 Späth and Zajic (169) 1939 Späth and Biniecki (249) 1946 Frankenburg (250) 1952 Frankenburg and Gotscho (97) 1953 Tso and Jeffrey (117)
581-49-7	2,3'-Bipyridine, 1,2,3,6-tetrahydro-, (S)- { <i>l</i> -anatabine}		1937 Späth and Kesztler (251, 252) 1946 Frankenburg (250) 1948 Shmuk (253) 1953 Tso and Jeffrey (117)
5953-51-5	2,3'-Bipyridine, 1,2,3,6-tetrahydro- 1-methyl-, (S)-		1937 Späth and Kesztler (254) 1946 Frankenburg (250)
7440-69-9	Bismuth		1934 Heffer <i>et al.</i> (180)
7440-42-8	Boron	1952 Bailey (118)	1923 Warrington (255) 1926 Sommer and Lipman (256) 1927 Swanback (257) 1929 McMurtrey (258) 1934 Van Schreven (259) 1935 McMurtrey (199) 1938 McMurtrey (200) 1938 McMurtrey and Robinson (120)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
7440-42-8	Boron (cont.)		1938 Morgan and Street (121) 1941 McMurtrey (203) 1950 Steinberg (260) 1951 Garner (81) 1952 Lashkevich (261)
123-72-8	Butanal	1908 Brasch and Neuberg (64) 1909 Brasch (65) 1931 Neuberg and Burkard (66) 1954 Kosak (1)	
107-89-1	Butanal, 3-hydroxy-	{aldol}	1931 Neuberg and Burkard (66)
107-85-7	1-Butanamine, 3-methyl-	{isoamyl amine}	1911 Ciamician and Ravenna (262) 1928 Shmuk (140)
110-15-6	Butanedioic acid	{succinic acid}	1924 Shmuk (85) 1929 Shmuk (87) 1930 Shmuk (263)
6915-15-7	Butanedioic acid, hydroxy-	{malic acid}	1904 Kissling (265) 1924 Shmuk (85) 1929 Shmuk (87) 1931 Yamafuji (88) 1930 Shmuk (263) 1935 Koenig (89) 1937 Pucher <i>et al.</i> (266) 1939 Shmuk (165) 1951 Bacon <i>et al.</i> (267) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1953 Phillips and Bacot (269) 1953 Wright and Burton (270) 1937 Pucher <i>et al.</i> (266) 1951 Garner (81)
16426-50-9	Butanedioic acid, hydroxy-, calcium salt		1937 Pucher <i>et al.</i> (266)
869-06-7	Butanedioic acid, hydroxy-, magnesium salt		1937 Pucher <i>et al.</i> (266)
585-09-1	Butanedioic acid, hydroxy-, potassium salt		1951 Garner (81)
431-03-8	2,3-Butanedione	1935 Neuberg and Kobel (271) 1939 Schmalfuss (272) 1950 Schmalfuss (273) 1953 Sasaki (274) 1954 Kosak (1)	1929 Schmalfuss and Barthmeyer (275) 1932 Schmalfuss and Schmalfuss (276) 1935 Neuberg and Kobel (271)
107-92-6	Butanoic acid	1843 Zeise (74) 1871 Vohl and Eulenberg (75, 76) 1900 Thoms (129) 1904 Thoms (277) 1931 Neuberg and Burkard (66) 1935 Wenusch (278) 1951 Garner (81) 1952 James and Martin (82) 1954 Kosak (1)	1871 Vohl and Eulenberg (75) 1909 Garner (84) 1924 Shmuk (85) 1929 Shmuk (87)
56-12-2	Butanoic acid, 4-amino-	{4-aminobutyric acid}	1952 Frankenburg and Gotscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99) 1946 Frankenburg (222)
503-74-2	Butanoic acid, 3-methyl-	{isovaleric acid}	
2055-23-4	1-Butanone, 4-(methylamino)-1-(3-pyridinyl)-	{pseudooxynicotine}	1939 Henry (176)
71278-11-0	1-Butanone, 4-amino-1-(3-pyridinyl)-	{poikililine}	1948 Wenusch (279)
538-79-4	3-Buten-1-amine, <i>N</i> -methyl-4-(3-pyridinyl)-	{metanicotine; nicotimine}	1928 Shmuk (140) 1948 Shmuk (253)
110-17-8	2-Butenedioic acid ( <i>E</i> )-	1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) {fumaric acid}	1924 Shmuk (85) 1929 Shmuk (87) 1930 Shmuk (263)
7440-43-9	Cadmium		1934 Heffer <i>et al.</i> (180)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>Dr</b> ), destructive ( <b>D</b> )]	Tobacco
7440-70-2	Calcium	1952 Bailey (118)	1907 Garner (280) 1928 Bailey and Anderson (281) 1935 Koenig (89) 1950 Steinberg (260) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1953 Bortner and Hamilton (282)
7440-44-0	Carbon		1934 Garner <i>et al.</i> (283, 284) 1951 Garner (81)
124-38-9	Carbon dioxide	1843 Zeise (74) 1899 Thoms (128) 1900 Thoms (129) 1901 Habermann (285) 1903/04 Moir (286) 1904 Habermann (287) 1909 Lehmann (135) 1914 Bush (288) 1922 Armstrong and Evans (289) 1929 Bogen (141) 1929 Gabelya and Kipriyanov (78) ( <b>Dr</b> ) 1938 Saruta (290) 1938 Wenusch and Schöller (291) 1939 De Voogd and Van der Linden (292) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939/40 de Campos (293) 1940 Haag (92) 1949 Fishel and Haskins (294) 1952 Larsen (167) 1954 Kosak (1)	1909 Boekhout and de Vries (295) 1934 Garner <i>et al.</i> (283, 284) 1936 Dixon <i>et al.</i> (69) 1951 Garner (81)
75-15-0	Carbon disulfide		1951 Garner (81)
630-08-0	Carbon monoxide	1843 Zeise (74) 1871 Vohl and Eulenberg (75, 76) 1874 Krause (296) 1877 Schwarz (297) 1879 Périgord (126) 1880 LeBon (127) 1884 Fokker (298) 1899 Thoms (128) 1899 Wahl (299) 1900 Thoms (129, 300) 1901 Habermann (285) 1902 Pontag (130) 1903 Pontag (131) 1903 Spitta (301) 1903/04 Moir (286) 1904 Habermann (287) 1907 Marcelet (302) 1907 Tani (303) 1907 Toth (304) 1908 Fleig (305) 1908 Lee (133) 1908 Lehmann (134) 1908 Marcelet (306) 1908 Toth (307) 1909 Garner (84) 1909 Lehmann (135) 1911 Marcelet (308) 1914 Bush (288) 1920 Hartridge (309) 1922 Armstrong and Evans (289) 1923 Baumberger (310) 1923 Heinz (311) 1923 Jones <i>et al.</i> (312) 1929 Bogen (141) 1929 Gabelya and Kipriyanov (78) ( <b>Dr</b> ) 1929 Schöller (313) 1932 McNally (147) 1934 Ehrismann and Abel (314) 1934 Leikola and Rautavaara (315) 1934 Waser and Stähli (316)	

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
630-08-0	Carbon monoxide ( <i>cont.</i> )	1935 Bastedo (187) 1935 Wenusch and Schöller (317) 1936 Bogen (150) 1937 Saruta (318) 1937 Tsumura (319) 1938 Roffo (320) 1938 Saruta (290) 1938 Wenusch and Schöller (291) 1939 De Voogd and Van der Linden (292) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939/40 de Campos (293) 1940 Haag (92) 1942 Hukusima (321) 1949 Copenhagen and Bigelow (322) 1949 Fishel and Haskins (294) 1951 Garner (81) 1951 Obersteg and Scoch-Kanter (323) 1954 Kosak (1)	Tobacco
463-79-6	Carbonic acid	1928 Shmuk (140)	
10361-29-2	Carbonic acid, ammonium salt	1939 Roffo (70, 71, 72, 73) ( <b>D</b> )	
584-08-7	Carbonic acid, dipotassium salt {potash}	1894 Behrens (154) 1935 Koenig (89)	
39409-82-0	Carbonic acid, magnesium salt	1923 Garner <i>et al.</i> (324, 325) 1951 Garner (81)	
7235-40-7	$\beta,\beta$ -Carotene { $\beta$ -carotene, all- <i>trans</i> }	1939 Nagel (326) 1947 Jeffrey and Griffith (327) 1951 Garner (81) 1952 Jensen (161) 1939 Nagel (326) 1951 Garner (81)	
127-40-2	$\beta,\varepsilon$ -Carotene-3,3'-diol {xanthophyll, lutein}	1939 Nagel (326) 1951 Garner (81)	
9001-05-2	Catalase	1936 Dixon <i>et al.</i> (69) 1937 Matsumina (171) 1938 Hukusima (328) 1946 Garner (173) 1951 Garner (81) 1951 Nakai and Inaba (174) 1953 Brown and Steinberg (329)	
9012-54-8	Cellulase	1950 Tracey (330) 1953 Barrett <i>et al.</i> (175)	
9004-34-6	Cellulose	1934 Pyriki (331) 1935 Koenig (89) 1936 Brückner (332) 1951 Garner (81)	
483-17-0	Cephalin	1939 Shabanov (333)	
7440-45-1	Cerium	1950 Yamagata (334)	
7440-46-2	Cesium	1862/63 Grandea (335) 1913 Traetta-Mosca (217)	
16887-00-6	Chloride	1892 Nessler (336) 1894 Behrens (154) 1899 Pritchard (337) 1923 Garner <i>et al.</i> (325) 1925 Krevs (338) 1928 Bailey and Anderson (281) 1935 Koenig (89) 1941 Ward (339) 1950 McEvoy (340) 1951 Garner (81) 1951 Mosley <i>et al.</i> (341) 1939 Nagel (326) 1951 Garner (81)	
479-61-8	Chlorophyll a	1939 Nagel (326) 1951 Garner (81)	
519-62-0	Chlorophyll b	1939 Nagel (326) 1951 Garner (81)	
1406-65-1	Chlorophyll a and b	1935 Koenig (89) 1939 Nagel (326) 1950 Steinberg (260) 1951 Bacon <i>et al.</i> (267) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1952 Jensen (161)	

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
	Chlorophyll degradation products	1937 Wenusch (342) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1954 Kosak (1)	
57-88-5	Cholest-5-en-3-ol (3 $\beta$ )-{cholesterol}	1928 Kennaway and Sampson (343) 1938 Roffo (344) 1939 Roffo (345, 346) 1941 Roffo (347) 1943 Kirby (348) 1949 Falk <i>et al.</i> (349)	1928 Kennaway and Sampson (343) 1938 Roffo (344) 1939 Roffo (345) 1941 Roffo (347) 1943 Kirby (348) 1949 Falk <i>et al.</i> (349)
7440-47-3	Chromium		1934 Heffer <i>et al.</i> (180) 1936 Johnson (350)
7440-48-4	Cobalt		1934 Heffer <i>et al.</i> (180) 1952 Nicholas (351) 1953 Nicholas and Thomas (352)
7440-50-8	Copper	1952 Bailey (118)	1934 Heffer <i>et al.</i> (180) 1937 Manns <i>et al.</i> (353) 1938 McMurtrey and Robinson (120) 1950 Swanback (354) 1951 Garner (81) 1952 Lashkevich (261) 1953 Brown and Steinberg (329)
57-12-5	Cyanide <sup>-</sup>	1932 McNally (147) 1954 Kosak (1)	
608-73-1	Cyclohexane, 1,2,3,4,5,6-hexachloro-{Lindane®}		1951 Vinzant (60)
327-97-9	Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-[1S-(1 $\alpha$ ,3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ )]-{chlorogenic acid; 3-O-caffeoylequinic acid}		1909 Gorter (355) 1930 Shmuk and Piatnicki (93) 1933 König and Dörr (356) 1935 Koenig (89) 1939 Shmuk (165) 1951 Garner (81) 1951 Roberts and Wood (96) 1953 Pearse and Novellie (98)
77-95-2	Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-{quinic acid}		1929 Shmuk (87) 1930 Shmuk (357, 358) 1939 Shmuk (165) 1951 Garner (81)
89-78-1	Cyclohexanol, 5-methyl-2-(1-methylethyl)-{menthol}	1941 Haggard and Greenberg (361) 1952 Rakieten <i>et al.</i> (362)	1941 Haggard and Greenberg (361)
	Pre-1954, considered as a flavorant applied to and identified on tobacco and found in its smoke; subsequently identified as naturally occurring in several different additive-free tobaccos (359) and its mechanism of formation as an isoprenoid defined (360)		
498-40-8	Cysteic acid		1953 Zacharius and Frankenburg (99)
52-90-4	L-Cysteine	{propanoic acid, 2-amino-3-mercaptop-}	1951 Garner (81) 1951 Sharmon (363) 1953 Zacharius and Frankenburg (99)
24645-67-8	Cystine		1951 Garner (81)
56-89-3	{propanoic acid, 2-amino-3,3'-dithiobis-}		1951 Sharmon (363) 1953 Zacharius and Frankenburg (99)
334-48-5	Decanoic acid {capric acid}	1952 James and Martin (82)	1953 Barrett <i>et al.</i> (175) 1953 Silberger and Skoog (364)
	Decarboxylase, $\alpha$ -ketoglutaric acid		1934 Pyriki (331)
	Deoxyribonucleic acid		1942 Ward (172)
9004-53-9	Dextrin		1951 Garner (81) 1953 Phillips and Bacot (269)
9000-92-4	Diastase		1914 Garner <i>et al.</i> (100) 1942 Ward (172) 1951 Garner (81)
	Distillate, destructive, tobacco	1937 Roffo (245) ( <b>D</b> ) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> )	

