

# CHEMICAL COMPOUND DATA SEARCHING

ALDRICH CATALOG - 2

Aldrich (Functional Group) Structure Index (e.g. Aromatic Acid Halides, Aromatic Amines, ...)  
S-A Library of Rare Chemicals (Functional Group) Structure Index (38K compounds).

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April 2003

## MERCK INDEX, 13th Edition, 2002

(MIL-8 QREF TABLE)

4,000 drugs and pharmaceuticals, 2,000 organic compounds/reagents, 2,000 naturally occurring substances, 1,000 elements/inorganic compounds, 1,000 agricultural compounds/biological agents.

Name, Formula, CAS RN, and Therapeutic Category & Biological Activity Indexes, Organic Name Reactions and Miscellaneous Tables (e.g. Greek alphabet, Isotonic Solutions, Latin Terms, Conversion Factors, etc.)

## ALDRICH CATALOG -- PRINT

(MIL-8 QREF Table)

Over 37,000 Products. Organics, Polymer Products, Organometallics, Inorganics, etc., Compounds arranged by 'product' name. Entries include physical properties, and references to Aldrich Library of NMR or FT-IR Spectra ... Molecular Formula, CAS RN indexes.

\*\*\*Aldrich (Functional Group) Structure Index (e.g. Aromatic Acid Halides, Aromatic Amines, ...)

\*\*\*S-A Library of Rare Chemicals (Functional Group) Structure Index (38K compounds).

## ALDRICH CATALOG -- <http://www.sigmaaldrich.com/Brands/Aldrich.html>

Physical properties, literature and spectra references and MSDS online, with registration.

Search by Name, CAS RN, Molecular Formula, Molecular Weight & Substructure.

## COMBINED CHEMICAL DICTIONARY

<http://www.chemnetbase.com/scripts/ccdweb.exe> (Netscape preferred)

The Combined Chemical Dictionary includes all the compounds contained in:

Dictionary of Organic Compounds (255,000)

Dictionary of Inorganic/Organometallic Compounds (101,000)

Dictionary of Natural Products (170,000)

Dictionary of Drugs (40,000)

Dictionary of Analytical Reagents (14,000)

The CCD provides descriptive and numerical data on chemical, physical and biological properties, systematic and common names, literature references, structural diagrams (click on the 'benzene' ring) and connection tables (for structure searching).

Search options include: Menu Search, and Structure Search.

Searching for CAS RNs (e.g. 50-06-6) is done without hyphens (e.g. 50066), but browsing is done with hyphens.

Browsing for 50066 displays a list beginning with 50256-18-3.

Browse provides a ranked list of each data set. In the MF dictionary there are sub-sets for 'all metals' and 'all-nonmetals' as well as all compounds with a given element (e.g. -ALL-Tc) and compounds with 'only CHNOX' and a variety of other element combinations.

## CCD COMPOUND SELECTION:

Basic fundamental organic and inorganic compounds ...

Virtually every known natural product

All currently marketed drugs

Compounds with an established use (e.g. catalysts, solvents, reagents, etc.)

Important coordination compounds

Organometallic compounds representative of all important structural types

Important biochemicals and minerals

Miscellaneous compounds of ... active research interest

A (220 page) user manual is available, in addition to a Quick Reference Guide.

(Mil-8 REF QD5 C65 1997)

ChemINDEX (Chemfinder.com) <http://chemindex.cambridgesoft.com/>

See: Chemfinder.com - ChemINDEX comes without popup ads and expanded results

## CHEMFINDER.COM <http://www.chemfinder.com/>

Nearly 80,000 chemical compounds, from over 350 public source sites, including: biochemicals, medications, MSDS, pesticides/herbicides, physical properties (including manufacturer's catalogs), regulations, structures, usage, regulatory data, and NIST. A site list is available: <http://chemfinder.cambridgesoft.com/about/chemfinder/indexedsites.asp>

Both a Simple Query (name, formula, molecular weight or CAS registry number) and a Structure Query (with ChemDraw or Chem3D plugins) are provided.

A full description is given at: [http://library.caltech.edu/learning/course\\_materials.htm](http://library.caltech.edu/learning/course_materials.htm)

## DIPPR <http://library.caltech.edu/databases/> (to retrieve password)

Temperature-dependent properties for over 1,600 pure chemicals

A property listing is given at: [http://library.caltech.edu/learning/course\\_materials.htm](http://library.caltech.edu/learning/course_materials.htm)

## JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA (JPCRD)

JPCRD provides well-defined physical and chemical properties of well-characterized materials or systems. Data is critically evaluated to assess accuracy of the compilations.

