

The Combined Chemical Dictionary

<http://www.chemnetbase.com/scripts/ccdweb.exe>

includes all compounds contained in the:

Dictionary of Inorganic and Organometallic Compounds (101,000 records)

Dictionary of Natural Products (170,000 records)

Dictionary of Organic Compounds (255,000 records)

Dictionary of Analytical Reagents (14,000 records)

Dictionary of Drugs (40,000)

The compounds indexed in the CCD can be generally characterized as follows:

- Fundamental **organic and inorganic compounds** of simple structure, including the elements, inorganic binary and ternary compounds (hydrides, halides, oxides, sulfides);
- Virtually every known **natural product** including those of unknown structure;
- All **currently marketed drugs**, including all those listed in generic name compilations (US Adopted Names, International Nonproprietary Names, British Approved Names, Japanese Accepted Names), as well as those undergoing clinical trials;
- Compounds with an established use such as **catalysts, solvents, starting materials, synthetic reagents, analytical reagents**;
- Important **co-ordination compounds**, e.g., amines, phosphines, alkoxy complexes, and major well-characterised bioinorganics;
- **Organometallic compounds** representative of all important structural types (in the case of ligands with organic substituents, typically the parent member of each series, where known, together with a selection of homologues);
- Important **biochemicals and minerals**;
- Other compounds of particular interest because of their chemical, structural or biological properties, including many **newly synthesised compounds of active research interest**.

The CCD is unique because it provides a wider variety of references, for the compounds it indexes, than Beilstein/Gmelin or SciFinder Scholar (e.g. Aldrich spectra catalogs; Fieser & Fieser's Reagents...; Ullmann's and Kirk-Othmer; Extra Pharmacopoeia; Bretherick's Handbook of Reactive Chemical Hazards; RSC's Hazards in the Laboratory; Sax's Dangerous Properties ...; Browning's Toxicity and Metabolism ...; Organic Syntheses (which Beilstein hasn't indexed since 1980); Encyclopedia of Reagents for Chemical Synthesis and references to book chapters).

Because of its currency and the indexing practices of Beilstein/Gmelin & SciFinder Scholar, it will also provide unique journal article references.

A web based tour is available at: <http://www.chemnetbase.com/tours/ccd/index.html>

Searching the Combined Chemical Dictionary

After entering the database, you can search with a compound name, molecular formula, physical property, etc. or browse some of the indexes for search terms.

Browse Index is very strongly recommended, as it will give a perspective on the variety of index terms.

Click on the Browse Index button, then type the first part of the required search term in the Index Stem box and click Go To. The correct part of the index will then be displayed. Alternatively, you can click on the alphabetical links above the Index Stem box and page thru the terms.

Click on the required search term to transfer it to the Search Terms box. Then click on Return to Search.

Each entry in the 'Browse Index' lists is hotlinked to the search box. Click on an entry, go to the top of the page and click 'Return to Search'. The term will now be in the correct search box. Click on 'Search' and then click on the compound name to display the compound record. Clicking on the 'Benzene' ring next to the compound name will display the structure.

SEARCH TIPS

The **Molecular Formula** 'Browse Index' first displays 'ALL' search terms for all compounds with a given element (e.g. -ALL-Ag is the search term for retrieving the 621 compounds containing Silver). Click on 'Next Entry' to display the next page which gives 'ONLY' search terms for compounds with only certain combinations of elements (e.g. -ONLY-C H P X) is the search term for retrieving the 820 compounds that contain only Carbon, Hydrogen, Phosphorus and Halogen. These two unique Molecular Formula search term families (-ALL- and -ONLY- are followed by the molecular formulas of individual compounds in Hill order.

Range searching for physical property data is allowed (e.g. For example, to search the Melting Point field for a melting point within the range of 47 to 51 degrees Celsius, key in 47 - 51. You can also use the following additional symbols:

> greater than < less than >= greater than or equal to <= less than or equal to

Truncation symbols are * and ? (for one character).

References are searchable by author, patent assignee, journal title, etc.

Type of Compound is useful in searching for specific structural types of inorganic compounds, very general classes of organic compounds, or classes of natural products.

Chemical Name contains all chemical names and synonyms for each compound in the database. It includes trade names, generic names for pharmaceuticals, CAS names, trivial names and semisystematic names.

The online **CCD Help File**: <http://www.chemnetbase.com/help/ccdhelp/ccdindex.htm>

Beilstein/Gmelin vs CCD vs SciFinder Scholar

SciFinder Scholar (Chemical Abstracts Plus) has completely different criteria for indexing articles than Beilstein/Gmelin or the Combined Chemical Dictionary.

Chemical Abstracts, per its stated policy, covers the full range of the 'chemical' literature, focusing on 'new' information and the main points of the article. This differs significantly from B/G and the CCD which index a much smaller subset of chemical journals and focus on chemical compounds.

Thus, the indexing of documents (SFS) vs. indexing compounds (B/G & CCD) obviously leads to significant differences in retrieval. In addition, the extensive coverage of the patent literature in SFS (which Beilstein dropped after 1979, and the CCD only covers selectively) strongly suggests that compound searches should be performed in all three databases.

SciFinder Scholar's Registry File contains nearly 36M substances, and Beilstein/Gmelin have indexed over 8M organic and about 1.4 M inorganic/organometallic compounds respectively. While this compares with only about 450K organic compounds and natural products and 100K inorganic/organometallic compounds in the CCD, a comparison of results from the three databases is strongly reinforces the need to search multiple databases. For example:

Lithium, [2-(dimethylamino)phenyl]- -- (2-Dimethylaminophenyl) lithium C₈H₁₀LiN -- 22608-37-3

Beilstein: 5 references (3 as a reactant, 2 prep references) from 1977-1997.
Three of the 5 references are unique to Beilstein.

Gmelin: 14 references as a reactant (including a German patent) from 1943-1990
Ten of the 14 references are unique to Gmelin.

CCD: 6 references to synthesis/reaction/use (1966-1990), including a book chapter.
Five of the 6 references are unique to the CCD.

SFS(CA): 28 references, from 1969-1998, of which 5 describe preparation (1997, 1996, 1984, 1983, 1973). The 1977 Beilstein synthesis reference is not included in SFS, since the main point of the article was the reactivity of the starting materials).
Twenty one of the 28 references are unique to SFS.

This multiple database search resulted in a total of 46 unique articles of which only 7 were duplicated.

Brian M. Stoltz (as an author)

Beilstein: 12 references. Gmelin: 2 references. (CuCl accelerated Stille ... in both databases).
(Enantioselective total synthesis of nicadrenones is indexed in Gmelin)

SFS(CA): 29 references (including all the references in Beilstein and Gmelin). In addition, there are references to his thesis, a patent, and ACS Abstracts -- as well as a recent JACS article (August 2001) and three articles that presumably should have been indexed for Beilstein (Novel annulation products ... the cardenolide ouabain, Total synthesis of (+)-RK-286c, (+)-MLR-52, (+) Staurosporine & (+)-K252a, and Total synthesis of (+) & (-)-K252a.