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>Dr</b> ), destructive ( <b>D</b> )]	Tobacco
	Distillate, dry, tobacco	1826 Unterordnen (365) ( <b>Dr</b> ) 1843 Zeise (74) ( <b>Dr</b> ) 1930 Gabelya and Kipriyanov (78) ( <b>Dr</b> )	
143-07-7	Dodecanoic acid Emulsin	{lauric acid} 1952 James and Martin (82)	1913 Oosthuizen and Shedd (170) 1951 Garner (81) 1950 Holden (366) 1951 Bacon <i>et al.</i> (267) 1952 Bacon <i>et al.</i> (268)
	Enzymes, general		1871 Vohl and Eulenberg (75, 76)
75-04-7	Ethanamine		1871 Vohl and Eulenberg (75)
62-49-7	Ethanaminium, 2-hydroxy- <i>N,N,N</i> -trimethyl- {choline}		1932 Nottbohm and Mayer (367) 1933 Vickery <i>et al.</i> (182) 1935 Vickery <i>et al.</i> (183) 1951 Garner (81)
460-19-5	Ethanedinitrile	{cyanogen} 1910 Toth (368, 369) 1911 Toth (370)	1884 Takayama (83) 1894 Behrens (154) 1904 Kissling (265) 1924 Shmuk (85) 1929 Shmuk (87) 1935 Koenig (89) 1939 Shmuk (165) 1951 Bacon <i>et al.</i> (267) 1952 Bacon <i>et al.</i> (268) 1953 Wright and Burton (270)
144-62-7	Ethanedioic acid	{oxalic acid} 1938 Wiley <i>et al.</i> (371)	1894 Behrens (154) 1937 Pucher <i>et al.</i> (266) 1951 Garner (81) 1938 Wiley <i>et al.</i> (371) 1954 Kosak (1)
563-72-4	Ethanedioic acid, calcium salt		
107-21-1	1,2-Ethanediol	{ethylene glycol} 1938 Forbes and Haag (372) 1949 Reif (373) 1954 Kosak (1)	1926 Neuberg and Kobel (68) 1937 Haag (375) 1937 Holck and Carlson (376) 1938 Newman (377) 1945 McNally <i>et al.</i> (374) 1952 Küchle <i>et al.</i> (378) 1954 Kosak (1)
64-17-5	Ethanol		
111-46-6	Ethanol, 2,2'-oxybis- {diethylene glycol}	1945 McNally <i>et al.</i> (374) 1951 Garner (81)	
	A tobacco additive applied to and identified in tobacco and its smoke	1954 Kosak (1)	
350-03-8	Ethanone, 1-(3-pyridinyl)- {3-acetylpyridine; methyl 3-pyridyl ketone}		1952 Frankenburg and Gottscho (97) 1953 Tso and Jeffrey (117)
74-86-2	Ethyne	{acetylene} 1934 Ehrismann and Abel (314) 1949 Copenhagen and Bigelow (322) 1949 Fishel and Haskins (294) 1954 Kosak (1)	
	Fat, tobacco		1883 Kissling (379)
	Fluorescent components	1932 Hirst (380)	1948 Best (228) 1951/52 Mizukami (381) 1953 Johanson (229)
7782-41-4	Fluorine	1948 Spira (382)	
50-00-0	Formaldehyde	1904 Thoms (277) 1904 Trillat (383, 384, 385) 1905 Trillat (386) 1909 Lehmann (135) 1926 Neuberg and Kobel (68) 1927 Neuberg and Ottenstein (387) 1931 Neuberg and Burkard (66) 1932 McNally (147) 1935 Bastedo (187) 1954 Kosak (1)	1929 Neuberg and Kobel (388)
64-18-6	Formic acid	1871 Vohl and Eulenberg (75, 76) 1929 Gabelya and Kipriyanov (78) ( <b>Dr</b> ) 1931 Neuberg and Burkard (66) 1937 Bradford <i>et al.</i> (79) 1940 Haag (92) 1951 Garner (81) 1952 James and Martin (82) 1954 Kosak (1)	1871 Vohl and Eulenberg (75) 1924 Shmuk (85) 1929 Shmuk (87) 1930 Shmuk (263) 1930 Shmuk and Kashirin (389) 1931 Neuberg and Burkard (66) 1935 Koenig (89) 1936 Dixon <i>et al.</i> (69)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
57-48-7	D-Fructose	{levulose}	1884 Attfield (390) 1929 Balabucha-Popzova (86) 1934 Pyriki (331) 1934 Shmuk (391) 1942 Ward (172) 1951 Bacon <i>et al.</i> (267) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1953 Pearse and Novellie (98)
	Furan derivative	1935 Schürch and Winterstein (392) 1954 Kosak (1)	
98-01-1	2-Furancarboxaldehyde	1904 Thoms (393) [opium study] 1912 Anonymous (138) 1912 Anonymous (139) 1914 Bush (288) 1929 Bogen (141) 1933 Molinari (394) 1935 Bastedo (187) 1936 Bogen (150) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939 Wenusch (226) 1954 Kosak (1)	1903 Jetta (395) 1909 Boekhout and de Vries (295) 1926 Neuberg and Kobel (396) 1939 Wenusch (226)
98-00-0	2-Furanmethanol (furfuryl alcohol)		1931 Hukusima and Ooike (397) 1950 Molinari (159)
59-23-4	D-Galactose		1929 Balabucha-Popzova (86) 1929 Gabelya and Kipriyanov (181)
526-99-8	Galactaric acid	(mucic acid)	1929 Gabelya and Kipriyanov (181)
14982-50-4	Galacturonic acid		1929 Balabucha-Popzova (86) 1929 Gabelya and Kipriyanov (181) 1931 Neuberg and Scheuer (398) 1951 Garner (81)
25990-10-7	Galacturonic acid, homopolymer		1929 Balabucha-Popzova (86)
554-91-6	Gentibiose		1943 Miller (399)
	Globulin		1932 Vickery (400)
498-07-7	β-D-Glucopyranose, 1,6-anhydro-	1938 Wenusch (401, 402) {levoglucosan}	1950 Molinari (159)
50-99-7	α-D-Glucose		1894 Behrens (154) 1934 Pyriki (331) 1935 Kurilo (230) 1936 Neuberg and Kobel (233) 1942 Ward (172) 1951 Bacon <i>et al.</i> (267) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1952 Hough <i>et al.</i> (160) 1953 Pearse and Novellie (98)
57-50-1	α-D-Glucopyranoside, β-D-fructofuranosyl-	{sucrose}	1894 Behrens (154) 1942 Ward (172) 1951 Bacon <i>et al.</i> (267) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1953 Pearse and Novellie (98) 1953 Phillips and Bacot (269) 1931 Yamafuji (88) 1952 Frankenburg and Gotscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
576-37-4	Glucuronic acid		1934 Vickery <i>et al.</i> (403)
6899-05-4	Glutamic acid		1937 Vickery <i>et al.</i> (214) 1951 Garner (81)
56-85-9	Glutamine		1952 Frankenburg and Gotscho (97) 1953 Pearse and Novellie (98)
56-40-6	Glycine		1953 Zacharius and Frankenburg (99)
70-18-8	Glycine, N-(N-L-γ-glutamyl-L-cysteinyl)-	{glutathione}	1935 Heiserich (404)
	Glycolase		
	Glycosides		1951 Garner (81) 1932 Yamafuji (405) 1939 Shmuk (165) 1952 Geissmann and Hinreiner (406)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
	Gudham = mixture of basic components of tobacco and its smoke (58)	1935 Wenusch and Schöller (56) 1954 Kosak (1)	1935 Wenusch and Schöller (56)
9034-32-6	Hemicellulose		1934 Pyriki (331) 1935 Koenig (89) 1951 Garner (81)
630-04-6	Hentriacontane	1843 Zeise (74) 1892 Abeles and Paschkis (77) 1894 Kissling (407) 1934 Wenusch (408) 1935 Schürch and Winterstein (392) 1937 Wenusch (409) 1954 Kosak (1)	1883 Kissling (379) 1931 Hukusima and Oika (397) 1934 Chibnall <i>et al.</i> (410) 1942 Pyriki (411) 1951 Garner (81)
502-73-8	16-Hentriacontanone	1935 Schürch and Winterstein (392)	
593-49-7	Heptacosane		1934 Chibnall <i>et al.</i> (410) 1931 Hukusima and Oika (397) 1935 Shirokaya (412) 1937 Shmuk (413) 1942 Pyriki (411) 1951 Garner (81)
123-19-3	Heptanoic acid 4-Heptanone {butyrone; dipropyl ketone}	1952 James and Martin (82) 1931 Neuberg and Burkard (66) 1954 Kosak (1)	1935 Neuberg and Kobel (271)
57-10-3	Hexadecanoic acid {palmitic acid}		1931 Hukusima and Oika (397) 1935 Shirokaya (412) 1937 Salisbury (414) 1937 Shmuk (413) 1944 Venkataraao <i>et al.</i> (466) 1945 Riemenschneider <i>et al.</i> (227) 1951 Garner (81) 1931 Hasegawa (415) 1936 Neuberg and Kobel (416) 1946 Frankenburg (222)
50-70-4	Hexane, hexahydroxy-{sorbitol; glucitol}		
142-62-1	Hexanoic acid {caproic acid}	1871 Vohl and Eulenberg (75, 76) 1931 Neuberg and Burkard (66) 1952 James and Martin (82) 1954 Kosak (1)	
71-00-1	Histidine		1931 Yamafuji (88) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99) 1883 Kissling (379) 1901 Thorpe and Homes (417)
	Hydrocarbons, aliphatic		1883 Kissling (379)
	Hydrocarbons, aliphatic C <sub>25</sub> -C <sub>32</sub>		
	Hydrocarbons, aromatic	1949 Fishel and Haskins (294) 1954 Kosak (1)	
	Hydrocarbons, unsaturated	1949 Fishel and Haskins (294) 1954 Kosak (1)	
74-90-8	Hydrocyanic acid {hydrogen cyanide}	1858 Vogel and Reischauer (418) 1870 Poggiale and Marty (419) 1871 Vohl and Eulenberg (75) 1880 LeBon (127) 1882 Molnár (420) 1899 Thoms (128) 1900 Thoms (129) 1901 Habermann (285) 1902 Pontag (130) 1903 Habermann (421) 1903 Pontag (131) 1903 Thoms (422) 1908 Lee (133) 1908 Lehmann (134) 1909 Habermann and Ehrenfeld (423) 1909 Garner (84) 1909 Lehmann (135) 1912 Lehmann and Gundermann (424) 1914 Bush (288) 1923 Heinz (311) 1934 Ehrismann and Abel (314) 1934 Waser and Stähli (316)	1871 Vohl and Eulenberg (75) 1950 Molinari (159) 1951 Garner (81)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
74-90-8	Hydrocyanic acid ( <i>cont.</i> ) {hydrogen cyanide}	1938 Schöller (425, 426) 1939 Wenusch (226) 1939/40 de Campos (293) 1948 Haag and Larson (427) 1949 Fishel and Haskins (294) 1951 Garner (81) 1954 Kosak (1)	
1333-74-0	Hydrogen	1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> )	
7783-06-4	Hydrogen sulfide	1858 Vogel and Reischauer (418) 1901 Habermann (285) 1909 Garner (84) 1909 Habermann and Ehrenfeld (423) 1909 Lehmann (135) 1913 Toth (428) 1914 Bush (288) 1932 McNally (147) 1935 Wenusch (429) 1938 Schöller (426) 1938 Wenusch and Schöller (291) 1939 De Voogd and Van der Linden (292) 1939 Wenusch (226) 1949 Fishel and Haskins (294) 1951 Garner (81) 1954 Kosak (1)	1913 Oosthuizen and Shedd (170) 1950 Molinari (159)
	Hydropectin		1929 Balabucha-Popzova (86)
	Hygroscopic agents	1937 Ballenger and Johnson (430) 1937 Haag (375) 1938 Ballenger (431) 1938 Forbes and Haag (372) 1939 Ballenger (432) 1940 Haag (92) 1945 McNally <i>et al.</i> (374) 1951 Garner (81)	1934 Mulinos and Osborne (433) 1935 Greenwald (434) 1935 Mulinos and Osborne (435) 1937 Holck and Carlson (376) 1938 Wiley <i>et al.</i> (371) 1952 Küchle <i>et al.</i> (378, 436)
6917-35-7	Inositol		1930 Shmuk (263, 358) 1935 Neuberg and Kobel (271) 1951 Garner (81)
3615-82-5	myo-Inositol, hexakis(dihydrogen phosphate), calcium magnesium salt Inulase	{phytin}	1930 Shmuk (263)
9001-57-4	Invertase		1913 Oosthuizen and Shedd (170) 1913 Oosthuizen and Shedd (170) 1936 Dixon <i>et al.</i> (69) 1937 Matsumina (171) 1946 Garner (173) 1951 Garner (81) 1951 Nakai and Inaba (174) 1953 Barrett <i>et al.</i> (175) 1930 Schwaibold (437) 1935 McMurtrey (199) 1938 McMurtrey (200) 1941 McMurtrey (203) 1953 Wolff <i>et al.</i> (208)
7553-56-2	Iodine		1988 Fesca and Imai (438) 1909 Boekhout and de Vries (295) 1929 Coolhaas (439) 1933 Starkenstein and Stejskal (440) 1937 McMurtrey (441) 1938 McMurtrey and Robinson (120) 1946 LeCompte (442) 1951 Garner (81) 1953 Brown and Steinberg (329) 1950 Steinberg (260) 1953 Zacharius and Frankenburg (99)
7439-89-6	Iron	1952 Bailey (118)	1914 Noga (443) 1913 Oosthuizen and Shedd (170) 1946 Garner (173) 1953 Barrett <i>et al.</i> (175)
7004-09-3	Isoleucine		1952 Hough <i>et al.</i> (160)
	Isonicotine		1935 Wenusch and Schöller (55)
	Lactase		1936 Wenusch and Schöller (177) 1954 Kosak (1)
63-42-3	Lactose		1935 Wenusch and Schöller (55)
	Lathrein = a mixture of basic components of tobacco and its smoke (58)		1935 Wenusch and Schöller (55)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
7439-92-1	Lead	1952 Bailey (118)	1861 Creegan (444) 1921 Caddenhead and Jacques (445) 1927 Prat (446) 1929/30 Reitzel (447) 1934 Heffer <i>et al.</i> (180) 1952 Bunce (207)
8002-43-5	Lecithins		1894 Behrens (154) 1937 Shabanov (448)
7005-03-0	Leucine		1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
9005-53-2	Lignin		1934 Pyriki (331) 1951 Garner (81) 1953 Phillips and Bacot (269)
9001-62-1	Lipase		1913 Oosthuizen and Shedd (170) 1946 Garner (173) 1951 Garner (81)
7439-93-2	Lithium		1909 Ravenna and Zamorani (449) 1913 Traetta-Mosca (217) 1921 Headden (220) 1935 McMurtrey (199) 1938 McMurtrey (200) 1941 McMurtrey (203) 1950 Yamagata (334) 1951 Garner (81)
Lohitam = mixture of basic components in tobacco and its smoke (58)		1935 Wenusch and Schöller (55) 1936 Wenusch and Schöller (177) 1954 Kosak (1)	1935 Wenusch and Schöller (55)
6899-06-5	Lysine		1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
7439-95-4	Magnesium	1952 Bailey (118)	1922 Garner <i>et al.</i> (450) 1923 Garner <i>et al.</i> (325) 1928 Bailey and Anderson (281) 1931 Anderson <i>et al.</i> (451) 1935 Koenig (89) 1936 Anderson <i>et al.</i> (452) 1937 McMurtrey (441) 1941 Ward (339) 1950 Steinberg (260) 1951 Garner (81) 1953 Bortner and Hamilton (282)
69-79-4	$\alpha$ -Maltose		1934 Pyriki (331) 1941 Pyriki (453) 1942 Ward (172) 1951 Garner (81) 1952 Hough <i>et al.</i> (160)
7439-96-5	Manganese	1952 Bailey (118)	1910 Mach (454) 1934 Heffer <i>et al.</i> (180) 1938 McMurtrey and Robinson (120) 1941 Ward (339) 1951 Garner (81) 1953 Brown and Steinberg (329) 1929 Shmuk (87)
3615-41-6	L-Mannose, 6-deoxy- { $\alpha$ -rhamnose}		
8049-97-6	Melanin		1934 Shmuk and Shirokaya (455)