Indexes are provided for both properties (e.g. Activity Coefficients) and classes of materials (e.g. Atmospheric Gases) and are cumulated (v.1-10, v.11-20, v.21-29). Beginning with the cumulated index for v.21-30, the AIP classification is used instead of an alphabetical index..

In addition to the journal, a series of monographic supplements has also appeared. See: [http://library.caltech.edu/learning/course\\_materials.htm](http://library.caltech.edu/learning/course_materials.htm)

## PHYSPROP (ENVIRONMENTAL) <http://esc.syrres.com/interkow/PhysProp.htm>

Environmental Physical Properties for ~25,000 Compounds. Search by CAS RN only.

## ORGANIC SOLVENTS, 4<sup>th</sup> ed., 1986 MIL-8 REF QC 544.5 R72

Physical Properties .. Purification (~500 solvents).

## SOLV-DB (SOLVENTS DATABASE) <http://solvdb.ncms.org/index.html>

Properties & Cost. Search by Name, CAS RN, Sax #, MF, Category or Property Range.

## MATHESON GAS DATA BOOK, 6<sup>th</sup> ed., 1980 MIL-8 REF TP 761 C65 M3

Physical/Thermodynamic Properties for (Industrial) Gases

## BRENDA <http://www.brenda.uni-koeln.de/>

Comprehensive Enzyme Information System. Search by Name, EC #, CAS RN, etc.

## HANDBOOK OF PROTEOLYTIC ENZYMES

[http://skinbark.caltech.edu/cdroms/Handbook\\_of\\_Proteolytic\\_Enzymes/](http://skinbark.caltech.edu/cdroms/Handbook_of_Proteolytic_Enzymes/)

Grouped by catalytic type (Serine-, Cysteine-, Aspartic-, Metallo- and Unclassified-Peptidases)

## NIST CRITICALLY SELECTED STABILITY CONSTANTS OF METAL COMPLEXES

[http://skinbark.caltech.edu/cdroms/NIST\\_Critically\\_Selected\\_Constants\\_of\\_Metal\\_Complexes\\_2001/campus\\_access/](http://skinbark.caltech.edu/cdroms/NIST_Critically_Selected_Constants_of_Metal_Complexes_2001/campus_access/)

Updated CD-ROM version of Martell's Critical Stability Constants (H considered a metal).

# NIST CHEMISTRY WEBBOOK

<http://webbook.nist.gov/chemistry/>

Database contains ~40,000 compounds (mostly organic with a few small inorganics).

Data Type	Number of Species
Gas phase thermochemical data	6,500+
Condensed phase thermodynamic data	5,600+
Phase change thermodynamic data	13,800+
Reaction thermodynamic data	9,800+
Gas phase ion energetics data	15,600+
Gas phase ion cluster data	1,100+
IR spectrum	8,700+
Mass spectrum	12,600+
UV/Vis spectrum	400+
Vibrational & electronic energy levels	4,100+
Constants of diatomic molecules	600+
Fluid property data	33

Search Options: Formula, Name, CAS RN

Enter a chemical species name (e.g., methane)

Select the desired units for thermodynamic data: SI or calorie based

Select the desired type(s) of data:

Thermodynamic Data	Other Data
<input type="checkbox"/> Gas phase	<input type="checkbox"/> Gas phase IR spectrum
<input type="checkbox"/> Condensed phase	<input type="checkbox"/> Mass spectrum
<input type="checkbox"/> Phase change	<input type="checkbox"/> UV/Vis spectrum
<input type="checkbox"/> Reaction	<input type="checkbox"/> Vibrational and/or electronic spectrum
<input type="checkbox"/> Ion energetics	<input type="checkbox"/> Constants of Diatomic Molecules
<input type="checkbox"/> Ion cluster	<input type="checkbox"/> Henry's Law

Search Options: Ionization Energy, Electron/Proton Affinity, Vibrational/Electronic Energy Levels, Molecular Weight.

Data Set: Thermophysical Properties of selected fluids.

## KIRK-OTHMER ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY

<http://www.mrw.interscience.wiley.com/kirk/>

Extensive Physical Property Data for Common Industrial compounds, e.g.

ACETIC ACID AND DERIVATIVES  
ACETYLENE  
ADIPIIC ACID  
ALUMINUM COMPOUNDS  
AMMONIA

Updated regularly, **Kirk-Othmer Online** will stay current with the latest developments in chemical technology and related fields. Articles will be updated and revised in response to actual changes and developments as they occur in the chemical industry.

