

THE MERCK INDEX

AN ENCYCLOPEDIA OF
CHEMICALS, DRUGS, AND BIOLOGICALS

FOURTEENTH EDITION

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Published by
Merck Research Laboratories
Division of

MERCK & CO., INC.
Whitehouse Station, NJ, USA

2006

THE MERCK INDEX

Library of Congress Catalog Card Number 89-60001

ISBN Number 0-911910-00-X

ISBN Number 978-0-911910-00-1

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Printed in the USA

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FOREWORD

For more than a century, *The Merck Index*, Chemistry's Constant Companion™, has provided quick and reliable answers to questions arising in the course of the scientist's work. The Fourteenth Edition continues this tradition to publish an authoritative, multidisciplinary reference handbook committed to scientific excellence.

Each edition is reflective of key scientific discoveries of its time period. Once again, significant new compounds have been carefully selected from biomedicine, agriculture, and various disciplines of chemistry. With the particular needs of the research scientist in mind, every effort has been made to include additional physical property information in the monographs. Coverage of important new tools for pharmacological research and organic synthesis has been expanded and includes more than 140 monographs on Name Reagents. The Organic Name Reactions have again been updated and now include 450 entries.

The Supplemental Tables have been extensively revised. More than 70 pages of hard-to-find information complement the material presented in the other sections. New for this edition is a table describing vaccine preparations for use in the prevention of infectious disease, an area of research never before covered in this reference work. Another new table provides the expanded meanings for acronyms encountered in biomedical and pharmaceutical research.

An important new feature introduced for this edition is the companion CD that accompanies the printed volume. This new multimedia reference set allows the scientist to use whichever format is most useful—hardcopy at the lab bench and CD in the laptop. The text searchable CD uses CambridgeSoft's ChemFinder® software to enable quick retrieval of data and provides access to nearly 1000 monographs retired from the 12th and 13th editions that are no longer available in print.

Merck & Co., Inc. is one of the world's largest pharmaceutical companies. Merck is committed to providing trusted medical and scientific information and continues to publish *The Merck Index* and all of the Merck Handbooks as a not-for-profit service to the scientific community and the public. We hope that this edition of *The Merck Index* will be an indispensable resource to all who use it.

ACKNOWLEDGMENTS

The successful publication of the Fourteenth Edition of *The Merck Index* would not have been possible without the close collaboration of many dedicated people who have generously contributed their expertise and special talents.

The Merck Index Staff wishes to acknowledge our coworkers whose contributions have been particularly significant: *Beverly Grodzinski* for system support and for organizing and tracking the production process; *John Ho* and *Bob Dougherty* for computer expertise, custom programming and technical guidance; *Sharon O'Brien* for designing the CD artwork; *Debra Shelinsky Greene* and *Hilary Wandall* for advice and counsel on intellectual property and contractual issues; *Pamela Barnes-Paul* for coordinating the advertising and marketing effort; *Margaret Hill*, *Ann Smith*, and the entire staff of the MRL Library for their ongoing assistance.

We are especially indebted to the many readers who took the time to contact us with comments, additions and corrections and to the generations of Merck scientists who have contributed to this and previous editions of *The Merck Index*.

Finally, special thanks are due to *Dr. John D. Irvin* of Merck Research Laboratories for his personal interest, encouragement and support; and to *Gary Zelko*, our publisher, for his collaboration and expertise in producing this edition.

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EXPLANATORY NOTES

The Fourteenth edition of *The Merck Index* contains 10,200 monographs describing significant chemicals, drugs, and biological substances. The entries cover a wide range of compounds which have been selected on the basis of present or historic importance and interest. Since the publication of the Thirteenth Edition in 2001, over 5,000 monographs have been significantly revised and updated. More than five hundred monographs have either been combined or deleted from the manuscript to make room for hundreds of new entries. Nearly 450 of these monographs, as well as 540 monographs archived from the Twelfth Edition, are presented in their original form on the companion CD which accompanies this volume.

Entries are generally limited to single substances and related compounds such as isomers or salts. While multi-component drugs are, for the most part, excluded, there are a number of monographs devoted to families of natural products or biological substances. Monographs vary greatly in length. The length of a monograph, however, is not necessarily indicative of the importance of a compound, but rather may simply be an indication of the amount of relevant published information available for the compound.

For the purpose of illustrating the general monograph format, a typical monograph is depicted and the components are identified. While all possible categories of information in a monograph are described below, it must be emphasized that not all categories are present in every monograph.

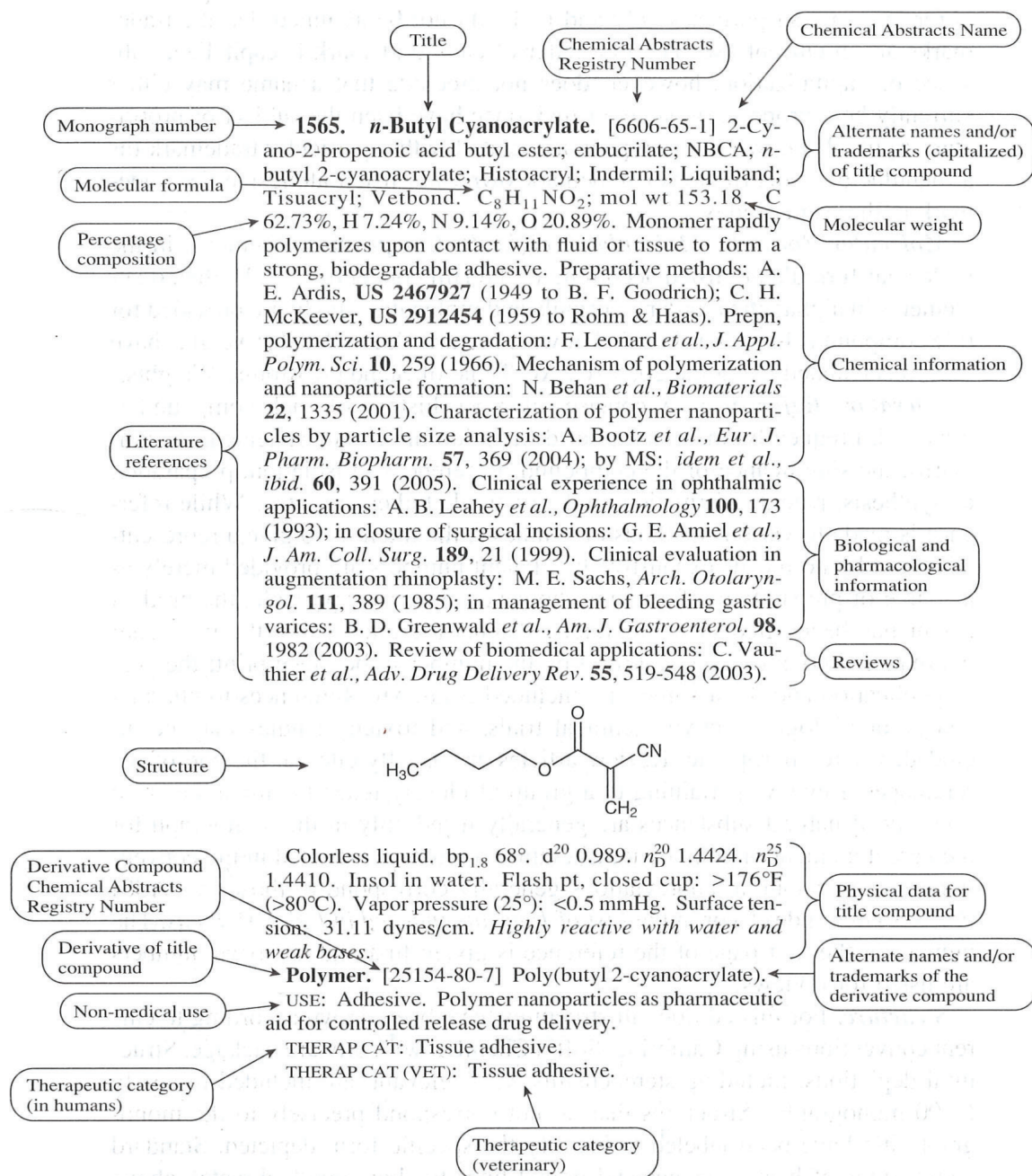
Monograph Number. Sequential accession numbers are assigned to monographs which are alphabetized by title. Entries in the indices are referenced to these accession numbers, not to page numbers. (*Note:* Monograph numbers in the Fourteenth Edition do not correspond to Thirteenth Edition monograph numbers.)

