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Merck & Co., Inc. Announces...

  - More than 25,000 copies sold
- Reference set now includes book *and* CD
- CD includes the content of the book *plus*
  almost 1000 monographs retired from the 12th (1996) & 13th (2001) editions
- Includes a free 1-year personal subscription to CambridgeSoft Internet Edition

*Chemistry’s Constant Companion™*
Merck began the development and publication of medical textbooks more than 100 years ago. The goal was to provide the scientific and medical communities with the very best information, on a not-for-profit basis. These books have grown to be considered the world’s most respected and best-selling texts in the fields of chemistry, medicine, veterinary science and geriatrics.

www.merckbooks.com

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What is *The Merck Index*?

- First published in 1889
- World renowned handbook of chemical, pharmaceutical and biomedical information
- Critically evaluated, peer-reviewed, and authoritative information
- Concise yet descriptive
The Merck Index:
Authoritative and Essential

- Editorial staff researches and analyzes a variety of sources to identify compounds, data and literature citations
- Focuses on compounds of significance in research, commerce and environmental impact
- Structures, physical properties, trademarks and CAS registry numbers critically evaluated and assigned to specific chemical entities
- Merck Index Monograph Number used as an international compound identifier by chemical suppliers and other reference works
The Merck Index: Broad Subject Coverage

- Drugs for humans and animals
- Organic chemicals used in research and manufacturing
- Plants and traditional medicines
- Natural products and biologicals
- Agriculturals, pesticides, herbicides
- Food additives and supplements
- Fragrances, cosmetics, dyes, colors

Chemistry’s Constant Companion™
It's all in *The Merck Index*
The Merck Index:
Your Index to Chemical Information

- Collection of monographs covering >18000 compounds with >50000 synonyms
- >15000 Trademarks and manufacturers
- CAS Registry Numbers for >12000 compounds
- >8500 Chemical Structures
  - Molecular formulae, line formulae, molecular weight, percentage composition

- Physical Properties
  - Melting point, boiling point, Log P, density, absorbance maxima, solubility, flash point, optical rotation…
The Merck Index:
Your Index to Chemical Information

- Toxicity, Handling, Cautions
- US Regulatory Information
  - Controlled Substances, Carcinogens
- Medical Uses for therapy and diagnosis
- Commercial Uses
- Key citations to the scientific literature
- International patent coverage

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What’s New in the Monograph Section

- New content – over 500 new monographs
- Extensively revised
  - More than half of the existing entries updated
  - Updated with new references and uses
  - Up-to-date US regulatory information for controlled substances and carcinogens
  - More physical properties
  - Molecular weights recalculated with the latest IUPAC standards

Chemistry’s Constant Companion™
Expanded Focus for Researchers

- >100 new monographs covering chemicals of significance in modern organic synthesis
  - Polymer additives, solvents, fluorescent stains, reagents
- 25 New Monographs on Named Reagents
- Expanded coverage on “Green Chemistry” and environmentally important compounds

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Reagents and Commercial Chemicals

- Texanol Isobutyrate
  - Plasticizer for manufacturing of vinyl flooring, toys, other vinyl products
- Triflic Acid
  - Catalyst and solvent; one of the strongest acids known
- Trifluoroethanol
  - Environmentally friendly alternative to CFCs
Reagents and Commercial Chemicals

- **Selectflor**
  - Electrophilic, versatile fluorinating reagent

- **Samarium Iodide**
  - One-electron reducing agent used in organic synthesis and electron transfer reactions

- **Herrmann-Beller Catalyst**
  - Highly efficient palladacycle catalyst; used in carbon-carbon bond forming reactions such as the Heck and Suzuki reactions
Research Probes and Stains

- Epicocconone
  - Fluorescent natural product isolated from the fungus *Epicoccum nigrum*; biodegradable fluorescent stain for protein detection

- Maitotoxin
  - One of the most toxic and largest (mol wt 3422 Da) natural products known to date; involved in ciguatera fish poisoning; research tool for ion flux

- PMSF or phenylmethanesulfonyl fluoride
  - Standard protease inhibitor in biological research
Human Pharmaceutical Products

- **Antidiabetic**
  - **Insulin Detemir**: Levemir (Novo); soluble long-acting basal insulin analog
  - **Sitagliptin**: Januvia (Merck & Co.); selective inhibitor of dipeptidyl peptidase IV (DPP-IV)