Also in print (4th ed. SFL REF) (1st-3d ed. MIL-8 REF) TP9 E685

## ULLMANN'S ENCYCLOPEDIA OF INDUSTRIAL CHEMISTRY

<http://www.mrw.interscience.wiley.com/ueic/>

Ullmann's describes chemical substances, ranging from raw materials and bulk products to fine and specialty chemicals, in detail.

Information on physical and chemical properties, production, applications, economic data, toxicology and occupational health is provided. Relevant patent information is supplied wherever available.

Fully international in scope and coverage and published in the English language, Ullmann's has been compiled under the supervision of a renowned global [Editorial Advisory Board](#). It contains nearly 1000 major articles, 10,000 tables, 30,000 figures, and innumerable literature sources and cross-references, written by some 3,000 authors affiliated to leading chemical companies or research institutes.

# BEILSTEIN / GMELIN CROSSFIRE

Organic / Inorganic-Organometallic compound databases for property data.

## What is CrossFire?

- CrossFire is a search system with a locally loaded client interface (Beilstein Commander) which provides access to the CrossFire server at the University of Wisconsin - Madison. Macintosh or MS Windows versions are available for downloading to Caltech workstations, from the library web page: <http://library.caltech.edu/publications/beilstein/default.htm>

## What is Beilstein?

- A database of over 35M property records (from about 1.8M articles) for 8.4M organic compounds (including salts, mixtures, peptides with <12 amino acids). Polymers or polycondensation products are not indexed.
- Covers the scientific literature from 1771 to the present.
- Reactions (9M) and properties are critically evaluated, with references to original articles.

## What is Gmelin?

- A database of properties for over 1.5M inorganic and organometallic compounds (including coordination compounds, alloys, glasses, ceramics, and minerals).
- Covers the scientific literature from 1772 to the present.
- Reactions (1.25M) and properties are critically evaluated, with references to original articles.

## How can I access Crossfire?

- Workstations with the Commander client are available in the Millikan, SFL, Astro & Geology libraries, under the START MENU (either as Beilstein or MDL Crossfire).
- Macintosh or MS Windows versions are available for downloading to Caltech workstations, from the library web page < [library.caltech.edu](http://library.caltech.edu) >

## Crossfire features:

- **Substance Searching.**  
Search with a name and copy the structure from the 'short display' into the structure editor, or draw a chemical structure or sub-structure or modify a copied structure and search. Beilstein has structure templates. Combine with property or text terms (e.g. NMR, malaria).
- **Reaction Searching**  
Role (reactant &/or product) of a compound or sub-structure in a reaction can be specified.
- **Fact Searching:**  
Names or portion(s) of chemical names. CAS Registry numbers. Author Names  
Property values - e.g. melting point between 100 and 102 degrees, solubility, spectra ...  
Dipole moment is now electrical moment. Biological function is now Pharmacological data.
- **Text Searching (new with version 6):**  
Search for keywords in title/abstract of references (1980+)
- **Combination Searching** of text terms and structures or sub-structures.
- **Autonom** - a program that generates IUPAC names from an organic structures.

## SCIFINDER SCHOLAR 2002

Databases of articles and property data, etc. Search by substances, reactions, keywords, author names, patent numbers, company/organization names, etc. Include/exclude Medline. Workstations with the SFS client are available in the Millikan, SFL, Astro & Geology libraries, under the START MENU. Macintosh or MS Windows versions are available for downloading to Caltech workstations, from the library web page < <http://library.caltech.edu/publications/scifinder/> >

## **CAplus**     <http://www.cas.org/casdb.html>

Chemical Abstracts 1907+ -- plus cover-to-cover indexing of 1,350 key chemical journals since Oct. 1994+, -- plus bibliographic information from both 'electronic' articles and from US, EP, WO patents (including machine translated abstracts for JP and DE patents), prior to CAS indexing. Records from 1907-1961 do NOT include CA Index Terms nor CAS Registry Numbers.

## **Registry File**     <http://www.cas.org/casdb.html>

A chemical structure and dictionary (CA Index Name, synonyms, CAS RN or MF) database - 1957+. Currently lists over 20M organic and inorganic compounds and over 24M biosequences. Provides links to 'Commercial Availability' and 'Regulated Chemicals Listing'. ACD calculated property data is provided for nearly 12.7M organic compounds along with basic (mp, bp, refractive index, ORD & density) experimental property data for over 800K compounds. 'Dictionary' searching is often faster than structure searching and avoids problems with structure searches that contain multi-component substances because of SFS' philosophy of 'maximizing retrieval'. SFS 2001 and 2002 offer an Additional Options dialog box to exclude: mixtures, isotopes, polymers ...