Monograph Title. Titles are usually simple chemical names or in the case of drugs, the commonly used generic name such as the USAN (United States Adopted Name) or INN (International Nonproprietary Name). Registered trademarks, designated by ®, are used for a small number of entry titles, primarily when nonproprietary terms are not available. Plant monographs are titled using a common name rather than the full botanical name.

Chemical Abstracts Registry Number(s). The Chemical Abstracts Service (CAS) Registry Number appears following the title. These unique identifiers are provided for title substances and for selected derivatives. Where appropriate, numbers for isomeric and unspecified forms of the compound are listed. Descriptors are appended to the entry if more than one registry number has been associated with the compound.

Chemical Abstracts Name(s). The uninverted form of the CAS Index Name appears in native font following the CAS Registry Number. When a specific isomer is being discussed, stereochemical descriptors have been included to more clearly delineate that isomer. CAS Registry Numbers and CAS Index Names are provided as aids for further searching of the compound of interest in *Chemical Abstracts* and elsewhere.

Alternate Name(s). Other chemical names, trivial names, experimental drug codes, and trademarks that identify the entry are listed. Listing of trademarks



is for information purposes only and it should not be assumed that the trademarks are in current use. The first letter of each trademark is capitalized; absence of capitalization, however, does not preclude that a name may either currently be a proprietary name, or may once have been the subject of proprietary rights. If known, the company associated with a particular trademark (as a manufacturer, distributor or trademark owner) is listed alongside the trademark in the Name Index.

Molecular Formula, Molecular Weight, % Composition. Elements in the molecular formula are listed according to the Hill convention (C, H, then other elements in alphabetical order). Formula and molecular weight are provided for title compounds having a specific known structure. All molecular weights have been recalculated using the 2005 IUPAC Table of Standard Atomic Weights.

Literature References. A concise reference history of each compound is provided. Frequently, there is a brief description or capsule statement to summarize the significance of the compound. References to isolation, preparation or synthesis, patent information, and structural studies are cited. While reference is made to various methods of synthesis, the intent is to give a representative, but by no means exhaustive list. Patent numbers are provided merely as a source of preparative information; however, whenever possible, the product patent has been cited in monographs. Patents are cited using the two letter international country code followed by the number in boldface print; the year of publication and the assignee are included if known. References to pharmacology or biological activity, clinical trials, and toxicity studies may be included, where appropriate. Review articles are usually cited at the end of the references. Reviews pertaining to a group of closely related compounds or to a family of natural substances are generally listed only in the monograph for the parent element or compound. Literature references are cited in the conventional manner; journal abbreviations generally correspond to those in CASSI (CAS Source Index[®]) or in the *List of Journals Indexed in Index Medicus*. The number of the first page of the reference is given; first and last page numbers are listed for reviews.

Structure. For this edition, all structures have been drawn according to current conventions using CambridgeSoft's ChemDraw[®] software package. Structural depictions, including stereochemistry, if relevant, are included in nearly 6,700 monographs. Structures that do not correspond precisely to the monograph title have been labeled to identify the specific form depicted. Standard conventions of heavy wedges and dotted lines to show bonds directed above or below the plane of the paper are used where appropriate. Whenever possible, double bond geometry has been defined within the structure. Amino acid residues are assumed to be L unless specified otherwise. In addition, 1,850 monographs contain line formulae showing molecular arrangements.

Physical Data. Data are cited as found in the literature. When several alternate data values appear in the literature, the data is evaluated and representative selections are made. The values are then reported with the corresponding source. Whenever possible, the color of a substance is stated, but the absence of color (white or colorless) is often omitted. Temperatures are given in degrees Celsius, unless otherwise noted. When solubilities are determined at room temperature (about 25°C), the temperature is generally omitted. When optical ro-

tations are measured in water, the solvent is usually not specified. For ultraviolet absorption measurements, the solvent is given within parentheses.

An effort has been made to provide toxicity data (e.g. LD₅₀, LC₅₀) and to identify the source of this information. **Caution** and/or **Note** statements are also provided in a number of monographs. Specific statements are given for compounds on the U.S. Government's Schedules of Controlled Substances in Title 21 of the Code of Federal Regulations (CFR), for compounds listed as suspected or confirmed carcinogens in the *Eleventh Report on Carcinogens* issued in 2004 by the U.S. Department of Health and Human Services (USDHHS), and for chemicals considered potential occupational hazards as described in sources such as the *NIOSH Pocket Guide to Chemical Hazards* (USDHHS). *Note:* Absence of toxicity data or specific cautions does not imply that toxic effects do not exist.

Derivatives. When derivatives (isomers, salts, etc.) of the title compound are described in a monograph, the information appears in the paragraph(s) directly following the physical data. These paragraphs may also be used to describe specific members of a large family of natural substances. Derivative data presentation mirrors that of the title compound and may include registry numbers, chemical and alternate names, molecular weights, percentage composition, literature references, and physical properties.

Use. Descriptions of specific uses, which are not medical or veterinary therapeutic applications, are summarized under this heading.