7439-97-6	Mercury		1934 Heffer <i>et al.</i> (180) 1936 Kincaid (456)
74-89-5	Methanamine {methylamine}	1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1954 Kosak (1)	1928 Shmuk (140)
75-50-3	Methanamine, <i>N,N</i> -dimethyl- {trimethylamine}	1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> )	1929 Gabelya and Kipriyanov (78, 181) 1936 Späth and Zajic (169) 1939 Späth and Biniecki (249)
124-40-3	Methanamine, <i>N</i> -methyl- {dimethylamine}	1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> )	1928 Shmuk (140)
107-43-7	Methanaminium, 1-carboxy- <i>N,N,N</i> - trimethyl-, inner salt {betaine}		1928 Shmuk (140) 1933 Vickery <i>et al.</i> (182) 1935 Vickery <i>et al.</i> (183) 1934 Nito and Kitamura (221) 1951 Garner (81) 1952 Willaman (457)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
74-82-8	Methane	1871 Vohl and Eulenberg (75, 76) 1909 Lehmann (135)	
67-56-1	Methanol	1909 Lehmann (135) 1927 Neuberg and Ottenstein (387) 1929 Neuberg and Kobel (388) 1929 Shmuk (458) 1931 Neuberg and Burkard (66) 1932 McNally (147) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939 Wenusch (226) 1951 Garner (81) 1954 Kosak (1)	1926 Neuberg and Kobel (68) 1929 Balabucha-Popzova (86) 1929 Neuberg and Kobel (388) 1929 Shmuk (458) 1931 Neuberg and Burkard (66) 1931 Neuberg and Scheuer (398) 1936 Lokschina (459) 1939 Shmuk (165) 1951 Garner (81)
63-68-3	<i>L</i> -Methionine		1951 Sharmon (363) 1953 Zacharius and Frankenburg (99)
7439-98-7	Molybdenum		1939 Arnon and Stout (460) 1947 Kozlowska (461) 1953 Brown and Steinberg (329)
9047-56-7	Mutase		1926 Neuberg and Kobel (68)
9033-12-9	Mutase, ketone-aldehyde		1951 Garner (81)
7440-02-0	Nickel	1952 Bailey (118)	1934 Heffer <i>et al.</i> (180) 1952 Nicholas (351) 1952 Hunter and Vergnano (462) 1952 Shira and Kodaira (463)
	Nicotine = nornicotine + anatabine		1914 Noga (443) 1928 Ehrenstein (111) 1928 Shmuk (140) 1935 Späth and Zajic (464) 1936 Späth <i>et al.</i> (465) 1939 Henry (176) 1914 Noga (443) 1894 Behrens (154) 1951 Garner (81)
14797-55-8	Nicotine Nitrate	1932 McNally (147) 1954 Kosak (1)	1885 Müller-Thurgen (153) 1894 Behrens (154) 1934 Garner <i>et al.</i> (283, 284) 1951 Garner (81)
7697-37-2	Nitric acid		1934 Chibnall <i>et al.</i> (410)
7757-79-1	Nitric acid, potassium salt		1928 Shmuk (140)
7727-37-9	Nitrogen	1877 Schwarz (297)	1929 Gabelya and Kipriyanov (78) 1935 Wenusch and Schöller (55, 56) 1950 Molinari (159)
630-03-5	Nonacosane Nonanoic acid Obelin = ammonia (58)	1952 James and Martin (82) 1935 Wenusch and Schöller (55, 56) 1936 Wenusch and Schöller (177) 1954 Kosak (1)	1935 Wenusch and Schöller (55, 56) 1937 Salisbury (414) 1937 Shmuk (413) 1944 Venkataraao <i>et al.</i> (466) 1945 Riemenschneider <i>et al.</i> (227) 1951 Garner (81)
506-21-8	9,12-Octadecadienoic acid {linoleic acid}		1937 Salisbury (414) 1944 Venkataraao <i>et al.</i> (466) 1945 Riemenschneider <i>et al.</i> (227) 1951 Garner (81)
57-11-4	Octadecanoic acid {stearic acid}		1937 Shmuk (413) 1944 Venkataraao <i>et al.</i> (466) 1945 Riemenschneider <i>et al.</i> (227) 1951 Garner (81)
463-40-1	9,12,15-Octadecatrienoic acid {linolenic acid}		1935 Shirokaya (412) 1944 Venkataraao <i>et al.</i> (466)
112-80-1	9-Octadecenoic acid {oleic acid}		1937 Salisbury (414) 1937 Shmuk (413) 1944 Venkataraao <i>et al.</i> (466) 1945 Riemenschneider <i>et al.</i> (227) 1951 Garner (81)
78-70-6	1,6-Octadien-3-ol, 3,7-dimethyl- {linalool}		1941 Sabetay <i>et al.</i> (90)
124-07-2	Octanoic acid {caprylic acid}	1871 Vohl and Eulenberg (75, 76) 1952 James and Martin (82)	1941 Sabetay <i>et al.</i> (467) 1946 Frankenburg (222)
372-75-8	<i>L</i> -Ornithine, <i>N</i> 5-(aminocarbonyl)- {citrulline}		1953 Zacharius and Frankenburg (99)
9035-73-8	Oxidase		1910 Betting (468) 1913 Oosthuizen and Shedd (170) 1928 Shmuk (140)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
9035-73-8	Oxidase (cont.)		1941 Roberts (469) 1946 Garner (173) 1951 Garner (81) 1953 Barrett <i>et al.</i> (175) 1953 Brown and Steinberg (329) 1953 Barrett <i>et al.</i> (175) 1950 Molinari (159) 1952 Jensen (161) 1901 Thorpe and Homes (417) 1946 Garner (173) 1951 Garner (81) 1884 Takayama (83) 1929 Balabucha-Popzova (86) 1931 Neuberg and Scheuer (398) 1951 Garner (81) 1953 Phillips and Bacot (269) 1903 Jetta (395) 1929 Balabucha-Popzova (86) 1929 Gabelya and Kipriyanov (181) 1931 Neuberg and Scheuer (398) 1934 Pyriki (331) 1935 Koenig (89) 1951 Garner (81) 1953 Phillips and Bacot (269) 1929 Gabelya and Kipriyanov (181) 1936 Späth and Zajic (169) 1871 Vohl and Eulenberg (75) 1929 Gabelya and Kipriyanov (78) ( <b>D</b> r) 1931 Neuberg and Burkard (66) 1952 James and Martin (82) 1954 Kosak (1)
9029-44-1	Oxidase, ascorbate		
9001-16-5	Oxidase, cytochrome c		
7782-44-7	Oxygen	1954 Kosak (1)	
79-83-4	Pantothenic acid		
	Paraffins	1893 Kissling (223)	
9025-98-3	Pectase		
9046-40-6	Pectic acid		
9000-69-5	Pectin		
	Pectinic acid		
	<i>I</i> -Peganin		
109-52-4	Pentanoic acid	{valeric acid} 1871 Vohl and Eulenberg (75, 76) 1929 Gabelya and Kipriyanov (78) ( <b>D</b> r) 1931 Neuberg and Burkard (66) 1952 James and Martin (82) 1954 Kosak (1)	1871 Vohl and Eulenberg (75) 1929 Gabelya and Kipriyanov (78) 1947 Sabetay and Panouse (470)
105-43-1	Pentanoic acid, 3-methyl-		1947 Sabetay and Panouse (470)
96-22-0	3-Pantanone	1927 Neuberg and Ottenstein (387) 1931 Neuberg and Burkard (66) 1954 Kosak (1)	1935 Neuberg and Kobel (271)
116001-96-8	Pentosan		
	Pentose		
	Pentosenucleic acid		
	Peptide		
9003-99-0	Peroxidase		
85-01-8	Phenanthrene	1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1954 Kosak (1)	1903 Jetta (395) 1914 Garner <i>et al.</i> (100) 1935 Koenig (89) 1953 Phillips and Bacot (269) 1931 Neuberg and Scheuer (398) 1934 Pyriki (331) 1951 Garner (81) 1953 Silberger and Skoog (364) 1937 Vickery <i>et al.</i> (214) 1951 Garner (81) 1910 Betting (468) 1937 Matsumina (171) 1951 Garner (81) 1951 Nakai and Inaba (174) 1953 Barrett <i>et al.</i> (175) 1953 Brown and Steinberg (329)
	Phenanthrene derivative		
108-95-2	Phenol	1871 Vohl and Eulenberg (75, 76) 1914 Bush (288) 1936 Bogen (150) 1936 Molinari (224) 1940 Haag (92) 1947 Ikeda (215) 1952 Rayburn (471) 1953 Rayburn <i>et al.</i> (472) 1954 Kosak (1)	1871 Vohl and Eulenberg (75) 1939 Wenusch (226) 1950 Molinari (159) 1953 Rayburn <i>et al.</i> (472)
90-05-1	Phenol, 2-methoxy-	1952 Rayburn (471)	1939 Wenusch (226)
	{guaiacol}	1953 Rayburn <i>et al.</i> (472)	1953 Rayburn <i>et al.</i> (472)
97-54-1	Phenol, 2-methoxy-4-(1-propenyl)- {isoeugenol}		1946 Frankenburg (222)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
97-53-0	Phenol, 2-methoxy-4-(2-propenyl)-{eugenol}		1941 Sabetay <i>et al.</i> (467) 1946 Frankenburg (222)
1319-77-3	Phenol, methyl-{cresol}	1936 Bogen (150)	
95-48-7	Phenol, 2-methyl-{o-cresol}	1952 Rayburn (471) 1953 Rayburn <i>et al.</i> (472)	
108-39-4	Phenol, 3-methyl-{m-cresol}	1952 Rayburn (471) 1953 Rayburn <i>et al.</i> (472)	1953 Rayburn <i>et al.</i> (472)
106-44-5	Phenol, 4-methyl-{p-cresol}		1934 Shmuk (391)
	Phenols, structure unspecified	1954 Kosak (1)	1934 Shmuk and Shirokaya (455)
63-91-2	Phenylalanine		1953 Pearse and Novellie (98)
14265-44-2	Phosphate		1953 Zacharius and Frankenburg (99)
	Phosphatase		1894 Behrens (154)
			1935 Koenig (89)
7803-51-2	Phosphine	1898 Cavalli (473)	1946 Garner (173)
56-38-2	Phosphorothioic acid, O,O-diethyl O-(4-nitrophenyl) ester {Parathion®}		1951 Garner (81)
7723-14-0	Phosphorus		1928 Bailey and Anderson (281)
	Phytosterol	1954 Kosak (1)	1941 Ward (339)
	Pigments		1950 Steinberg (260)
110-89-4	Piperidine		1951 Garner (81)
535-75-1	2-Piperidinecarboxylic acid {pipecolic acid}		1953 Bortner and Hamilton (282)
	Poikiline = 1-Butanone, 4-amino-1-(3-pyridyl)-	1954 Kosak (1)	1913 Traetta-Mosca (474)
7440-09-7	Potassium	1952 Bailey (118)	1935 Kobel and Neuberg (235)
			1935 Schürch and Winterstein (392)
			1937 Shmuk (413)
147-85-3	Proline		1935 Koenig (89)
			1939 Nagel (326)
78-98-8	Propanal, 2-oxo-{pyruvaldehyde; methylglyoxal}		1936 Späth and Zajic (169)
141-82-2	Propanedioic acid {malonic acid}		1953 Zacharius and Frankenburg (99)
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy- {citric acid}	1939 Roffo (70, 71, 72, 73) ( <b>D</b> )	1948 Wenusch (279)
			1923 Garner <i>et al.</i> (325)
			1928 Bailey and Anderson (281)
			1950 Steinberg (260)
			1951 Garner (81)
			1953 Bortner and Hamilton (282)
			1953 Wolff <i>et al.</i> (208)
			1952 Frankenburg and Gottscho (97)
			1953 Pearse and Novellie (98)
			1953 Zacharius and Frankenburg (99)
			1929 Kobel and Scheuer (475)
			1953 Wada and Kobashi (94)
813-94-5	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, calcium salt		1884 Takayama (83)
3344-18-1	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, magnesium salt		1894 Behrens (154)
6100-05-6	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, potassium salt		1904 Kissling (265)
			1924 Shmuk (85)
			1930 Shmuk (357)
			1930 Shmuk and Piatnicki (93)
			1931 Yamafuji (88)
			1935 Koenig (89)
			1939 Shmuk (165)
			1951 Bacon <i>et al.</i> (267)
			1952 Bacon <i>et al.</i> (268)
			1953 Phillips and Bacot (269)
			1953 Wright and Burton (270)
			1937 Pucher <i>et al.</i> (266)
			1951 Garner (81)
			1937 Pucher <i>et al.</i> (266)
			1951 Garner (81)
			1937 Pucher <i>et al.</i> (266)
			1951 Garner (81)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
56-81-5	1,2,3-Propanetriol A tobacco additive applied to and identified in tobacco and its smoke; in 1964, it was identified as a component of additive-free, uncased tobacco (478)	{glycerol} 1938 Forbes and Haag (372) 1945 McNally <i>et al.</i> (374) 1951 Garner (81) 1954 Kosak (1)	1937 Holck and Carlson (376) 1937 Shmuk (413) 1945 McNally <i>et al.</i> (374) 1946 Frankenburg (222)
79-09-4	Propanoic acid	{propionic acid} 1871 Vohl and Eulenberg (75, 76) 1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1952 James and Martin (82)	1924 Shmuk (85) 1929 Gabelya and Kipriyanov (78) 1929 Shmuk (87)
50-21-5	Propanoic acid, 2-hydroxy- (lactic acid) 1-Propanone, 1-(3-pyridinyl)- (pyridyl ethyl ketone)	1919 Kissling (477) 1935 Schöller (478) 1939 Wenusch (226) 1954 Kosak (1)	1953 Wada and Kobashi (94) 1928 Shmuk (140)
67-64-1	2-Propanone	{acetone} 1937 Wenusch (409)	1871 Vohl and Eulenberg (75)
107-02-8	2-Propenal	{acrolein} 1932 McNally (147) 1936 Bogen (150) 1937 Ribeiro (479) 1954 Kosak (1)	
331-39-5	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-	{caffeic acid} 1939 Shmuk (165)	1894 Behrens (154) 1929 Shmuk (87) 1930 Shmuk (357, 480) 1930 Shmuk and Piatnicki (93) 1935 Koenig (89) 1939 Shmuk (165) 1951 Garner (81)
78990-62-2	Protease		1913 Oosthuizen and Shedd (170) 1951 Garner (81)
	Protein		1886 Mendel (481) 1894 Behrens (154) 1930 Smirnov and Izvoshchikov (155) 1933 Vickery <i>et al.</i> (182) 1935 Koenig (89) 1935 Vickery <i>et al.</i> (183) 1951 Garner (81)
20-73-0	1 <i>H</i> -Purine		1950 Steinberg (260)
73-24-5	1 <i>H</i> -Purin-6-amine	{adenine}	1931 Yamafuji (88) 1933 Vickery <i>et al.</i> (182) 1935 Vickery <i>et al.</i> (183) 1934 Nito and Kitamura (221) 1951 Garner (81)
73-40-5	6 <i>H</i> -Purin-6-one, 2-amino-1,7-dihydro-	{guanine}	1935 Vickery <i>et al.</i> (183) 1934 Nito and Kitamura (221) 1951 Garner (81)
69-93-2	1 <i>H</i> -Purine-2,6,8(3 <i>H</i> )-trione, 7,9-dihydro-	{uric acid} 1937 Wenusch (342) 1954 Kosak (1)	
129-00-0	Pyrene	1953 Cooper and Lindsey (179)	1871 Vohl and Eulenberg (75)
110-86-1	Pyridine	1871 Vohl and Eulenberg (75, 76) 1880 LeBon (127) 1894/95 Brunton and Tunnicliffe (482) 1899 Thoms (128) 1900 Thoms (129) 1903 Pontag (131) 1904 Thoms (277) 1906 Warburg (483) 1908 Lee (133) 1908 Lehmann (134) 1909 Lehmann (135) 1910 Toth and Krampera (136) 1914 Bush (288) 1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1932 McNally (147) 1933 Pfyl (148) 1935 Bastedo (187) 1936 Bogen (150) 1936 Preiss (151, 152, 156) 1937 Bradford <i>et al.</i> (79) 1937 Pyatnitskii and Kashirin (484)	1900 Eulenburg (486) 1928 Shmuk (140) 1929 Gabelya and Kipriyanov (78) 1933 Dobrin (487) 1936 Preiss (156) 1948 Pyriki (166)