## **ChemCats**     <http://www.cas.org/CASFILES/chemcats.html>

Commercially available chemical compounds and suppliers. Requires a 'compound' search, with Registry File records providing links to ChemCats/ChemList. Search 'Chemical Substance or Reaction' (it will be much faster with a CAS Registry Number) although names or molecular formulas can also be used. Clicking on the 'Commercial Sources' hotlink provides a list of suppliers, catalog date, order number, product name and description. Suppliers must be contacted directly for prices.

## **CA Patent Family Information**     <http://www.cas.org/EO/caspat.html>

Chemical Abstracts Patent Concordance/Index (1967+). Patent Family Information is only available after searching, 'getting' the references and clicking on the 'microscope icon' for a patent record, which displays the full bibliographic record including the 'Patent Family Information'.

Since CA generally abstracts European, German or WO applications first, this is a good way to find U.S. equivalents, as is the [Esp@cenet](http://ep.espacenet.com/) Worldwide database at: <http://ep.espacenet.com/>

Please note CA may provide a more descriptive patent title for U.S. patents.

## **CASReact**     <http://www.cas.org/CASFILES/casreact.html>

Reaction information (journal articles 1907+ and patents 1982+) from both the organic/organometallic sections of Chemical Abstracts and InfoChem. Only available while performing a structure search.

## **CHEMLIST**     <http://www.cas.org/CASFILES/chemlist.html>

CHEMLIST (Regulated Chemicals Listing) was originally built from data in the 1985 TSCA Inventory and supplements, and the Federal Register for 1978-1987. Sources for updates are greatly expanded (e.g. EINECS, EPA, etc.). Links from Registry File records. The file covers 1979 to the present, with more than 227K records (4/2002). It is updated weekly. Includes: ACGIH Threshold Limit Values

# SFS 2001/2002 - New Features

2001 [http://www.cas.org/SCIFINDER/help/2001/SCH\\_Help/Ctxt\\_eps/default.htm](http://www.cas.org/SCIFINDER/help/2001/SCH_Help/Ctxt_eps/default.htm)

2002 <http://www.cas.org/SCIFINDER/SCHOLAR/index.html#whatsnew>

## 1. Structure Searching - (Stereobonds can be included)

a. After drawing a structure ...

Clicking 'Get Substances' and 'Additional Options' displays a dialog box that allows you to include or exclude; mixtures, polymers, isotopes, metal-containing substances and incompletely described structures. This option does not allow exclusion of 'multicomponent substances'.

b. After retrieving an 'Answer Set' of compounds ...(Display buttons for references / 3D model / commercial source / registry file record / reactions.

You can 'Refine' the compounds by 'Calculated Property Data' (i.e. # of hydrogen donors or acceptors, MW, Log POW, Freely Rotatable Bonds, Log DOW (i.e. Log POW as a function of pH), pKa, and solubility (in water as a function of pH). 12.7M compounds have the ACD property data in their Registry File record. A Stereoanalysis feature is now included.

2. **Cited References** from articles and patents are included (since 1999+). After retrieving a list of references, you can:

a. check off an article of interest and click the 'Microscope Icon' to see the cited references (many of which are 'hot linked' to their CA abstract record), or

b. check off one or more articles of interest and either:

Click 'Get Related' and then '**Cited** References'. This will display the records for all the 'hot linked' cited references in the document/s, or ...

Click 'Get Related' and then '**Citing** References' to display records (1999+) that have cited the document/s.

3. **Reaction Searching** has been expanded to 5M reactions -- journal articles, 1974+ and patents 1982+.

4. **Research Topic Searching** has additional limit options (publication year, document type, author, company/institution name)

5. **Registry Numbers** in many document records are 'hot linked' to their Registry File records (which include CAS name, synonyms, MW, structure diagram, etc).

6. **Previous enhancements** (SFS 2000) included:

Company / Institutional name searching / refining, functional group reaction searching, refining reactions by; yields, type, number of steps).

7. **Importing Data** from SciFinder Scholar to **EndNote**, ProCite and Reference Manager is described at: <http://www.cas.org/Support/scifinder2001/bibapps/download.html>