Therapeutic Category and Therapeutic Category (Veterinary). In most cases, therapeutic categories reflect the accepted terminology in the medical literature. When available, mode of action information is included in the literature references section of the monograph. Monographs for human drugs have been indexed by both therapeutic category and biological activity beginning on page THER-1.

The Merck Index is not intended as an official therapeutic guide. Inclusion of a drug or any other compound in this book is not an endorsement, but merely a statement of the fact that such a substance exists. THERAPEUTIC CATEGORY and THERAPEUTIC CATEGORY (VETERINARY) paragraphs are intended only as summary statements of major pharmacological properties or indications for the individual compounds. For additional information on uses, dosage, side effects, and adverse reactions, readers are directed to consult pertinent scientific and professional publications, product circulars, information sheets or material safety data sheets prepared or published by the respective manufacturers.

Indices. Four indices—Name, Formula, CAS Registry Number and Therapeutic Category—are included; each entry directs the reader to the number of the monograph in which the substance of interest is described. More than 60,000 synonyms, including titles, CAS names, alternate names, trademarks, and derivative names are contained in the **Name Index**. If known, trademarks have been matched with an associated company. An abbreviated form of the company name appears in brackets following the trademark. The complete company name and location is listed in an updated and expanded Company Register in the TABLES section of the book. Company names are provided as a source of additional information and do not necessarily imply trademark ownership. Due

to reorganizations or mergers, some company names may have changed since the original matching process was completed.

More than 7,500 entries appear in the **Formula Index**. This index contains the molecular formula for the title compounds and derivatives other than acid addition salts, hydrates or isomers.

The **CAS Registry Number Index** of more than 12,000 entries arranged in ascending Registry Number order. Descriptors are appended to the entry if more than one registry number may be associated with the compound.

In the **Therapeutic Category and Biological Activity Index**, monographs describing human drugs have been listed by one or more therapeutic indications and/or mechanisms of action. Cross references to closely related categories and mechanisms have been included. Whenever appropriate, subclassifications have been developed by grouping compounds according to chemical or pharmacological similarities.

Organic Name Reactions. This section is comprised of 450 named reactions and an index. A concise reference history and associated reaction schema are provided for each reaction or subreaction.

Tables. A compilation of over 70 pages of tables is provided to supplement the material presented in the monographs. This section has been extensively revised for this edition and now includes tables of Acronyms, Vaccines, and Physical Constants.

Great care has been taken to assure the accuracy of the information contained in *The Merck Index*. However, the Editorial Staff and the Publisher cannot be responsible for errors incurred in publication or for any consequences arising from use of the information published in *The Merck Index*. Accordingly, reference to original sources is strongly encouraged, as is reporting of errors and omissions in order to assure that appropriate changes may be made in the next edition.

Abbreviations

Included are abbreviations commonly used in *The Merck Index*. Please consult the Acronyms and Glossary (Suppl. Tables Section) for additional definitions.

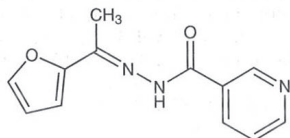
α_D^{25}	specific optical rotation at 25° C for D (sodium) line; absence of brackets indicates optical rotation of a liquid in a 1 decimeter cell, neat	d	density; specific gravity (d_4^{19} specific gravity at 19° referred to water at 4°)
Å	angstrom	d-	<i>dextro</i> (rotatory); the opposite of <i>l</i>
A	absorbance	D-	<i>Dextro</i> configuration; opposite of <i>L</i>
Ab	antibody	Da	daltons
abs	absolute; absorption	dec; decomp; decompn	decompose(s); decomposition
abs config	absolute configuration	deg	degree
Ag	antigen	deliques	deliquescent
alc	alcohol; ethanol; ethyl alcohol	deriv	derivative
alk	alkali(ne)	determn	determination
a_M	molar absorptivity	dil	dilute; diluted; dilution
amps	ampules; amperes	distln	distillation
anhydr	anhydrous	dl-	racemic
Ann.	<i>Justus Liebig's Annalen der Chemie</i>	DL-	optically inactive by external compensation as contrasted with <i>meso</i> -
approx; ~	approximate(ly)	dyn	dynes
aq	aqueous	ϵ (epsilon)	molar extinction coefficient; dielectric constant
as-; asym-	asymmetrical; unsymmetrical	η (eta)	viscosity
at.	atomic	E.C. No.	Enzyme Commission Number
at. no.	atomic number	e.g.	(<i>exempli gratia</i>) for example
at. wt.	atomic weight	$E_{1\text{cm}}^{1\%}$	the absorbance of a solution containing one gram per 100 ml contained in a cell having an absorption path of one cm
atm	atmosphere(s)	Ed(s).	editor(s)
B.P.C.	British Pharmaceutical Codex	ed.	edition
Bé	Baumé (a specific gravity scale)	<i>eidem</i>	the same (authors); plural of <i>idem</i>
Beilstein	<i>Beilstein's Handbuch der Organischen Chemie</i>	E_M	molar extinction coefficient (concn in g-moles/l)
Ber.	<i>Chemische Berichte</i> (Berichte der Deutschen Chemischen Gesellschaft)	equiv	equivalent
bp	basepair; boiling point	<i>et al.</i>	(<i>et alii</i>) and others
°C	Celsius degrees	etc.	(<i>et cetera</i>) and so forth
c	concentration	eV	electron volt
ca.	(<i>circa</i>) about	evac	evacuated
cal	calorie(s)	evapn	evaporation
calc(d)	calculate; calculated	exptl	experimental(ly)
cc	cubic centimeter(s) (milliliter)	ext(d)	extract; extracted
cf.	(<i>confer</i>) compare	extern	externally
Ci	curie	°F	Fahrenheit degrees
coll. vol.	collective volume	fp	freezing point
compd	compound	Frdl.	<i>P. Friedlander Fortschritte der Teerfarbenfabrikation</i> , a collection of patents
compn	composition	g	gram(s)
concd	concentrated	Gmelin's	<i>Gmelin's Handbuch der Anorganischen Chemie</i>
concn	concentration	habit.	habitat
config	configuration	Houben	a German collection of medicinal patents
constit	constituent(s)	Houben Weyl	<i>Houben-Weyl Methoden der Organischen Chemie</i>
contd	continued	hr	hour
contg	containing	i.e.	(<i>id est</i>) that is
corr	corrected	i.g.	intra gastric
corresp	corresponding; corresponds	i.m.	intramuscular
C_p	heat capacity (constant pressure)	i.p.	intraperitoneal
crit press	critical pressure	I.U.	international unit
crit temp	critical temperature	i.v.	intravenous
cryst	crystalline; crystals		
crystn	crystallization		
Δ (delta)	indicates the locant of the double bond		

Abbreviations (Continued)