- **Antineoplastic**
  - **Aprinocarsen**: Affinitac (Lilly); antisense oligonucleotide designed to inhibit protein kinase C-a (PKC-a) expression
  - **Cetuximab**: Erbitux (ImClone); chimeric mAb directed against human epithelial growth factor receptor (EGFR); in treatment of colorectal cancer
Human Pharmaceutical Products

- **Immunomodulator**
  - **Sipuleucel-T**: Provenge (Dendreon); therapeutic vaccine designed to stimulate immunity against human prostatic acid phosphatase; antineoplastic

- **Immunosuppressant**
  - **Abatacept**: Orencia (BMS); recombinant chimeric fusion protein composed of CTLA-4 fused to human IgG; antipsoriatic

- **Diagnostic Aid**
  - **Ferumoxtran 10**: Combidex (Advanced Magnetics); Sinerem (Guerbet); dextran covered superparamagnetic iron oxide magnetite nanoparticles; MRI imaging agent to detect metastatic cancer in lymph nodes
Plants and Herbal Medicines

- **Andrographis**

- **Bilberry and Bilberry Extract**
  - Deciduous, dwarf shrub, *Vaccinium myrtillus* L., *Ericaceae*; extract used in eyecare and skin products; used in treatment of night blindness

- **Hoodia**
  - Genus of succulent plants in the family *Apocynaceae*; used in African traditional medicine as an appetite suppressant

*Chemistry’s Constant Companion™*

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The Merck Index: More than Just the Monographs

- 450 Organic Name Reactions
  - Unique compilation of reactions
  - Schema and key references
  - Excellent teaching tool for organic chemistry
377. **Sonogashira Coupling** (Sonogashira-Hagihara Coupling)


\[ \text{R-X} \xrightarrow{\text{Palladium catalyst (e.g. PdCl}_2\text{(PPh}_3)_2\text{)}} \text{H-} \xrightarrow{\text{Copper catalyst (e.g. Cul), base (e.g. NEt}_3\text{)}} \text{R-} \xrightarrow{} \text{R}^1 \]

Palladium(0)-copper(I) catalyzed cross-coupling between sp\(^2\)-hybridized organic halides and terminal acetylenes.

The Merck Index:
Expanded Supplemental Tables

32 Tables/70 Pages of hard-to-find information

- **New tables**
  - Vaccines
  - Acronyms
  - Physical & mathematical constants
  - Selected hexoses & pentoses

- **Updated Tables**
  - Company register
  - Glossary
  - Periodic table
  - USAN and INN terms for radical and groups
  - Manufacturer codes
  - International patent codes
  - Table of atomic weights

Chemistry’s Constant Companion™
14th Edition Electronic Products

CD-ROM
- Included as companion to the book
- Text searchable with structure upgrade available
- Single user or single workstation
- Windows compatible
- Stand alone product requires no internet access

Internet Edition
- Platform independent
- Text and structure searchable
- Updated semi-annually
- 1 year personal subscription included with book/cd purchase

Dialog/STN Databases
- The Merck Index Online to be updated with the new edition

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Getting Started

Install The Merck Index
User Help Guides
Technical Support
Web Access & CD Enhancements

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Getting Started: CD Installation

Two part installation:
Part 1: Required of all Users
Part 2: Required only if using a version of ChemOffice less than 10
Getting Started: CD Registration

- To use the CD it must be registered.
- Register the CD after selecting Compound Search at the Main Menu.
- The registration (serial) number is found on the CD envelope in the back of your book.
- Use this same number to sign-up for the 1-year personal subscription to the internet edition at:

  http://scistore.cambridgesoft.com/software/fulfill_includedproducts.cfm?CFID=10460394&CFTOKEN=15199970%20
Features of CD and Web Product

- Revised search interface
- Can search text fields, properties, or a combination of both
Chemistry’s Constant Companion™

Search Guide: Text Search

**Compound Names** searches:
- Monograph Title (Bisorclozole)
- CAS Name (5-butylpicolinic acid)
- Additional Names (betrolic acid)
- Trademark (Coumadin)
- Manufacturer Code (H-168)
- Derivative Type (hydrochloride)

**Literature References and Notes** searches:
- Literature References Notes
- Search by keywords (inhibitor, antioxidant), author, journal title, reference type (prepn, isoln, determn, clinical, pharmacology, patent, review), caution statement (carcinogen, overexposure).

**Monograph Title**
(Entecavir, Mepact, Noviflumuron)

Searches only the monograph title as it appears in the book

**Non-Medical Uses**
(solvent, catalyst, herbicide)

**Human Therapeutic Use**
(vasodilator)

Search the therapeutic category database field and associated index terms

**Veterinary Therapeutic Use**
(antibacterial, anthelmintic)

Consult Therapeutic Category and Biological Activity Index in the back of book.