Table 1. (cont.)

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
110-86-1	Pyridine (cont.)	1939 Dittmar (162, 164) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939 Wenusch (226) 1939/40 de Campos (293) 1942 Hofmann (485) 1948 Pyriki (166) 1951 Garner (81) 1954 Kosak (1)	
27175-64-0	Pyridine, dimethyl-	{lutidine} 1871 Vohl and Eulenber (75) 1932 McNally (147) 1908 Lehmann (134) 1954 Kosak (1)	1871 Vohl and Eulenber (75) 1928 Shmuk (140)
108-48-5	Pyridine, 2,6-dimethyl-	{2,6-lutidine} 1932 McNally (147)	
1333-41-1	Pyridine, methyl-	{picoline} 1871 Vohl and Eulenber (75, 76) 1908 Lehmann (134) 1914 Bush (288) 1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1954 Kosak (1)	1871 Vohl and Eulenber (75) 1928 Shmuk (140) 1929 Gabelya and Kipriyanov (78)
109-06-8	Pyridine, 2-methyl-	{2-picoline} 1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1932 McNally (147) 1944 Woodward <i>et al.</i> (488)	1928 Shmuk (140)
29611-84-5	Pyridine, trimethyl-	{collidine} 1871 Vohl and Eulenber (75, 76) 1908 Lee (133) 1908 Lehmann (134) 1954 Kosak (1)	1871 Vohl and Eulenber (75) 1928 Shmuk (140)
108-75-8	Pyridine, 2,4,6-trimethyl-	{2,4,6-collidine} 1932 McNally (147)	
532-12-7	Pyridine, 3-(3,4-dihydro-2H-pyrrrol-5-yl)-	{/-myosmine} 1933 Wenusch and Schöller (53) 1935 Wenusch and Schöller (55) 1936 Wenusch and Schöller (177) 1939 Wenusch (226) 1954 Kosak (1)	1934 Wenusch and Schöller (54) 1936 Späth <i>et al.</i> (465) 1944 Woodward <i>et al.</i> (489) 1946 Frankenburg (250) 1952 Frankenburg and Gottscho (97) 1953 Tso and Jeffrey (117) 1946 Frankenburg (250) 1949 Swain <i>et al.</i> (490) 1952 Willaman (457) 1937 Späth and Kesztler (254) 1946 Frankenburg (250) 1953 Sadykov <i>et al.</i> (491)
24380-92-5	Pyridine, 3-(1-methyl-2-piperidinyl)-, (S)- {N-methylanabasine}	Pyridine, 3-(3,4-dihydro-1-methyl-2H-pyrrrol-5-yl)- {N-methylmyosmine}	
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-	{/-nicotine} 1826 Unterdorden (365) ( <b>D<sub>r</sub></b> ) 1843 Melsens (492) 1844 Melsens (493) 1871 Vohl and Eulenber (75, 76) 1872 Heubel (494) 1882 Kissling (495, 496) 1892 Lowenthal (497) 1898 Kissling (498) 1899 Thoms (128) 1900 Thoms (129) 1901 Habermann (285) 1902 Ludwig (499) 1903 Pontag (131) 1904 Bamberger (500) 1904 Paschkis (501) 1904 Schmidt (502) 1905 Theodorovits (503) 1906 Rattner (504) 1906 Warburg (483) 1907 Bitter (505) 1907 Kuhles (506) 1908 Lee (133) 1908 Noda (507) 1908 Biederbeck (132) 1908 Toth (508) 1909 Habermann and Ehrenfeld (423) 1909 Toth (509) 1909 Weger (510) 1910 Toth and Krampera (136)	1807 Cerioli (524) 1809 Vauquelin (264) 1822 Hermbstädt (525) 1826 Unterdorden (365) 1828 Posselt and Reimann (526) 1842 Barral (527) 1842 Ortigosa (528) 1843 Melsens (492) 1847 Barral (529) 1852 Vleminckx (530) 1867 Huber (531) 1868 Jullien (532) 1969 Kopff (533) 1873 Weidel (534) 1877 Von Laiblin (535) 1879 Von Laiblin (536) 1880 Prescott (537) 1884 Takayama (83) 1886 Liebrecht (538) 1892 Gautier (539) 1893 Blau (540) 1893 Étard (541) 1893 Pinner (542, 543) 1894 Behrens (154) 1894 Étard (544) 1895 Pinner (545) 1897 Pictet and Genequand (546) 1904 Kissling (265) 1904 Pictet and Rotschy (547)