<i>ibid.</i>	(<i>ibidem</i>) at the same place	pK	log of the reciprocal of the dissociation constant
<i>idem</i>	the same (author); plural: <i>eidem</i> , the same (authors)	ppm	parts per million
incl	including	ppt; pptd	precipitate; precipitated
incompat	incompatibility	prepd; prepn	prepared; preparation
inorg	inorganic	press.	pressure
insol	insoluble	pt	point
Intl	International	<i>q.q.v.</i>	(<i>quae vide</i>) which see, plural
isoln	isolation	<i>q.v.</i>	(<i>quod vide</i>) which see
K	dissociation constant; equilibrium constant; Kelvin temperature	<i>r-</i>	racemic
λ (lambda)	wavelength; microliter	recryst(n)	recrystallize; recrystallization
l	liter	ref	reference
<i>l-</i>	<i>levo</i> (rotatory); the opposite of <i>d</i>	rep [REP]	"roentgen equivalent physical" means a dose of ionizing radiation capable of producing energy absorption of 93 ergs per gram of tissue
<i>L-</i>	<i>Levo</i> configuration; opposite of <i>D</i>	resp	respectively
LC ₅₀	median lethal concentration; the concn of a chemical that is estimated to be fatal to 50% of the organism tested	s.c.	subcutaneous
LD ₅₀	median lethal dose; the quantity of a chemical that is estimated to be fatal to 50% of the organisms tested	sapon(if)	saponification
<i>loc. cit.</i>	(<i>loco citato</i>) in the place cited	satd	saturated
log	logarithm (common)	sec	second(s)
log <i>P</i>	logarithm of the partition coefficient	sepn	separation
<i>M</i>	molar (concentration; moles/liter)	sol	soluble
<i>m-</i>	<i>meta</i> chemical locant for ring substituents	soly	solubility
Mab; mAb	monoclonal antibody	solidif	solidifies; solidification
mass spec	mass spectrometry	soln	solution
MD	molecular rotation $\frac{[\alpha]_D \times \text{mol wt}}{100}$	sp gr	specific gravity
<i>Mellor's</i>	<i>Mellor's Comprehensive Treatise on Inorganic and Theoretical Chemistry</i>	<i>sp.</i>	species
Mfg; manuf	manufacturing	spec	spectroscopy; spectrum; spectral
mfr	manufacturer	<i>spp.</i>	species (plural)
misc	miscible	<i>sqq</i>	(<i>sequentia</i>) and following
mixt	mixture	subl	sublimes
mol wt	molecular weight	suppl	supplement
<i>Monatsh.</i>	<i>Monatshfte für Chemie</i>	<i>sym-</i>	symmetrical
mp	melting point	<i>t</i> _{1/2}	half-life
<i>M_r</i>	relative molecular mass	tabl	tablet(s)
<i>N</i>	normal concentration or nitrogen as a locant	tech	technical
<i>n</i>	index of refraction (<i>n</i> _D ²⁰ for 20° and sodium light); normal, as <i>n</i> -propyl	temp	temperature
<i>o-</i>	<i>ortho</i> chemical locant for ring substituents	uncor(r)	uncorrected
<i>op. cit.</i>	(<i>opere citato</i>) in the work cited	<i>unsym-</i>	unsymmetrical; asymmetrical
org	organic	UV; uv	ultraviolet
OsM	osmolar; osmole	v	volt(s)
ψ (psi)	pseudo	<i>v-</i>	(<i>vicinal</i>) adjacent
P	poise	v/v	percent "volume in volume" expresses the number of milliliters of an active constituent in 100 milliliters of solution
<i>p-</i>	<i>para</i> chemical locant for ring substituents	var	variety
p; pp	page(s)	viz.	(<i>videlicet</i>) that is to say; namely
Pa	pascal	vol	volume
<i>passim</i>	here and there; scattered	vs	versus
pat.	patent	w/v	percent "weight in volume" expresses the number of grams of an active constituent in 100 milliliters of solution, and is used regardless of whether water or another liquid is the solvent
petr	petroleum	w/w	percent "weight in weight" expresses the number of grams of an active constituent in 100 grams of solution or mixture
pH	acid-base scale; log of reciprocal of hydrogen ion concentration	wt	weight
pI	isoelectric point		

Methyl ester. Methyl furoate; methyl pyromucate. $C_6H_6O_3$. Liquid. Agreeable odor. bp 181.3°; d_4^{21} 1.1786; n_D^{21} 1.4871. Slightly sol in water; sol in alcohol.

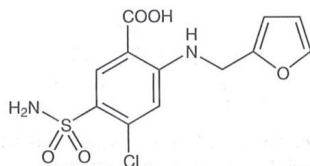
4308. Furonazide. [3460-67-1] 4-Pyridinecarboxylic acid [1-(2-furanyl)ethylidene]hydrazide; isonicotinic acid α -methylfurfurylidenehydrazide; 2-furyl methyl ketone isonicotinoylhydrazone; α -methylfurfurylidenehydrazide of isonicotinic acid; INF; Furilazone; Clitizina; Menazone. $C_{12}H_{11}N_3O_2$; mol wt 229.23. C 62.88%, H 4.84%, N 18.33%, O 13.96%. Prepn: Miyatake *et al.*, *J. Pharm. Soc. Jpn.* **75**, 1066 (1955).



Crystals, mp 199-201.5°.

THERAP CAT: Antibacterial (tuberculostatic).

4309. Furosemide. [54-31-9] 5-(Aminosulfonyl)-4-chloro-2-[(2-furanylmethyl)amino]benzoic acid; 4-chloro-*N*-furfuryl-5-sulfamoylanthranilic acid; frusemide; furosemide; LB-502; Aisemide; Bernald; Desdemin; Discoid; Diural; Dryptal; Durafurid; Errolon; Eutensin; Frusetic; Frusid; Fulsix; Fuluvamide; Furesis; Furo-Puren; Furosedon; Hydro-rapid; Impugan; Katlex; Lasilix; Lasix; Lowpston; Macasirool; Mirfat; Nicorol; Odemase; Oedemex; Profemin; Rosemide; Rusedy; Trofurit; Urex. $C_{12}H_{11}ClN_2O_5S$; mol wt 330.74. C 43.58%, H 3.35%, Cl 10.72%, N 8.47%, O 24.19%, S 9.69%. Prepn: K. Stürm *et al.*, **DE 1122541**; *idem*, **US 3058882** (both 1962 to Hoechst). Molecular and crystal structure: J. Lamotte *et al.*, *Acta Crystallogr.* **B34**, 1657 (1978). Review of pharmacokinetics: L. Z. Benet, *J. Pharmacokinet. Biopharm.* **7**, 1-27 (1979); R. E. Cutler, A. D. Blair, *Clin. Pharmacokinet.* **4**, 279-296 (1979). Pharmacodynamics and pharmacokinetics of a slow-release formulation in man: A. Ebihara *et al.*, *Arzneim.-Forsch.* **33**, 163 (1983). Toxicity: E. I. Goldenthal, *Toxicol. Appl. Pharmacol.* **18**, 185 (1971). Comprehensive description: A. M. Al-Obaid *et al.*, *Anal. Profiles Drug Subs.* **18**, 153-193 (1989).