**Manufacturer** (BASF)
Consult Company Register in the Supplemental Tables section of the book for company abbreviations.

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Search Guide: Properties Search

**Properties (Full Text)**
Search by keywords (solid, yellow, vapor pressure)

**Molecular Formula searches:**
- Line Formula
- Molecular Formula
- Derivative Molecular Formula
- Extra Formula

*Use Hill Convention (C, then H, then other elements in alphabetical order)*

**Molecular Weight**
Search parent and derivative molecular weights as numerical ranges

---

*Please note: The Search Screen Help Guide can be printed from the User Help Guides on the Main Menu.*
Navigation: Within an Answer Set
Navigation: To additional resources

The Merck Index
Fourteenth Edition

Name Reactions | Tables | Help

Search Monographs

Supplemental Tables

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Search for a Specific Compound

The Merck Index
Fourteenth Edition

Cyanuric Chloride

Monograph Title
Searches only the monograph title as it appears in the book

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Use:

Intermediate in the synthesis of active dyes, agricultural products, and drug substances. Reagent in organic synthesis. Coupling agent for nucleic acids and proteins; cyanuric chloride-activated paper is used in capillary and electrophoretic applications, dot tests, and hybridization protocols.

CAUTION: Eye irritant; avoid skin contact and inhalation (Hunger, 1986).

Use:

Searching for a Specific Compound

Cyanuric Chloride

Monograph Number: 0002699
Title: Cyanuric Chloride
CAS Registry Number: 108-77-0
CAS Name: 2,4,6-Trichloro-1,3,5-triazine
Additional Names: Trichloro-triazine
Molecular Formula: C₃Cl₆N₃
Molecular Weight: 164.41

Percent Composition: C 19.54%, Cl 57.88%, N 22.78%

Literature References:

Properties:
- Crystals from ether, mp 145.5°, bp 186°.
- Crystal density: 1.93 g/cm³.

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Search for Compounds by a Specific Company

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Fourteenth Edition

**TEXT SEARCH**
- Compound Names
- CAS Registry Number
- Literature References and Notes
- Manufacturer: BASF

**PROPERTIES SEARCH**
- Properties (Full text)
- Mol Formula

*Chemistry's Constant Companion™*

Consult Company Register in the Supplemental Tables section of the book for company abbreviations.
Search for Compounds by a Specific Company

Used to switch between monograph view and table view.
Step #1: Click on compound of interest

Step #2: Return to the monograph view for details
Search for a Specific Author

Chemistry's Constant Companion™
Active vs. Retired Monographs

Monographs that have been removed from the 12th and 13th editions have been provided on *The Merck Index* 14th edition CD in a retired state.

- The search default is to search over all active and retired monographs.
- Searches can be conducted over the active monographs only.
- After each search the default is restored and searches will be conducted over active and retired monographs unless the box next to “Search Active Monographs Only” is checked.
Search Active and Retired Monographs for Insecticides
Active and Retired Monographs on Insecticides

Example of Active Monograph

Abamectin

The Merck Index

Example of Retired Monograph

Sesamex

There are 285 active and retired monographs on compounds with a use as an insecticide.
Active Monographs on Insecticides

Step #1: Check the box next to Search Active Monographs Only

Step #2: Enter keyword “insecticide” into Non-Medical Use field

Chemistry’s Constant Companion™

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There are 257 active monographs on compounds with a use as an insecticide. Therefore, 28 monographs are retired.
**Multiple Terms in a Single Field**

<table>
<thead>
<tr>
<th>TEXT SEARCH</th>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Compound Names</td>
<td></td>
<td>Monograph Title</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CAS Registry Number</td>
<td></td>
<td>Non-Medical Uses</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Literature References</td>
<td><strong>controlled substance AND anabolic steroid</strong></td>
<td>Human Therapeutic Use</td>
<td></td>
<td></td>
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<tr>
<td>and Notes</td>
<td></td>
<td>Veterinary Therapeutic Use</td>
<td></td>
<td></td>
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<tr>
<td>Manufacturer</td>
<td></td>
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</tbody>
</table>

*Please note:* Boolean operators must be capitalized when using the internet edition.
Multiple Terms in a Single Field

Sampling of results from searching “controlled substance AND anabolic steroid” in Literature References and Notes.

The table view allows quick review of the structures to assess similarities.
Multiple Terms in Separate Fields

Searching for monographs with a human therapeutic use of antilipemic that have toxicity data (or where toxicity data exists).