Table 1. (cont.)

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>Dr</b> ), destructive ( <b>D</b> )]	Tobacco
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- ( <i>l</i> -nicotine) ( <i>cont.</i> )	1911 Fröhlich (511) 1911 Von Frankl-Hochwart (512) 1912 Anonymous (138, 139, 513) 1914 Bush (288) 1914 Favenger (514) 1915 Kütt (515) 1916 Toth and Dangelmajer (516) 1919 Silberbauer (517) 1919 Van Leeuwen (518) 1920 Asherson (519) 1920 Hahn and Langer (520) 1920 Hirschfelder <i>et al.</i> (521) 1921 Bogner (522) 1922 Popp and Contzen (549) 1923 Baumberger (523) 1923 Heinz (311) 1923 Rhode (550) 1927 Dixon (561) 1927 Pfyl and Schmitt (554) 1927 Winterstein and Aronson (562) 1927/28 Schöller (563) 1927/28 Wenusch (564) 1928 Wenusch (565) 1928 Winterstein and Aronson (566) 1929 Bogen (141) 1929 Gabelya and Kipriyanov (78) ( <b>Dr</b> ) 1929 Wenusch (567, 568, 569, 570) 1929 Winterstein and Aronson (571, 572) 1930 Bodnár (573, 574) 1930 Bolm (575) 1930 Braun (613, 614) 1930 Heiduschka (617) 1930 Storp (576) 1930 Wenusch (577, 578) 1931 Barta and Toole (579) 1931 Ehrismann (580) 1931 Frank (581) 1931 Hahn and Ehrismann (582) 1931 Herrmann (583) 1931 Kovalenko (584) 1931 Pyriki (585, 586) 1931 Van Druten (587) 1931 Wenusch (588, 589, 590) 1932 Barta and Toole (145, 146) 1932 Heiduschka and Post (591) 1932 Kissling (592, 593) 1932 Margasinski (594) 1932 McNally (147) 1932 Michalowsky (595) 1932 Molinari (596) 1932 Nagy (597, 598) 1932 Paffgen (599) 1932 Post (621) 1932 Pyriki (600, 601, 602) 1932 Schaarschmidt <i>et al.</i> (603) 1932 Schlossmann and Schlesinger (604) 1932 Shmuk <i>et al.</i> (605) 1932 Skumburdis and Kissling (606) 1932 Traube (607) 1932 Van Druten (608) 1932 Waser and Stähli (609, 610) 1933 Hofmann (623) 1933 Nagy and Dickman (611, 612) 1933 Pfyl (67, 148) 1933 Pyriki (654) 1933 Schlossmann (655) 1933 Stähli (656) 1933 Starkenstein and Stejskal (440) 1933 Toole (624) 1934 Graham (657) 1934 Koperina (658)	1904 Schmidt (502) 1908 Lee (133) 1909 Garner (84) 1909 Weger (510) 1912 Chuard and Mellet (548) 1914 Bush (288) 1922 Popp and Contzen (549) 1923 Rhode (550) 1927 Heiduschkska and Muth (551, 552, 553) 1927 Pfyl and Schmitt (554) 1927 Winterstein and Trier (555) 1928 Harlan and Hixon (556) 1928 Popp (557) 1928 Shmuk (140) 1929 Heiduschkska and Muth (558, 559, 560) 1930 Braun (613, 614) 1930 Faitelowitz (615) 1930 Harlan and Hixon (616) 1930 Heiduschka (617) 1930 Windus and Marvel (618) 1931 Auprecht (619) 1931 Hukusima and Oika (397) 1931 Tonn (620) 1932 Post (621) 1932 Waser (622) 1933 Dobrin (487) 1933 Hofmann (623) 1933 Toole (624) 1936 Cuvelier (168) 1935 Koperina and Kalibab (625) 1935 Späth and Kesztler (626) 1935 Wenusch (627) 1935 Wenusch and Schöller (55) 1936 Busbey and McIndoo (628, 629) 1936 Dixon <i>et al.</i> (69) 1936 Malaquin (630) 1936 McIndoo <i>et al.</i> (631, 632, 633) 1937 Bailey and Petre (682) 1937 Späth and Kainrath (634) 1937/38 Mulinos and Cockrill (635) 1938 Molinari (636) 1939 Avens and Pearce (637) 1939 Shmuk (165) 1939 Shmuk and Borozdina (638) 1940 Reif (639) 1942 Dawson (640) 1942 Haag and Larson (641) 1943 Pyriki (642) 1944 Larson and Haag (643) 1945 Clemo and Swann (644) 1945 Haag <i>et al.</i> (645) 1945 Larson and Haag (646) 1946 Frankenburg (250) 1948 Brice (647) 1948 Dawson (648) 1948 Griffith and Jeffrey (649) 1948 Pyriki (166) 1948 Shmuk (253) 1948 Wenusch (279) 1948 Willits (650) 1949 Porter <i>et al.</i> (651) 1949 Swain <i>et al.</i> (652) 1950 Dawson (653) 1950 Willits <i>et al.</i> (696) 1951 Garner (81) 1952 Weybrew <i>et al.</i> (697) 1953 Bortner and Hamilton (282) 1953 Cundiff and Markunas (698) 1953 Sadykov <i>et al.</i> (491)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> r), destructive ( <b>D</b> )]	Tobacco
54-11-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- (cont.)	{/ <i>-nicotine}</i> 1934 Koperina and Shageeva (659) 1934 Nagy and Barta (660) 1934 Preiss (661) 1934 Pyriki (662, 663, 664) 1934 Waser and Stähli (665) 1934 Wenusch (666, 667, 668, 669, 670) 1934 Wulfert (671, 672) 1935 Bastedo (187) 1935 Bodnár <i>et al.</i> (673, 674) 1935 Jensen and Haley (675) 1935 Koperina and Kalibab (625) 1935 Preiss (676) 1935 Pyriki (677, 678) 1935 Schürch and Winterstein (392) 1935 Wenusch (627) 1935 Wenusch and Schöller (55) 1936 Bogen (150) 1936 Cuvelier (168) 1936 Heiduschka (679) 1936 Malaquin (630) 1936 Preiss (152) 1936 Wenusch (680, 681) 1936 Wenusch and Schöller (57) 1937 Bailey and Petre (682) 1937 Bradford <i>et al.</i> (79) 1937 Derr <i>et al.</i> (683) 1937 Pierce (684) 1937 Pyriki (685) 1937 Wenusch (409, 686, 687) 1938 Justin-Müller (688) 1938 Molinari (636) 1938 Nagy (689) 1939 Wenusch (226) 1939/40 Haag (690) 1940 Haag (92) 1940 Haag and Neale (691) 1940 Haag <i>et al.</i> (692) 1940 Wenusch (693, 694, 695) 1941 Hofmann (485) 1941 Pierce (699) 1941 Wenusch (700) 1942 Wenusch (701, 702, 703, 704) 1943 Pyriki (642, 705) 1944 Larson and Haag (643) 1944 Woodward <i>et al.</i> (489) 1944 Woodward <i>et al.</i> (488, 706) 1945 Larson and Haag (646) 1946 McCormick and Smith (707) 1947 Finnegan <i>et al.</i> (708) 1948 Pyriki (166) 1948 Shmuk (253) 1948 Sollmann (709) 1949 Dabrowska (710) 1949 Ling and Wynn Parry (711) 1949 Wenusch (712) 1950 Rayburn (713) 1950 Willits <i>et al.</i> (696) 1951 Garner (81) 1951 Marchand and Renard (714) 1951 Vettors (715) 1952 Bailey (118) 1952 Greenberg <i>et al.</i> (716) 1952 Larsen (167) 1952 Rakieten <i>et al.</i> (362) 1953 Cundiff and Markunas (698) 1953 Staub and Furrer (717, 718) 1953 Wahl and Heil (719) 1953 Wolman and Stark (720, 721) 1954 Kosak (1)	1953 Tso and Jeffrey (117) 1953 Wright and Burton (270)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
2820-55-5	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, 1-oxide, (S)-{nicotine N-oxide}	1950 Rayburn <i>et al.</i> (722)	1885 Pinner (723) 1950 Rayburn <i>et al.</i> (722) 1952 Frankenburg and Gottscho (97) 1953 Tso and Jeffrey (117)
	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, organic acid salts	1937 Wenusch (724)	1809 Vauquelin (264) 1822 Hermbstädt (525) 1823 Hermbstädt (725) 1939 Shmuk (165)
487-19-4	Pyridine, 3-(1-methyl-1 <i>H</i> -pyrrol-2-yl)-{nicotyrine}	1935 Wenusch and Schöller (55) 1939 Wenusch (226) 1954 Kosak (1)	1898 Pictet and Crépieux (726) 1928 Wibaut and Overhoff (727) 1932 Wibaut and Hackman (728) 1935 Wenusch (729) 1937 Späth and Kesztler (254) 1946 Frankenburg (250)
494-52-0	Pyridine, 3-(2-piperidinyl)-, (S)-{/anabasine}	1933 Haag (730)	1931 Ehrenstein (111) 1931 Smith (731) 1932 Smith (732) 1935 Olchansky (733) 1935 Smith (734) 1937 Späth and Kesztler (251) 1939 Shmuk and Borozdina (638) 1942 Smith and Smith (735) 1946 Dubinin and Chelintsev (736) 1946 Frankenburg (250) 1948 Matveev (737) 1048 Sadykov <i>et al.</i> (738) 1948 Shmuk (253) 1949 Porter <i>et al.</i> (651) 1951 Garner (81) 1953 Sadykov <i>et al.</i> (491) 1953 Tso and Jeffrey (117)
	Pyridine, 3-(2-piperidinyl)-, 6-oxo-{6-oxoanabasine}		1939 Henry (176)
494-97-3	Pyridine, 3-(2-pyrrolidinyl)-, (S)-{/nornicotine}	1944 Larson and Haag (643) 1945 Larson and Haag (646)	1928 Shmuk (140) 1935 Späth and Zajic (739) 1936 Wenusch (740) 1936 Späth <i>et al.</i> (741) 1937 Späth and Kesztler (251) 1944 Larson and Haag (643) 1945 Larson and Haag (646) 1946 Frankenburg (250) 1948 Brice (647) 1948 Dawson (648) 1948 Shmuk (253) 1949 Swain <i>et al.</i> (652) 1951 Garner (81) 1952 Weybrew <i>et al.</i> (697) 1953 Tso and Jeffrey (117) 1953 Wright and Burton (270)
494-98-4	Pyridine, 3-(1 <i>H</i> -pyrrol-2-yl)-{nornicotyrine}		1946 Frankenburg (250)
	Pyridine bases	1932 McNally (147) 1954 Kosak (1)	
98-92-0	3-Pyridinecarboxamide {nicotinamide}		1953 Tso and Jeffrey (117)
100-54-9	3-Pyridinecarbonitrile {nicotinonitrile}	1944 Woodward <i>et al.</i> (488)	
59-67-6	3-Pyridinecarboxylic acid {nicotinic acid}	1944 Woodward <i>et al.</i> (488)	1879 Von Laiblin (536) 1938 Chen <i>et al.</i> (742) 1952 Gottscho and Frankenburg (743) 1953 Tso and Jeffrey (117)
289-95-2	Pyrimidine {1,3-diazine}		1950 Steinberg (260)
107-49-3	Pyrophosphoric acid, tetraethyl ester {TEPP} a metabolite of phosphorus-containing pesticides		1951 Vinzant (60)
109-97-7	Pyrrole	1909 Lehmann (135) 1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1939 Roffo (70, 71, 72, 73) ( <b>D</b> ) 1939/40 de Campos (293) 1954 Kosak (1)	1928 Shmuk (140) 1937 Fromm (157)

Table 1. (cont.)