Crystals from aq ethanol, mp 206°. uv max (95% ethanol): 288, 276, 336 nm ($E_{1cm}^{1\%}$ 945, 588, 144); (0.1*N* NaOH): 226, 273, 336 nm ($E_{1cm}^{1\%}$ 1147, 557, 133). Slightly sol in water, chloroform, ether. Sol in acetone, methanol, DMF, aq solns above pH 8.0. Less sol in ethanol. *Pharmaceut. Incompat*: Calcium gluconate, ascorbic acid, tetracyclines, urea, epinephrine. LD₅₀ orally in female, male rats: 2600, 2820 mg/kg (Goldenthal).

THERAP CAT: Diuretic; antihypertensive.

THERAP CAT (VET): Diuretic.

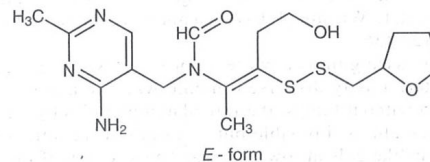
4310. Furoyl Chloride. [1300-32-9] Furancarbonyl chloride. $C_5H_3ClO_2$; mol wt 130.53. C 46.01%, H 2.32%, Cl 27.16%, O 24.51%. C_4H_3OCl .

Colorless liquid; mp -2°. bp 170°. Dec by water or alcohol. Sol in ether.

Caution: Vapors irritate the eyes.

4311. Fursultiamine. [804-30-8] *N*-[(4-Amino-2-methyl-5-pyrimidinyl)methyl]-*N*-[4-hydroxy-1-methyl-2-[(tetrahydro-2-furanyl)methyl]dithio]-1-butenyl]formamide; thiamine tetrahydrofurfuryl disulfide; Alinamin F; Diteftin; Judolor; TTFD. $C_{17}H_{26}N_4O_3S_2$; mol wt 398.54. C 51.23%, H 6.58%, N 14.06%, O 12.04%, S 16.09%. Prepn: S. Yurugi, T. Fushimi, **US 3016380** (1962 to Takeda). Metabolism: S. Kikuchi *et al.*, *Eur. J. Pharmacol.* **9**, 367 (1970); C. Mitoma, *Drug Metab. Dispos.* **1**, 698 (1973). Series

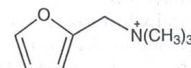
of papers on function of tetrahydrofurfuryl mercaptan moiety: *J. Biochem.* **74**, 717 (1973). Crystal structure: W. Shin, Y. C. Kim, *Bull. Korean Chem. Soc.* **7**, 331 (1986).



Colorless prisms from ethyl acetate, mp 132° (dec). d 1.29. Sparingly sol in water; sol in organic solvents, dil mineral acids. LD₅₀ in rats (mg/kg): 2200 orally; 540 i.p. (Yurugi, Fushimi).

THERAP CAT: Vitamin (enzyme cofactor).

4312. Furtrethonium. [7618-86-2] *N,N,N*-Trimethyl-2-furamethanaminium; furfuryltrimethylammonium; trimethylfurfurylammonium; furtrimethonium; Furmethide. $[C_8H_{14}NO]^+$. Prepn of salts: Nabenhauer, **US 2185220** (1938 to SK & F); Weilmuenster, Jordan, *J. Am. Chem. Soc.* **67**, 415 (1945); Khromov-Borisov *et al.*, *J. Gen. Chem. USSR* **24**, 2021 (1954).



Iodide. [541-64-0] Furamon; Furanol. $C_8H_{14}INO$; mol wt 267.11. Crystals from ethanol + ethyl acetate, mp 116-117° (Weilmuenster, Jordan); also reported as mp 118-120° (Khromov-Borisov). Soluble in water, alcohol. Practically insol in benzene. pH of 1% aq soln, 5.3-6.0.

Benzenesulfonate. Benzamon. $C_{14}H_{19}NO_4S$; mol wt 297.37. Crystals from ethanol + butyl acetate, mp 134-135° (Kromov-Borisov). Soluble in water, alcohol.

p-Toluenesulfonate. Fisostina. $C_{15}H_{21}NO_4S$; mol wt 311.40.

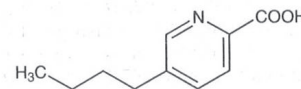
THERAP CAT: Cholinergic. Iodide as parasympathomimetic.

4313. Fusafungine. [1393-87-9] S-314; Biofusil; Fusaloyos; Fusarine; Locabitol. Antibiotic used as an aerosol for local application. Isoln from *Fusarium* species: Couchoud, **FR 1164181** (1958), *C.A.* **54**, 20074b (1960); Servier, **BE 612474** (1962), *C.A.* **57**, 11320b (1962); *idem*, **GB 1018626** (1966 to Biofarma), *C.A.* **64**, 16585b (1966). Bacteriological activity: D. Haler, *J. Int. Med. Res.* **5**, 61 (1977); *idem*, *Vie Med.* **61**, 507 (1980).

Solid, mp 125-129°. Stable up to 180°. Practically insol in water. Sol in glycols and fats.

THERAP CAT: Antibacterial.

4314. Fusaric Acid. [536-69-6] 5-Butyl-2-pyridinecarboxylic acid; 5-butylicolinic acid. $C_{10}H_{13}NO_2$; mol wt 179.22. C 67.02%, H 7.31%, N 7.82%, O 17.85%. Antibiotic (wilting agent) first isolated from the fungus *Fusarium heterosporium*, Nees; Yabuta *et al.*, *J. Agric. Chem. Soc. Jpn.* **10**, 1059 (1934). Isoln from other *Fusarium* species and from *Gibberella fujikuroi* and synthesis: Plattner *et al.*, *Helv. Chim. Acta* **37**, 1379 (1954). Prepn: Hardegger, Nikles, *ibid.* **39**, 505 (1956); **40**, 2428 (1957); Schreiber, Adam, *Ber.* **93**, 1848 (1960); Umezawa, Nagatsu, **DE 2005255** (1970 to Microbiochem. Res. Found.); R. Tschesche, W. Führer, *Ber.* **111**, 3502 (1978). Dopamine β -hydroxylase inhibitor and hypotensive activity: Suda *et al.*, *Chem. Pharm. Bull.* **17**, 2377 (1969); Nagatsu *et al.*, *Biochem. Pharmacol.* **19**, 35 (1970). Toxicity study: Ishii *et al.*, *Arzneim.-Forsch.* **25**, 55 (1975).