The asterisk “*” can be used for “wild cards” and “exists” searches.
Properties Range Searching

Fields within the Properties Search section are range searchable.
Please note: Properties searches will cover both parent and derivative values as illustrated below.
Human Therapeutic Use of Astringent

Monograph Number: 000257
Title: Alkannin
CAS Registry Number: 517-92-4
CAS Name: 5,8-Dihydroxy-2-[(1S)-1-hydroxy-4-methyl-3-penteny]-1,4-naphthalenedione
Additional Names: (S)-5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-penteny)-1,4-naphthalenedione; anchusa acid; anchusin; alkanna red; alkannet extract, (1-hydroxy-3-isohexenyl)naphthalazine; 2-(1-hydroxy-4-methyl-3-penteny)-5,8-dihydroxy-1,4-naphthalenedione, C.I. Natural Red 20, C.I. 75530.
Molecular Formula: C_{30}H_{36}O_{5}
Molecular Weight: 650.5
Percent Composition: C 86.66%, H 6.59%, O 27.75%
Properties: Brownish-red prisms with a metallic sheen from benzene, mp 149°. Can be sublimed in high vac at 140-150°. [α]_{D}^{20} -165° (benzene), -226° (chloroform). Also reported as -254 ± 7° (chloroform) (Toribara). Sol in organic solvents, sparingly sol in water. Buffered aq solns are red at pH 6.1; purple at pH 8.3; blue at pH 10.0. L.D_{50} in male, female mice, rats (g/kg): 3.0 ± 1.0; 3.1 ± 0.1; > 1.0 orally (Malakova).
Limit Human Therapeutic Use of Astringent
Search to Those with Aluminum

### TEXT SEARCH

<table>
<thead>
<tr>
<th>Compound Names</th>
<th>Monograph Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Registry Number</td>
<td>Non-Medical Uses</td>
</tr>
<tr>
<td>Literature References and Notes</td>
<td>Human Therapeutic Use</td>
</tr>
<tr>
<td>Manufacturer</td>
<td>Veterinary Therapeutic Use</td>
</tr>
</tbody>
</table>

### PROPERTIES SEARCH

<table>
<thead>
<tr>
<th>Properties (Full text)</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar Formula</td>
<td>Index of Refraction</td>
</tr>
<tr>
<td>Molar Weight</td>
<td>Optical Rotation</td>
</tr>
</tbody>
</table>

*astringent*
Human Therapeutic Use: Astringent

Molecular Formula: Al

Aluminum Ammonium Sulfate

Monograph Number: 0000327
Title: Aluminum Ammonium Sulfate
CAS Registry Number: 7784-25-0
Additional Names: Burnt ammonium alum, exsiccated ammonium alum
Molecular Formula: AlNH4SO4
Molecular Weight: 237.15
Percent Composition: Al 11.38%, H 1.70%, N 5.91%, O 53.97%, S 27.04%
Line Formula: AlNH4SO4
Properties: About 97-98% pure; the balance is chiefly excess Al2O3. White powder. One gram dissolves in about 20 ml cold, 1.5 ml boiling water, usually incompletely, practically insol in alcohol. Keep well-closed.

Derivative Type: Decahydrate

Additional Names: Ammonium alum
Properties: It is about 98.5% pure. Colorless crystals, white granules or powder, styptic taste. d 1.66, mp 94.5°. Al about 350°. Becomes weaker, disintegrates above 200°. One gram dissolves in 7 ml water. 0.6 ml hot water freely soluble in alcohol, nearly miscible.
The Search Monographs function can be coupled with other features of the CD.

For example: To find a definition for the term “lakes,” the glossary can be very helpful.

Selecting Tables links to the Glossary and other tables. The Supplemental Tables can also be accessed from the Main Menu.

Use: Important intermediate in the manuf of alizarin and indanthrene dyestuffs; forms insol Ca, Ba, Pb lakes. Antioxidant in synthetic lubricants; fungicide.
After selecting Tables while in the monograph view, the full listing of the Supplemental Tables appears.

Scroll through the list and double-click to view the table of interest.
The "Search" feature of Adobe Acrobat enables quick retrieval of glossary terms.
Searching for Structure and Properties†

To conduct a substructure search on anthracene:

Step #1: Double-click in structure box for drawing toolbar to appear.

Step #2: Use toolbar to draw structure.

Step #3: Click outside of the structure box and execute by clicking on “Search.”

† Please note that the following examples are conducted using the structure upgrade form of the CD. For further information on this upgrade, please contact CambridgeSoft.