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
	Pyrroles, structure unspecified	1932 McNally (147) 1937 Fromm (157) 1954 Kosak (1)	
123-75-1	Pyrrolidine	1909 Lehmann (135)	1908 Pictet and Court (110) 1928 Shmuk (140)
120-94-5	Pyrrolidine, <i>N</i> -methyl-	1932 McNally (147) 1954 Kosak (1)	1905 Pictet (744) 1908 Pictet and Court (110) 1928 Shmuk (140) 1939 Späth and Biniecki (249)
91-22-5	Quinoline	1929 Gabelya and Kipriyanov (78) ( <b>D<sub>r</sub></b> ) 1944 Woodward <i>et al.</i> (488)	
7440-14-4	Radium		1937 Drobkov (103)
10043-92-2	Radon		1937 Drobkov (103)
	Reconstituted tobacco sheet		1857 Von der Porten (745)
9037-80-3	Reductase		1913 Oosthuizen and Shedd (170) 1946 Garner (173) 1951 Garner (81)
	Resin	1893 Kissling (223) 1932 Koperina (746) 1934 Koperina (747) 1935 Wenusch (278, 748) 1937 Wenusch (342, 749) 1949 Dabrowska (710) 1950 Mazzulli (750) 1954 Kosak (1)	1904 Kissling (265) 1914 von Degrazia (751) 1924 Shmuk (85) 1931 Hukusima and Oika (397) 1935 Shirokaya (412) 1938 Gaertner (752) 1940 Pyriki (753)
	Resin acids	1893 Kissling (223) 1954 Kosak (1)	
	Resinol		1924 Shmuk (85)
3615-41-6	Rhamnose		1936 Neuberg and Kobel (233)
	Rhoeadin		1936 Späth and Zajic (169)
83-88-5	Riboflavin		1952 Jensen (161)
7440-17-7	Rubidium		1862/63 Grandea (335) 1950 Yamagata (334)
	Saccharides	1940 Dittmar (754)	1940 Dittmar (754) 1941 Pyriki (453)
129990-04-1	Saponin (from tobacco)		1935 Kobel and Neuberg (235)
7782-49-2	Selenium		1933 Martin and Trelease (755)
6898-95-9	Serine		1952 Frankenburg and Gottscho (97) 1953 Pearse and Novellie (98)
7631-86-9	Silica		1953 Zacharius and Frankenburg (99)
7440-21-3	Silicon	1952 Bailey (118)	1894 Behrens (154) 1925 MacIntyre <i>et al.</i> (756) 1928 Bailey and Anderson (281) 1951 Garner (81)
7440-22-4	Silver		1936 Johnson (350)
	$\alpha$ -Socratine = {nicotyrine + 2,3'-bipyridine + nicotinic acid + nornicotine + anatabine} (58)	1919 Kissling (477) 1933 Wenusch and Schöller (53) 1935 Wenusch and Schöller (55) 1936 Wenusch and Schöller (177) 1954 Kosak (1)	1934 Wenusch and Schöller (54) 1935 Wenusch and Schöller (55)
	$\beta$ -Socratine = {nicotyrine + 2,3'-bipyridine + nicotinic acid + nornicotine + anatabine} (58)	1919 Kissling (477) 1933 Wenusch and Schöller (53) 1935 Wenusch and Schöller (55) 1936 Wenusch and Schöller (177) 1954 Kosak (1)	1934 Wenusch and Schöller (54) 1935 Wenusch and Schöller (55)
	$\gamma$ -Socratine = <i>l</i> -nornicotine (58)	1919 Kissling (477) 1933 Wenusch and Schöller (53) 1935 Wenusch and Schöller (55) 1936 Wenusch and Schöller (177) 1954 Kosak (1)	1928 Shmuk (140) 1934 Wenusch and Schöller (54) 1935 Wenusch and Schöller (55)
7440-23-5	Sodium	1952 Bailey (118)	1928 Bailey and Anderson (281) 1938 Gaertner (752) 1950 Frankenburg (757) 1950 Yamagata (334) 1951 Garner (81) 1953 Wolff <i>et al.</i> (208)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D<sub>r</sub></b> ), destructive ( <b>D</b> )]	Tobacco
9005-25-8	Starch		1885 Müller-Thurgen (153) 1894 Behrens (154) 1914 Garner <i>et al.</i> (100) 1934 Pyriki (331) 1935 Koenig (89) 1942 Ward (172) 1951 Bacon <i>et al.</i> (267) 1951 Garner (81) 1952 Bacon <i>et al.</i> (268) 1952 Willaman (457) 1953 Phillips and Bacot (269)
7440-24-6	Strontium	1952 Bailey (118)	1897 Trimble (758) 1921 Headden (220)
57-50-1	Sugar		1885 Müller-Thurgen (153) 1914 Garner <i>et al.</i> (100) 1934 Pyriki (331) 1935 Koenig (89) 1936 Dixon <i>et al.</i> (69) 1951 Garner (81)
8013-17-0	Sugar, invert		1951 Garner (81)
14808-79-8	Sulfate		1923 Garner <i>et al.</i> (325) 1935 Koenig (89) 1951 Garner (81)
7704-34-9	Sulfur		1914 Shedd (759) 1928 Bailey and Anderson (281) 1934 Heiserich (404) 1937 McMurtrey (441) 1941 Ward (339) 1951 Garner (81)
71010-48-5	$\alpha$ -Tabacenic acid { $\alpha$ -tobacco acid}		1914 von Degrazia (751) 1924 Shmuk (85) 1934 Shmuk and Shirokaya (455) 1951 Garner (81)
71010-46-3	$\beta$ -Tabacenic acid { $\beta$ -tobacco acid}		1914 von Degrazia (751) 1924 Shmuk (85) 1934 Shmuk and Shirokaya (455) 1951 Garner (81)
71010-47-4	$\gamma$ -Tabacenic acid { $\gamma$ -tobacco acid}		1914 von Degrazia (751) 1924 Shmuk (85) 1934 Shmuk and Shirokaya (455) 1951 Garner (81)
1401-55-4	Tannins	{tannic acid}	1894 Behrens (154) 1924 Shmuk (85) 1935 Koenig (89) 1953 Phillips and Bacot (269)
494-04-2	3,2':4',3"-Terpyridine	{nicotelline}	1901 Pictet and Rotschy (108) 1914 Noga (443) 1928 Shmuk (140)
544-63-8	Tetradecanoic acid	{myristic acid}	1944 Venkataraao <i>et al.</i> (466)
7440-28-0	Thallium		1932 McMurtrey (760) 1934 Heffer <i>et al.</i> (180) 1938 Van Der Veen (761) 1940 Shear and Ussery (762) 1952 Jensen (161)
59-43-8	Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride {thiamine}		1938 Schöller (426) 1954 Kosak (1)
463-56-9	Thiocyanic acid		1938 Schöller (426) 1950 Molinari (159)
505-14-6	Thiocyanogen		1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
72-19-5	Threonine		1934 Heffer <i>et al.</i> (180) 1941 Ward (339)
7440-31-5	Tin		1941 Ward (339)
7440-32-6	Titanium	1952 Bailey (118)	1913 Traetta-Mosca (217) 1921 Headden (220) 1941 Ward (339) 1898 Cavalli (764)
	Tobacco, combustion products		

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>Dr</b> ), destructive ( <b>D</b> )]	Tobacco
	Tobacco, general		1793 Murray (765) 1895 Carpenter (766) 1905 Kissling (767) 1907 Lehmann (768) 1908 Kissling (769) 1910 Kissling (770) 1913 Traetta-Mosca (474) 1919 Kissling (477) 1930 Ehrenstein (771) 1930 Gabelya and Kipriyanov (772) 1931 Shmuk (773) 1934 Garner <i>et al.</i> (283) 1935 Waser (774) 1935 Wenusch (775) 1936 Brückner (332) 1937 Schöller and Molinari (776) 1938 Brandt (777, 778) 1939 Gaertner (158) 1940 Bodnár and Votisky (779) 1940 Smirnov <i>et al.</i> (780) 1941 Palfray <i>et al.</i> (781) 1943 Pyriki (782) 1950 Pyriki (783)
	Tobacco smoke, general		1923 Baumberger (784) 1930 Gabelya and Kipriyanov (772) 1931 Koperina (785) 1933 Kurilo (786) 1934 Tschebull (787) 1937 Pyriki (788) 1937 Rohrbach (789) 1937 Wenusch (724, 790) 1938 Brandt (777, 778) 1939 Smirnov and Sirotenko (791) 1939 Wenusch (792) 1940 Bodnár and Votisky (779) 1941 Hillsman (793) 1941 Matthews (794) 1946 Fromm (795) 1948 Matthews (796) 1951 Laskowski (797) 1953 Warner and Hobbs (798)
638-68-6	Triacontane		1937 Shmuk (413)
	17-Tritriacontanone		
	Triglycerides		1944 Venkatarao <i>et al.</i> (466)
73-22-3	Tryptophan	1935 Schürch and Winterstein (392) 1954 Kosak (1)	1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
	Tyrosinase		1953 Barrett <i>et al.</i> (175)
60-18-4	Tyrosine		1952 Frankenburg and Gottscho (97) 1953 Pearse and Novellie (98) 1953 Zacharius and Frankenburg (99)
112-37-8	Undecanoic acid	1952 James and Martin (82)	
7440-61-1	Uranium		1937 Drobkov (103) 1949 Drobkov (799)
97-59-6	Urea, (2,5-dioxo-4-imidazolidinyl)- {allantoin}		1933 Vickery <i>et al.</i> (182) 1935 Vickery <i>et al.</i> (183) 1946 Garner (173) 1951 Garner (81)
9002-13-5	Urease		1953 Barrett <i>et al.</i> (175)
	Uronic acids		1935 Kobel and Neuberg (235) 1953 Phillips and Bacot (800)
7004-03-7	Valine		1952 Frankenburg and Gottscho (97) 1953 Zacharius and Frankenburg (99) 1941 Ward (339)
7440-62-2	Vanadium		1884 Takayama (83)
7732-18-5	Water	1857 Vogel (123) 1929 Gabelya and Kipriyanov (78) ( <b>Dr</b> ) 1930 Braun (613, 614) 1932 McNally (147) 1940 Haag (92)	1936 Dixon <i>et al.</i> (69) 1948 Barnhardt (801)

**Table 1. (cont.)**

CAS No.	Name (per CA Collective Index)	Tobacco smoke and/or tobacco distillate [dry ( <b>D</b> <sub>r</sub> ), destructive ( <b>D</b> )]	Tobacco
7440-66-6 Zinc			1926 Sommer and Lipman (256) 1934 Heffer <i>et al.</i> (180) 1938 McMurtrey and Robinson (120) 1941 Ward (339) 1951 Garner (81) 1952 Nicholas (351)