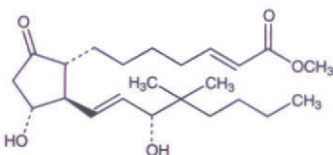


Colorless crystals, mp 96-98°. LD₅₀ orally in mice: 230 mg/kg (Ishii).

Copper salt. Bluish-violet crystals from water, mp 258-259°.

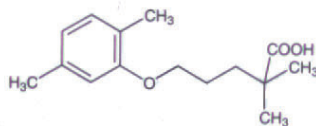
4315. Fusarubin. [1702-77-8] 3,4-Dihydro-3,6,9-trihydroxy-7-methoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-5,10-dione; 5,8-dihydroxy-2-(hydroxymethyl)-6-methoxy-3-(2-oxopropyl)-1,4-

4387. Gemeprost. [64318-79-2] (2E,11 α ,13E,15R)-11,15-Dihydroxy-16,16-dimethyl-9-oxoprostano-2,13-dien-1-oic acid methyl ester; 16,16-dimethyl-*trans*- Δ^2 -PGE₁ methyl ester; ONO-802; Cergem; Cervagem(e); Preglandin. C₂₃H₃₈O₅; mol wt 394.54. C 70.02%, H 9.71%, O 20.28%. Analog of prostaglandin E₁, *q.v.* Prepn: M. Hayashi *et al.*, *DE 2700021*; *idem.*, *US 4052512* (both 1977 to Ono); H. Suga *et al.*, *Prostaglandins* **15**, 907 (1978). Effects on uterine contractility and steroid hormone plasma levels: K. Oshima *et al.*, *J. Reprod. Fertil.* **55**, 353 (1979). Effects on reproductive function: K. Matsumoto *et al.*, *Nippon Yakurigaku Zasshi* **79**, 15 (1982), *C.A.* **96**, 98392 (1982). Use in termination of first trimester pregnancy: O. Reiertsen *et al.*, *Prostaglandins Leukotrienes Med.* **8**, 31 (1982).



THERAP CAT: Abortifacient; oxytocic.

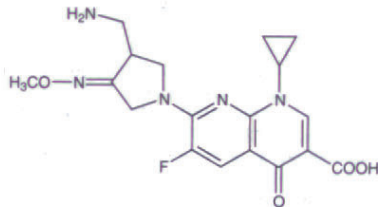
4388. Gemfibrozil. [25812-30-0] 5-(2,5-Dimethylphenoxy)-2,2-dimethylpentanoic acid; 2,2-dimethyl-5-(2,5-xyl-oxo)valeric acid; CI-719; Decrelip; Genlip; Gevilon; Lipozid; Lipur; Lopid. C₁₅H₂₂O₃; mol wt 250.33. C 71.97%, H 8.86%, O 19.17%. Serum lipid regulating agent. Prepn: P. L. Creger, *DE 1925423*; *idem.*, *US 3674836* (1969, 1972, both to Parke, Davis). Production: O. P. Goel, *US 4126637* (1978 to Warner-Lambert). Pharmacology: A. H. Kissebach *et al.*, *Atherosclerosis* **24**, 199 (1976); M. T. Kahonen *et al.*, *ibid.* **32**, 47 (1979). Series of articles on metabolism, clinical pharmacology, kinetics and toxicology: *Proc. R. Soc. Med.* **69**, Suppl. 2, 1-120 (1976). Toxicity data: S. M. Kurtz *et al.*, *ibid.* **15**. Clinical trial in hyperlipidemia: J. E. Lewis *et al.*, *Pract. Cardiol.* **9**, 99 (1983). Clinical reduction of cardiovascular risk in patients with low HDL levels: H. B. Rubins *et al.*, *N. Engl. J. Med.* **341**, 410 (1999).



Crystals from hexane, mp 61-63°. bp_{0.02} 158-159°. LD₅₀ in mice, rats (mg/kg): 3162, 4786 orally (Kurtz).

THERAP CAT: Antilipemic.

4389. Gemifloxacin. [175463-14-6] 7-[3-(Aminomethyl)-4-(methoxyimino)-1-pyrrolidinyl]-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid; SB-265805; LB-20304. C₁₈H₂₀FN₃O₄; mol wt 389.38. C 55.52%, H 5.18%, F 4.88%, N 17.99%, O 16.44%. Third generation fluorinated quinolone antibacterial. Prepn: J. H. Kwak *et al.*, *EP 688772*; C. Y. Hong *et al.*, *US 5633262* (1995, 1997 both to LG Chemical); C. Y. Hong *et al.*, *J. Med. Chem.* **40**, 3584 (1997). Antibacterial spectrum *in vitro*: R. Wise, J. M. Andrews, *J. Antimicrob. Chemother.* **44**, 679 (1999). HPLC-tandem MS determn in human plasma: E. Doyle *et al.*, *J. Chromatogr. B* **746**, 191 (2000). Clinical pharmacokinetics: A. Allen *et al.*, *Antimicrob. Agents Chemother.* **44**, 1604 (2000). Review of antibacterial activity, pharmacology, and clinical trials: J. M. Blondeau, B. Missaghi, *Expert Opin. Pharmacother.* **5**, 1117-1152 (2004).



Off-white, amorphous solid from chloroform-ethanol, mp 235-237°.

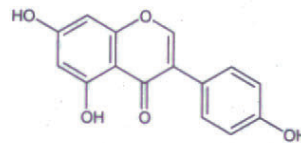
THERAP CAT: Antibacterial.

4390. Gemtuzumab Ozogamicin. [220578-59-6] CDP-771; CMA-676; Mylotarg. Immunoconjugate of *N*-acetyl- γ -calicheamicin with the humanized mouse monoclonal IgG4 κ antibody, hP67.6, directed against the human CD33 antigen located on the surface of normal and leukemic myeloid cells, but not on normal hematopoietic stem cells. Designed to deliver antibody-targeted chemotherapy for treatment of acute myelocytic leukemia (AML). Prepn of conjugate: P. R. Hamann *et al.*, *EP 689845*; *idem.*, *US 5773001* (1996, 1998 both to Am. Cyanamid). *In vitro* antineoplastic activity: K. Naito *et al.*, *Leukemia* **14**, 1436 (2000). Clinical evaluation in AML: E. L. Sievers *et al.*, *Blood* **93**, 3678 (1999). Reviews of development and therapeutic potential: I. D. Bernstein, *Leukemia* **14**, 474-475 (2000); I. Niculescu-Duvaz, *Curr. Opin. Mol. Ther.* **2**, 691-696 (2000); of clinical experience: F. J. Giles, *Expert Rev. Anticancer Ther.* **2**, 630-640 (2002).

Sensitive to light; protect from direct and indirect sunlight and unshielded fluorescent light.