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Structure and Properties Searching

To further refine the substructure search.

Anthracene

Monograph Number: 0000682
Title: Anthracene
CAS Registry Number: 120-12-7
Molecular Formula: C_{14}H_{10}
Molecular Weight: 178.23
Percent Composition: C 94.34%, H 5.66%

Literature References: Obtained from coal tar. q.v.: Dumas, Laurent, Ann. 5, 10 (1833); Laurent, Ann. 31, 237 (1840); Anderson, Ann. 122, 234 (1882); J. Chem. Soc. 15, 44 (1892); Auerbach, Das Anthracen und seine Derivate (Braunschweig, 1890); Pflüger, J. Soc. Arts 27, 572 (1879); Lunge, Coal Tar and Armatores (1916); Barnett, Anthracene and Anthraquinone (London, 1921); Naman, Text. Color. 48, 605, 676, 751 (1926); 49, 19, 246, 557, 593 (1927); Houben, Fischer, Das Anthracen und die Anthraquinone (Leipzig, 1929); Borrmann, Der Tee (Leipzig, 1940); Schumann, Kokerette (Stuttgart, 1940). Extensive patent literature on purification.

Properties: Monoclinic plates from coal. Sublimes. Yellow or colorless with violet fluorescence; when impure (due to tetracene, naphthacene), yellowish with green fluorescence. Strongly triboluminescent and triboelectric. d_{20}^\circ = 1.25, mp 218°, bp_{300}^\circ = 342°.

Absorption spectrum: Clar, Ber. 65, 506 (1932). Less soluble than the isomeric phenanthrene. Insol in water, one gram dissolves in 57 ml abs alcohol, 70 ml methanol, 82 ml benzene, 85 ml chloroform, 200 ml ether, 31 ml carbon disulfide, 86 ml carbon tetrachloride.
A structure search can be further refined by adding additional search terms.

For example: To refine the substructure search on anthracene, the keyword “violet” is added.
Search results from the refined substructure search on anthracene and violet among the properties.
Organic Name Reactions

Access the Organic Name Reactions from the Main Menu or from any monograph.
Organic Name Reactions

- 450 Organic Name Reactions are included
- Each contains:
  - Reference history
  - Associated reaction schema

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Organic Name Reactions
Browse Reaction Names Alphabetically

The Organic Name Reactions (ONR) section is intended to serve the professional chemist and student by describing organic chemical reactions which have come to be recognized and referred to by name within the chemistry community. A select group has been chosen for addition to this section. Each reaction description is designed to be informative and representative of the pertinent literature, however, it is not meant to be comprehensive. The descriptions are composed of the following: (1) name(s) associated with the reaction, (2) the original and/or primary contributor(s) connected with the discovery and/or development of the reaction, (3) a concise description of the transformation, (4) a reaction scheme, (5) key references, and (6) cross references to other ONR based on commonality. The index included in this section also lists supplementary terms.

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Select the Search tab to find a specific reaction by using keywords.

020. Bartoli Indole Synthesis


One-step reaction of ortho-substituted anilines with vinyl Grignard reagents to yield 7-substituted indoles.

Organic Name Reactions
To Create a List of Favorites

Step #1: While viewing a reaction of interest, select the “Favorites” tab.

020. Bartoli Indole Synthesis


One-step reaction of ortho-substituted nitroarenes with vinyl Grignard reagents to yield 7-substituted indoles:


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Organic Name Reactions
To Create a List of Favorites

Step #2: At the bottom of the window, in the “Current Topic” box, the reaction name will appear.
- Select “Add” to include the reaction among the Favorites.
Organic Name Reactions
To Create a List of Favorites

The added reaction name will appear among the Favorites.

To view a reaction, select the Favorites tab and either double-click on the reaction name or highlight the reaction name and select Display.

To remove a reaction from the list of Favorites, highlight the reaction name and select Remove.

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Highlights for the 14th Edition

- Book/CD reference set is now available
  - List Price $125 USD; show discount 15%
- Reference set now includes book and CD
- Over 700 new and majorly revised monographs, expanded supplemental tables, 450 Organic Name Reactions
- CD includes almost 1000 monographs retired from the 12th & 13th editions
- Includes a free 1-year personal subscription to CambridgeSoft Internet Edition
- Internet subscriptions and site licenses visit CambridgeSoft at www.cambridgesoft.com

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Suggestions…Please Contact Us

Have an idea for a new monograph?
    Found an ONR that is not included?
    A recommendation to improve the product?

Please contact us…

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