While noting that both ammonia and nicotine were previously identified as tobacco smoke components, KOSAK elected not to list references to them because their number of references, in his opinion, was too numerous to list. Also the number of references to carbon dioxide and carbon monoxide were limited by KOSAK. Table 1 lists many of the pre-1954 references to ammonia, nicotine, carbon dioxide, and carbon monoxide in tobacco and/or tobacco smoke. Included in Table 1 are several pesticide residues, e.g., arsenic/arsenic oxide, Toxaphene®, Lindane®, Parathion®, DDT, and TEPP (tetraethyl pyrophosphate), plus several pesticide residue degradation products, e.g., *o,p'*-DDD and *m,p'*-DDD, identified by VINZANT in 1951 (60). Listed in Table 1 are a few compounds used as flavorants on tobacco products, most notably menthol which, however, occurs naturally in trace amounts in several tobacco types. Table 1 also cites numerous references to pre-1954 studies of a general nature. These include references to arsenical insecticides, alkaloids, aliphatic acids, aliphatic hydrocarbons amino acids, bases, tobacco distillates, tobacco fats, chlorophyll degradation products, enzymes (general information), hydrocarbons, hygroscopic agents, paraffins, pigments, sugars, tobacco combustion products, tobacco (general), tobacco smoke (general), and triglycerides. These items are not included in the total of 325. Among metals, nonmetals, and ions, KOSAK in his 1954 catalogue listed only arsenic plus four ions as smoke components and KOSAK questioned the identification of each of the latter. Examination of Table 1 reveals that over 50 metals, nonmetals, and ions were identified in tobacco prior to late 1953. However, it was post-1953 when a concerted effort was made to determine the transfer of numerous metals from tobacco to tobacco smoke during the smoking process, e.g., the 1957 study by COGBILL and HOBBS (61). The references for numerous additional studies of this type are listed by RODGMAN and PERFETTI [see Chapter XX in (2)]. Among the metals and nonmetals in tobacco smoke, the one much studied pre-1954 was of course arsenic (As). Between 1917 and 1951, the As level in tobacco rose from about 12 to 57 µg/g (62). As, usually considered as As<sub>2</sub>O<sub>3</sub> in tobacco, was removed from tobacco agronomy in 1952.

While our REFERENCES section contains numerous references on the isolation, identification, and quantitation of many of the tobacco components listed in Table 1, also available are literally hundreds of pre-1954 references on studies that dealt with the effect of several components in tobacco smoke, e.g., nicotine, carbon monoxide, or in chewing tobacco, e.g., nicotine and related alkaloids, on a host of human biological activities. Many such studies are catalogued in the 1961 LARSON *et al.* book on experimental and clinical studies on tobacco (63).

In Table 1 are listed two dozen enzymes identified in tobacco prior to 1954. This early research was done primarily to obtain an insight into the mechanism of tobacco curing, fermentation, and aging. With the subsequent escalation of technologies pertinent to the isolation and characterization of enzymes, their number in plants, including the various types of tobacco, has increased dramatically. The number of completely identified tobacco enzymes listed by RODGMAN and PERFETTI approximated 500 but many thousands of enzymes present in the tobaccos have been catalogued [see Chapter XXII in (2)]. Paralleling the increase in identified chemical components in tobacco smoke from the fewer than 100 in 1954 (1) to more than 5200 recently catalogued (2) has been the increase in identified chemical components of tobacco from 325 (see Table 1) to the nearly 5000 recently catalogued (2).

## CONTROVERSIES OVER THE ROFFO INVESTIGATIONS

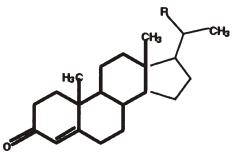
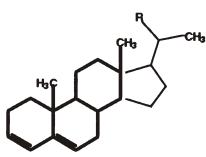
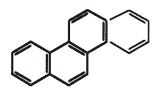
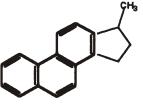
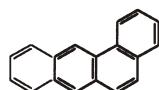
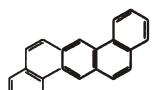
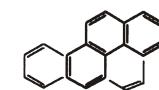
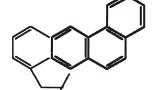
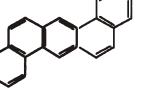
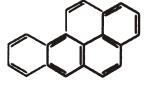
Because the results of a 1930 biological study reported by ROFFO (802) on a tobacco-related material, a destructive distillate from tobacco, coincided with the demonstration of the tumorigenicity to rodent skin of the PAH DB[*a,h*]A in 1930 (803) and preceded the demonstration of similar tumorigenicity of B[*a*]P in 1932 (804), questions were frequently raised about the pertinence to tobacco smoke of the subsequent ROFFO findings in which the destructive distillate tar was not only reported to be tumorigenic to laboratory animal skin but also to contain the tumorigenic B[*a*]P (see Table 2).

In their comments on the ROFFO's reports of their investigations on the chemical composition and biological properties of a destructive distillate from tobacco and the presence of B[*a*]P in the distillate (claims based on spectroscopic data), WYNDER *et al.* (5) noted that ROFFO had claimed to have identified B[*a*]P in the tobacco destructive distillate, but his finding was not confirmed by E. HOFFMANN *et al.* (10). However, WYNDER *et al.* did note that EBY (805), in his examination of the cigarette tar used in the WYNDER *et al.* 1953 biological study, did not detect B[*a*]P. They made little comment about EBY's failure to identify B[*a*]P or any other tumorigenic PAH in the WYNDER *et al.* cigarette tar or the 1957 summary by FIESER (806) on 1) the inadequacy of the spectroscopic data purported to indicate the presence of B[*a*]P in cigarette tar or 2) the failure of FIESER's colleagues to detect B[*a*]P in cigarette tar despite their success in identifying B[*a*]P in roast coffee.

**Table 2. Comparison of ROFFO's findings on the destructive distillate of tobacco vs. research findings reported by others on tobacco smoke**

Roffo and the destructive distillate of tobacco, other related research	Tobacco smoke and other related research
Roffo (320, 811) defined CO derived from tobacco as a hazard.	Many investigators pre-1954 (see Table 1) and post-1953 proposed the CO in tobacco smoke as a hazard. Subsequently, because of its hazard, CO became categorized as a "Hoffmann analyte" [see Chapter XXIII in (2)].
A.E. Roffo (245, 812) identified several PAHs (anthracene, B[a]P, phenanthrene) in the destructive distillate of tobacco.	In 1953, several PAHs (anthracene, pyrene) were identified in cigarette smoke by R.I. Cooper and Lindsey (179).
B[a]P was identified in the destructive distillate of tobacco (178, 240, 246, 247, 248, 812). Note: The Roffos reported 1,2-benzpyrene in the tobacco destructive distillate. 1,2-Benzpyrene was the name originally assigned by Cook <i>et al.</i> (804) to their coal-tar isolate. Subsequently, the nomenclature 1,2-benzpyrene was changed to 3,4-benzpyrene and then to benzo[a]pyrene by the International Union of Pure and Applied Chemistry (IUPAC).	<ul style="list-style-type: none"> <li>▶ E.A. Cooper <i>et al.</i> (10) stated that they could not confirm Roffo's finding of B[a]P in the destructive distillate of tobacco.</li> <li>▶ However, it should also be noted that Eby (805) could not detect B[a]P in the "tar" used by Wynder <i>et al.</i> (5) in their noted 1953 biological study.</li> <li>▶ In 1957, Fieser (806) classified as inadequate the ultraviolet spectrographic data claimed by R.L. Cooper and Lindsey (814) and by Rand personnel (815, 816, 817) as indicating B[a]P in cigarette "tar".</li> <li>▶ Fieser's colleague could not detect B[a]P in cigarette "tar" but identified it in roast coffee (806).</li> <li>▶ B[a]P was eventually accepted universally as a cigarette smoke component after the published report in 1959 of its isolation in crystalline form from cigarette smoke by Wynder and Hoffmann (818).</li> <li>▶ Fourteen PAHs, including benz[a]anthracene (B[a]A), B[a]P, and DB[a,h]A had previously been isolated individually from cigarette smoke (819), 12 in crystalline form, two as oils [see Table 1 in Rodgman (820)].</li> </ul>
In 1930 and 1939, Roffo reported the tumorigenicity to animal skin of the destructive distillate of tobacco (70, 72, 802, 821, 822, 823, 824).	In 1953, cigarette "tar" was reported to be tumorigenic to mouse skin in the renowned study by Wynder <i>et al.</i> (3–5) and subsequently reported to be tumorigenic to several other species [see Tables VII 1–3 in (808)].
Roffo reported that the specific tumorigenicities of the destructive distillates from the different tobacco types were essentially the same (70, 71, 72, 73, 825).	As reported by Wynder and Hoffmann in 1963 (826), subsequent findings with tobacco smoke did differ from those reported by Roffo (70, 71, 72, 73, 825). The specific tumorigenicities (mouse skin) of the cigarette "tars" from different tobacco types varied as follows: flue-cured = Oriental > Maryland > burley. The B[a]P levels in the CSC varied as follows: flue-cured > Oriental > Maryland > burley
Roffo (827) claimed that the destructive distillate "tar" from tobacco showed greater specific tumorigenicity to laboratory animals than did coal tar.	Later, Jaffe <i>et al.</i> (828) and Hueper (829) described findings that disagreed with those of Roffo, i.e., they reported that coal tar showed greater specific tumorigenicity to laboratory animals than did tobacco "tar".
The yields of B[a]P and other PAHs in the destructive distillate from organic solvent-extracted tobacco were less than those in the destructive distillate from the control (unextracted) tobacco (248).	The per cigarette yields of B[a]P and other PAHs were less in the "tar" [cigarette smoke condensate (CSC)] from organic solvent-extracted tobacco than those in the CSC from control (unextracted) tobacco (830, 831, 832, 833) [see Table 3 in Rodgman (820)].
The destructive distillate from the organic solvent-extracted tobacco showed less tumorigenicity than the destructive distillate from the control (unextracted) tobacco (248).	The CSC from organic solvent-extracted tobacco showed lower specific tumorigenicity than CSC from control tobacco but the % decrease in specific tumorigenicity was less than the % decrease in the B[a]P content (833) of the CSC.
Roffo proposed that the precursor in tobacco of the PAHs in the destructive distillate from tobacco (248) was phytosterol. Note: In 1939 and 1941, cholesterol was not a known component of tobacco. Also, high molecular weight terpenoids such as solanesol, neophytadiene, and the cyclotetradecane derivatives had not yet been identified as tobacco components. Each cyclotetradecane derivative had a 14-carbon structure similar to that in anthracene or phenanthrene. Subsequently, the high molecular weight terpenoids and derivatives (solanesyl esters) were identified in tobacco (and tobacco smoke) as were cyclotetradecane derivatives plus numerous phytosterols and their long-chained aliphatic esters plus cholesterol, its glycoside, and many long-chained aliphatic cholesteryl esters.	<ul style="list-style-type: none"> <li>▶ Subsequently, identified in tobacco were several phytosterols [stigmasterol (834), sitosterol (835), campesterol (836), ergosterol (835)] and cholesterol (837, 838) and their long-chained aliphatic esters (839). All were also identified in tobacco smoke components (838, 840, 841).</li> <li>▶ The saturated aliphatic hydrocarbons <sup>a</sup>, the phytosterols <sup>b</sup>, and terpenoids <sup>c</sup> (such as solanesol and its long-chained aliphatic esters) in tobacco, were demonstrated to be major precursors of PAHs in CSC in a 1979 study by Severson <i>et al.</i> (842) of the United States Department of Agriculture and in a 1958 study in which the levels of each category in the cigarette tobacco were doubled and tripled (843).</li> <li>▶ In 1963 and 1964, Rowland <i>et al.</i> (844) described the conversion of a cyclotetradecane derivative to a phenanthrene derivative.</li> </ul>