THERAP CAT: Antineoplastic

4391. Genistein. [446-72-0] 5,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one; 4',5,7-trihydroxyisoflavone; prunetol; genisteol. C₁₅H₁₀O₅; mol wt 270.24. C 66.67%, H 3.73%, O 29.60%. Phytoestrogen found in soy products; the aglucon of genistin and of sophoricoside. Specific protein kinase inhibitor. Prepn from the glucoside by hydrolysis with emulsin: Charaux, Rabaté, *J. Pharm. Chim.* [9] **1**, 404 (1941); by hydrolysis with HCl in methanol: Walter, *J. Am. Chem. Soc.* **63**, 3273 (1941). Isoln from *prunus* spp., *Rosaceae*: Hasegawa *ibid.* **79**, 1738 (1957); from *Podocarpus spicata* R.Br., *Podocarpaceae*: Briggs, Cebalo, *Tetrahedron* **6**, 145 (1959). Structure: Baker, Robinson, *J. Chem. Soc.* **1925**, 1981; **1926**, 2713; Walz, *Ann.* **489**, 118 (1931). Synthesis: Baker, Robinson, *J. Chem. Soc.* **1928**, 3115; Narasimhachari *et al.*, *J. Sci. Ind. Res.* **12**, 287 (1953); Yoder *et al.*, *Proc. Iowa Acad. Sci.* **61**, 271 (1954); Zemplén *et al.*, *Acta Chim. Acad. Sci. Hung.* **19**, 277 (1959). HPLC determn in biological fluids: J. G. Supko, L. R. Phillips, *J. Chromatogr. B* **666**, 157 (1995); A. A. Franke *et al.*, *Proc. Soc. Exp. Biol. Med.* **208**, 18 (1995). Review of synthesis and isotopic labeling: K. Wähälä *et al.*, *ibid.* 27-32. Series of articles on chemopreventive properties and mechanism of action: *ibid.* 103-115, 120-130; *J. Nutr.* **125**, Suppl. 3, 777S-797S (1995).



Rectangular or six-sided rods from 60% alcohol. Dendritic needles from ether. mp 297-298° (slight decompn). Sol in the usual organic solvents, in dil alkalis with yellow color. Practically insol in water. uv max: 262.5 nm (ϵ 138).

Sophoricoside. [152-95-4] Genistein-4'-glucoside. C₂₁H₂₀O₁₀. From the green pods of *Sophora japonica* L., *Leguminosae*: Charaux, Rabate, *Bull. Soc. Chim. Biol.* **20**, 454 (1938). Structure: Zemplén *et al.*, *Ber.* **76**, 267 (1943). Synthesis: Bognár, Szabo, *Acta Chim. Acad. Sci. Hung.* **4**, 383 (1954); *Chem. Ind. (London)* **1954**, 518. Crystals from alcohol, mp 298°. [α]_D²⁰ -47° (pyridine). [α]_D²⁰ -32° (10% aq pyridine). uv max (abs ethanol): 262 nm. Sparingly sol in water, alc, acetic acid; more sol in hot alc, hot acetic acid; sol in pyridine, dil alkalis. Practically insol in ethyl acetate, acetone.

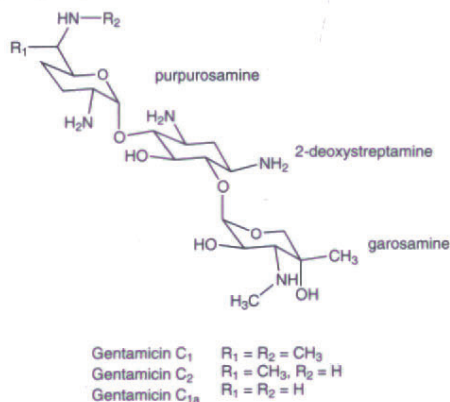
Genistin. [529-59-9] Genistein-7-O- β -D-glucoside. C₂₁H₂₀O₁₀. For isoln and structure see Walter, Hasegawa, Walz, *loc. cit.* Synthesis: Zemplén, Farkas, *Ber.* **76B**, 1110 (1943). Pale yellow plates from 80% ethanol, mp 256°. [α]_D²¹ -28° (c = 0.6 in 0.02N NaOH); [α]_D²⁶ -21.4° (pyridine). uv max (85% ethanol): 262.5 nm (a 90.5). Practically insol in cold water. Slightly sol in hot water, hot ethanol, hot methanol; sol in hot 80% ethanol, hot 80% methanol, hot acetone, pyridine.

Olmelin. 5,7-Dihydroxy-4'-methoxyisoflavone; biochanin A; 4'-methyl ether. C₁₆H₁₂O₅. Isoln from red clover: Pope *et al.*,

Chem. Ind. (London) **1953**, 1092; Wong, *J. Sci. Food Agric.* **13**, 304 (1962); from *Andira inermis* (Swartz) H.B.K., *Leguminosae*: Crocker *et al.*, *J. Chem. Soc.* **1962**, 4906. Identity with olmelin: Gakhokidze, *J. Appl. Chem. USSR* **23**, 789 (1950), *C.A.* **46**, 9098i (1952). Structure: Bose, Siddiqui, *J. Sci. Ind. Res.* **9B**, no. 1, 25 (1950). Synthesis: Baker *et al.*, *Nature* **169**, 706 (1952). Yellow needles from methanol, mp 212-216°.

USE: Chemical probe to explore signal transduction pathways.

4392. Gentamicin. [1403-66-3] Gentamycin. Antibiotic complex produced by fermentation of *Micromonospora purpurea* or *M. echinospora* and variants thereof: M. J. Weinstein *et al.*, *Antimicrob. Agents Chemother.* **1963**, 1. Isoln, purification and characterization: J. P. Rosselet *et al.*, *ibid.* **14**. Industrial pats.: G. M. Luedemann, M. J. Weinstein; Charney, **US 3091572**; **US 3136704** (1963, 1964, both to Schering). Consists of three closely related components, gentamicins C₁, C₂, C_{1a}, and also gentamicin A which differs from the other members of the complex but is similar to kanamycin C, *q.v.* Separation of gentamicin C components: H. Maehr, C. P. Schaffner, *J. Chromatogr.* **30**, 572 (1967); Wagman *et al.*, *ibid.* **34**, 210 (1968). Structures contain 2-deoxystreptamine, *q.v.*, linked to two saccharide units, these being **garosamine** and a **purpurosamine** in the C series gentamicins. Structure studies: D. J. Cooper *et al.*, *J. Chem. Soc. C* **1971**, 960, 2876, 3126. Structure of gentamicin A: H. Maehr, C. P. Schaffner, *J. Am. Chem. Soc.* **89**, 6787 (1967); **92**, 1697 (1969). Seps and structures of gentamicins A₁ to A₄: Nagabhushan *et al.*, *J. Org. Chem.* **40**, 2830, 2835 (1975). Synthetic studies: W. Meyer zu Reckendorf, Bischof, *Ber.* **105**, 2546 (1972); M. Chmielewski *et al.*, *Carbohydr. Res.* **70**, 275 (1979). Review of activity, toxicity and clinical pharmacology: J. Black *et al.*, *Antimicrob. Agents Chemother.* **1963**, 138-147. Comprehensive description: B. E. Rosenkrantz *et al.*, *Anal. Profiles Drug Subs.* **9**, 295-340 (1980). Determn in serum by immunoassay: H. A. Holt *et al.*, *J. Antimicrob. Chemother.* **34**, 747 (1994). Review of clinical use: S. B. Shrimpton *et al.*, *ibid.* **31**, 599-606 (1993). Clinical effect on chloride transport in cystic fibrosis: M. Wilschanski *et al.*, *Am. J. Respir. Crit. Care Med.* **161**, 860 (2000).