**Table 2. (cont.)**

Roffo and the destructive distillate of tobacco, other related research	Tobacco smoke and other related research
<p>In 1939, Roffo demonstrated that the pyrolysate from cholesterol was tumorigenic (345, 347), a confirmation of the 1928 findings of Kennaway and Sampson (343) and a prelude to the 1949 findings of Falk <i>et al.</i> (845).</p> <p>Note: In 1939 and 1941, cholesterol was not a known component of tobacco.</p> <p>Roffo reported that the tumorigenicity of his cholesterol pyrolysate was due to derivatives of phenanthrene (345).</p>	<p>A cholesterol pyrolysate was demonstrated to be tumorigenic in 1928 by Kennaway and Sampson (343), in 1945 by Beck <i>et al.</i> (846), and again in 1949 by Falk <i>et al.</i> (845).</p> <ul style="list-style-type: none"> <li>Pyrolysis of cholesterol and cholestryl esters yielded two tumorigenic compounds, 4-cholestren-3-one and 3,5-cholestadiene (845, 847), both of which may be considered as phenanthrene derivatives.</li> </ul>
	<p style="text-align: center;">     <b>4-Cholestren-3-one</b>                            <b>3,5-Cholestadiene</b> </p> <ul style="list-style-type: none"> <li>In the 1935 report on his pyrolysis of cholesterol, Cohen <i>et al.</i> (848) described the generation of phenanthrene derivatives, the so-called Diels' hydrocarbon (17-methyl-17H-cyclopenta[a]phenanthrene) and chrysene. At one time, chrysene was classified as a carcinogenic by the International Agency for Research on Cancer (IARC) (849) but subsequently the IARC cancelled its carcinogen classification.</li> <li>By 1951, many phenanthrene derivatives had been reported as tumorigenic, e.g., 1,2,3,4-tetramethylphenanthrene (850).</li> <li>Also, chrysene, the Diels' hydrocarbon, and several tumorigenic PAHs such as benz[a]anthracene B[a]A, DB[a,h]A, and B[a]P are obviously related structurally to phenanthrene since each has one or more additional benzene rings fused to a phenanthrene structure.</li> </ul> <p style="text-align: center;">     <b>Chrysene</b>                                    <b>Diels' hydrocarbons</b> </p> <p style="text-align: center;">      <b>Benz[a]anthracene</b> </p> <p style="text-align: center;">      <b>Cholanthrene</b>                            <b>Dibenz[a,h]anthracene</b>                            <b>Benzo[a]pyrene</b> </p>

**Table 2. (cont.)**

Roffo and the destructive distillate of tobacco, other related research	Tobacco smoke and other related research
In 1939, Roffo reported the tumorigenicity to laboratory animals of heated/oxidized "fat" (851, 852).	<ul style="list-style-type: none"> <li>▶ Subsequent studies on heated fats essentially confirmed the findings of Roffo, e.g., Peacock and Beck (853), Lane <i>et al.</i> (854), but a study by Morris <i>et al.</i> (855) did not.</li> <li>▶ Fat components such as saturated hydrocarbons were shown to yield tumorigens on heating, e.g., (856, 857).</li> <li>▶ Fat components such as high molecular weight aliphatic esters and triglycerides yield tumorigens on heating (858, 859, 860).</li> </ul>
Duplicating his tobacco destructive distillate procedure, Roffo reported in 1940 that the destructive distillate from tea was tumorigenic (861) as was the destructive distillate of Yerba mate (862). Note: Yerba mate is a tea-like substance containing xanthines and used for drink preparations, including toasted Yerba mate used in drink preparation.	<ul style="list-style-type: none"> <li>▶ In the late 1950s, tumorigenic PAHs were reported in tea and coffee by Kuratsune (863) and Kuratsune and Hueper (864).</li> <li>▶ In his 1988 review, Maga (865) summarized the identification of numerous tumorigenic PAHs in foodstuffs and beverages, including tea and coffee.</li> </ul>
In 1939, Roffo reported that the destructive distillate from coffee was tumorigenic to laboratory animals (866).	<ul style="list-style-type: none"> <li>▶ In 1939, Widmark (867) reported that an extract of roasted coffee was tumorigenic to laboratory animals.</li> <li>▶ With improved analytical technology available in the mid-1950s, B[a]P was identified in roast coffee by Fieser's colleagues (806, 863, 864) but no B[a]P was identified by them in cigarette "tar".</li> </ul>

<sup>a</sup>Considered a major precursor of PAHs by Lam and by Wynder; demonstrated to be significant but less significant than phytosterols and terpenoids such as solanesol.

<sup>b</sup>Considered a major precursor of PAHs by Wynder and Wright; demonstrated to be major by Rodgman and Cook (843) and by Severson *et al.* (842).

<sup>c</sup>Considered a major precursor of PAHs by Wright; demonstrated to be major by Rodgman and Cook (843) and Severson *et al.* (842).

Later, in their lengthy 1964 review [see p. 259 in 807] and 1967 book [see p. 94 in (808)], WYNDER and HOFFMANN essentially dismissed the research by ROFFO on a tobacco destructive distillate by tersely noting that the preparation by ROFFO of a tobacco "tar" for a carcinogenicity test involved the mere destructive distillation of tobacco, thus excluding the ROFFO investigations from any discussion of tobacco smoke.

Of course, most criticisms of ROFFO's research findings were based on his production of a tobacco tar by destructive distillation of tobacco, a process not considered comparable to the normal combustion of tobacco in a cigarette in the presence of air and its oxygen. It is indeed true that, during the cigarette puff, the oxygen level immediately ahead of the fire cone is depleted from the ≈21% level of air, but as NEWSOME and KEITH (809) demonstrated, the oxygen level is not 0% as it might be during destructive distillation. During the smoking process, the cigarette system has access to air (and its oxygen content) surrounding the cigarette both during and between puffs. Cigarette paper porosity also dictates some air flow through the cigarette paper during the puff.

In 1961, LARSON *et al.* [see pp. 422–424 in (810)] provided a critique of ROFFO's rabbit skin-painting studies with destructive distillates from tobaccos. ROFFO succeeded in producing tumors, many of which were described as carcinomas or epitheliomas, in the treated rabbits. Because of the small number of tumors generated in the ROFFO biological Studies, LARSON *et al.* considered that one must be very hesitant in placing too great weight on ROFFO's reiterated description of a solitary tumor.

ROFFO also claimed that his tobacco tar generated by destructive distillation was more tumorigenic than equivalent doses of coal tar, a finding at odds with those of

many investigators, even those who compared the tumorigenicity in mice of various tobacco-tar preparations with that of equivalent doses of coal tar solutions (see Table 2). Despite the numerous criticisms of the information provided by ROFFO in his numerous publications issued in the 1930s and early 1940s on the destructive distillate from tobacco because of the purported lack of pertinence of such information to that derived from studies on tobacco-derived smoke, it is interesting to compare the results reported by ROFFO on the chemical and biological properties of the tobacco destructive distillate with those obtained post-1953 with tobacco smoke, particularly cigarette smoke. Also interesting is the comparison of the findings of ROFFO on the pyrolysis of several tobacco components with reports by other investigators. Such comparisons are also presented in Table 2.

Although many of the findings reported by ROFFO on the tobacco destructive distillate differ in degree from findings reported for tobacco smoke, many of the tobacco destructive distillate and tobacco smoke findings do parallel each other generally. As indicated in Table 2, two ROFFO findings do differ substantially from those reported by other investigators: 1) The relationship between the tumorigenicity of tobacco destructive distillate vs. coal tar tumorigenicity. 2) The similarity of the tumorigenicities of the destructive distillates from different tobacco types reported by ROFFO (70, 71, 72, 73, 825) vs. the difference in tumorigenicities of the mainstream smoke "tars" from various tobacco types reported by WYNDER and HOFFMANN (826). Recently, PROCTOR (868) summarized the contributions of ROFFO to our tobacco-pertinent knowledge and noted several of the investigators who were either supportive of or critical of his findings.

**Table 3. Some compounds applied to tobacco for treatment of diseases and pests prior to 1953**

CAS No.	Name	Reference
<i>Fungicides:</i>		
50-00-0	Formaldehyde	1945 Clayton (869)
7761-88-8	Silver nitrate	1951 Garner (870)
7487-94-7	Corrosive sublimate {mercuric chloride} HgCl <sub>2</sub>	1951 Garner (870)
71-43-2	Benzol {benzene}	1951 Garner (870)
106-46-7	<i>p</i> -Dichlorobenzene	1951 Garner (870)
1317-39-1	Copper oxide {yellow cuprocide}	1951 Garner (870)
577-11-7	Sulfosuccinate	1951 Garner (870)
14882-18-9	Bismuth subsalicylate	1951 Garner (870)
14484-64-1	Ferric dimethyl-dithiocarbamate {Fermate}	1951 Garner (870)
7758-98-7	Copper sulfate, anhydrous {Bordeaux mixture}	1951 Garner (870)
<i>Pesticides:</i>		
12002-03-8	Copper acetoarsenite {Paris Green}	1951 Garner (870)
592-01-8	Calcium cyanide	1951 Garner (870)
98-95-3	Nitrobenzene	1951 Garner (870)
7784-40-9	Lead arsenate {Diplumbic lead arsenate }	1901 Marlatt (209) 1908 Marlatt (210) 1951 Garner (870)
15096-52-3	Sodium aluminofluoride = Sodium fluoaluminate {Cryolite}	1951 Garner (870)
83-79-4	Rotenone	1937 Chamberlin and Madden (871) 1951 Garner (870)
16893-85-9	Sodium fluosilicate	1951 Garner (870)
107-49-3	Tetraethyl pyrophosphate	1951 Garner (870)
56-38-2	Parathion dust	1951 Garner (870)
8003-34-7	Pyrethrum	1936 LaForge and Haller (872) 1944 LaForge and Barthel (873) 1951 Garner (870)
74-90-8	Hydrogen cyanide	1951 Garner (870)
75-21-8	Ethylene oxide	1951 Garner (870)
124-38-9	Carbon dioxide	1951 Garner (870)
75-15-0	Carbon disulfide	1951 Garner (870)
65-30-5	Nicotine sulfate	1917 Moore and Graham (874) 1936 Busbey and McIndoo (628, 629) 1951 Garner (870)
68038-71-1	<i>Bacillus thuringiensis</i> {B.t.} {Dipel®}	1924 Staudinger and Ruzicka (875)

#### OTHER COMPOUNDS APPLIED TO TOBACCO BUT NOT SPECIFICALLY IDENTIFIED IN TOBACCO OR TOBACCO SMOKE PRIOR TO 1953

In reviewing the tobacco and smoke literature prior to 1953, two additional sets of compounds are provided for historical purposes. These include either 1) compounds applied on tobacco prior to 1953 for the treatment of disease (molds, spores, fungi, viruses, etc) and pests, or 2) compounds applied on tobacco as flavorants, casings and/or humectants. The listings are not complete as farmers did not always reliably report such usage for their crops and tobacco manufacturers rarely reported the composition of flavor additives, casings, and humectants used on tobacco prior to 1953. Table 3 and Table 4 are primarily of historical value as the chemicals applied to tobacco for disease control and the types of additives applied to tobacco have markedly changed over time. Most of the chemicals in Tables 3 and 4 are not listed in Table 1 because they were not isolated and confirmed to be present on tobacco samples that were analyzed in the articles reviewed. Nonetheless, these compounds were applied to tobacco and may have been present as residues in the case of the fungicides and pesticides or at larger levels in the case of flavorants and humectants. These compounds are listed in Tables 3 and 4.

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**Table 4. Some flavorants, casings, and humectants applied to tobacco prior to 1953**

CAS No.	Name	Reference
8008-94-4	Liquidambar {sap of the sweet gum tree}	1632 Diaz del Castillo (876)
68916-91-6	Licorice	1951 Garner (877)
57-50-1	Sugar	1951 Garner (877)
50-99-7	Glucose	1951 Garner (877)
8013-17-0	Invert sugar	1951 Garner (877)
8028-66-8	Honey	1951 Garner (877)
9000-40-2	St. John's bread	1951 Garner (877)
68476-78-8	Molasses	1951 Garner (877)
8024-04-2	Tonka bean	1951 Garner (877)
	Deer's tongue	1951 Garner (877)
91-64-5	Coumarin	1951 Garner (877)
90604-31-1	Rum	1951 Garner (877)
91450-09-8		1951 Garner (877)
56-81-5	Glycerol	1951 Garner (877)
111-46-6	Diethylene glycol	1951 Garner (877)

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