White amorphous powder, mp 102-108°. [α]_D²⁵ +146°. Freely sol in water; sol in pyridine, DMF, in acidic media with salt formation; moderately sol in methanol, ethanol, acetone. Practically insol in benzene, halogenated hydrocarbons.

Gentamicin C₁. [25876-10-2] C₂₁H₄₃N₅O₇; mol wt 477.60. mp 94-100°. [α]_D²⁵ +158°.

Gentamicin C₂. [25876-11-3] C₂₀H₄₁N₅O₇; mol wt 463.57. mp 107-124°. [α]_D²⁵ +160°.

Gentamicin C_{1a}. [26098-04-4] O-3-Deoxy-4-C-methyl-3-(methylamino)- β -L-arabinopyranosyl-(1 $\rightarrow$ 6)-O-[2,6-diamino-2,3,4,6-tetradeoxy- α -D-erythro-hexopyranosyl-(1 $\rightarrow$ 4)]-2-deoxy-D-streptamine; gentamicin D. C₁₉H₃₉N₅O₇; mol wt 449.54.

Gentamicin A. [13291-74-2] O-2-Amino-2-deoxy- α -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-[3-deoxy-3-(methylamino)- α -D-xylopyranosyl-(1 $\rightarrow$ 6)]-2-deoxy-D-streptamine. C₁₈H₃₆N₄O₁₀; mol wt 468.50.

Hydrochloride. mp 194-209°. [α]_D²⁵ +113°. Freely sol in water, methanol; slightly in ether. Practically insol in other organic solvents.

C complex sulfate. [1405-41-0] Alcomycin; Cidomycin; Dura-gentam; Garamycin; Garasol; Genoptic; Gentacin; Gent-Ak; Gentalline; Gentalyne; Gentibiopral; Genticin; Gentocin; Gentogram; Gent-Optal; Lugacin; Optagran; Pangram; Refobacin; Septopal; Sulmycin. White, hygroscopic powder, mp 218-237°. [α]_D²⁵ +102°. Sol in ethylene glycol, formamide. LD₅₀ in mice (mg base/kg): 430 i.p.; 485 s.c.; 75 i.v.; >9050 orally (Black).

THERAP CAT: Antibacterial.

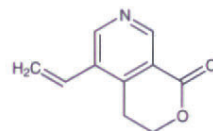
THERAP CAT (VET): Antibacterial.

4393. Gentian. Yellow gentian; pale gentian; bitter root. Dried rhizome and roots of *Gentiana lutea* L., *Gentianaceae*. *Habit.* Central and Southern Europe. *Constit.* Gentiin, gentiamarin, gentisin, gentisic acid, gentiopicroin, gentianose (a sugar), pectin.

THERAP CAT: Bitter tonic.

THERAP CAT (VET): Bitter tonic.

4394. Gentianine. [439-89-4] 5-Ethenyl-3,4-dihydro-1H-pyrano[3,4-c]pyridin-1-one; 4-(2-hydroxyethyl)-5-vinylnicotinic acid δ -lactone; erythricine. C₁₀H₉NO₂; mol wt 175.18. C 68.56%, H 5.18%, N 8.00%, O 18.27%. From *Gentiana kirilowi*, *Gentianaceae*: Proskurnina, *J. Gen. Chem. USSR* **14**, 1148 (1944), *C.A.* **40**, 7213 (1946); from *Anthocleista procera* Afz. and *Fagraea fragrans* Roxb., *Loganiaceae*: Lavie, Taylor-Smith, *Chem. Ind. (London)* **1963**, 781; Wan, Chow, *J. Pharm. Pharmacol.* **16**, 484 (1964). Isoln from *Slevogtia orientalis* Gris., *Gentianaceae*, structure and synthesis: Govindachari *et al.*, *J. Chem. Soc.* **1957**, 551, 2725.

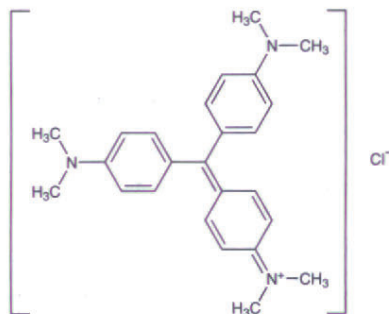


Needles from ether or petr ether, mp 82-83°. uv max: 220 nm (log ϵ 4.38). Sol in alkali.

Hydrochloride. C₁₀H₉NO₂·HCl. Needles from alcohol + ether, dec 169-170°.

Dihydrogentianine. C₁₀H₁₁NO₂. Crystals from ether + petr ether, mp 74-76°. uv max: 270 nm (log ϵ 3.4).

4395. Gentian Violet. [548-62-9] N-[4-[Bis[4-(dimethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methylmethanaminium chloride; C.I. Basic Violet 3; hexamethylparosaniline chloride; hexamethyl-p-rosaniline chloride; aniline violet; crystal violet; methylrosanilinium chloride; C.I. 42555; Axuris; Badil; Gentiaverm; Pyoktanin. C₂₅H₃₀ClN₃; mol wt 407.98. C 73.60%, H 7.41%, Cl 8.69%, N 10.30%. Prepn and properties: *Colour Index* vol. 4 (3rd ed., 1971) p 4391. Toxicity studies: H. C. Hodge *et al.*, *Toxicol. Appl. Pharmacol.* **22**, 1 (1972). Review of metabolism and mode of action: R. Docampo, S. N. Moreno, *Drug Metab. Rev.* **22**, 161-178 (1990); of use as a biological stain: *Conn's Biological Stains*, R. W. Horobin, J. A. Kiernan, Eds. (BIOS Scientific Publishers Ltd, Oxford, UK, 10th ed., 2002) 193-195.



Dark green powder or greenish, glistening pieces with metallic luster. Soly (%): water 0.2-1.7; ethanol 3-14; acetone 0.4; chloroform 5.1. Insol in xylene. Absorption max (water): 590 nm.

Consult the Name Index before using this section.

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