

Beilstein/Gmelin CrossFire V.6

Quick Review -- Spring 2004

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BEILSTEIN'S HANDBUCH ... & ... GMELIN'S HANDBUCH ...

Beilstein's Handbuch der Organischen Chemie was, until the 1980's, considered an absolutely essential subscription in any chemistry research library. Since that time, a dramatic increase in the number of new organic compounds, a decline in the study of German language, and the relative weakness of the US\$ vs. the German DM (which increased subscription costs to ~\$40K by 1990), led to Beilstein's virtual unaffordability in all but the largest university and industry libraries. In addition, the print volumes continued to be out-of-date, which has been a chronic problem since the inception of the Handbuch. For example...

	H	E I	E II	E III/IV	E V
Literature Coverage	1779-1909	1910-19	1920-29	1930-59	1960-79
Publication period	1918-1938	1928-38	1941-55	1958-86	1984-95

Caltech cancelled its Beilstein subscription in 1986, at the end of the 4th supplement (Erganzungswerk IV), because the literature coverage was only complete through 1959 and there was virtually no prospect that this situation would significantly improve. This became a fairly universal view as Beilstein's 3300 Handbuch subscriptions in 1965 were reduced to 294 by 1990.

The Beilstein Institute finally realized that they had to create an electronic version of their work that was reasonably up-to-date. Following the editorial preparation of the 5th supplement, they refocused their coverage to 120 significant organic chemistry journals (1980+) and began development of an online / internet based product - Beilstein CrossFire. It was also decided to publish the entire database in English (using a German to English translation algorithm for the existing data).

Beilstein currently covers about 180 journals, with an emphasis on synthesis, and a time lag between 9-12 months. This allows chemists to search for data on more than 9M organic compounds (including salts and addition compounds, amino acids, carbohydrates, nucleosides, porphyrins and steroids) and more than 9.5M reactions. Beilstein does not include polymers & has not covered patents since 1980.

The Beilstein Database contains searchable synthetic (preparation, formation, isolation, & purification), chemical (including characterization and analysis), physical, structural and biological data from nearly 2M literature references (since 1789) which include author abstracts since 1980. Sophisticated graphical and text based query options and hyper-linking capabilities are provided and the ability to use ranges of chemical and physical data as search terms greatly enhances its value.

The Gmelin Handbuch ... suffered similar problems with literature coverage and pricing. Instead of providing comprehensive coverage of the literature over specific time periods, Gmelin offered comprehensive coverage of specific elements and their compounds with elements having 'lower' Gmelin numbers. This system was necessitated by the convenience of having a metal (Nickel, for example,) and its compounds with non-metals (e.g. NiCl₂) grouped together. This approach resulted in very uneven coverage. Sodium covers the literature thru 1960, but Potassium only thru 1936. Mellor's Comprehensive Treatise ... Supplements provides updates on the halogens, alkali metals, nitrogen and phosphorus. The handbooks published after 1975 are not included, as Gmelin transitioned to indexing ~120 of the most important journals beginning with 1976.

Gmelin is a comprehensive collection of factual data on inorganic, organometallic and coordination compounds, alloys, glasses, ceramics and minerals. The Gmelin Database currently contains data for nearly 2 million compounds & more than 1.5M reactions from about 1M literature references (since 1772). The database includes information about analytical chemistry, atomic physics, ores, electrochemistry, geochemistry, coordination chemistry, corrosion and passivity, crystallography, geology, metallography, metallurgy, mineralogy, physical properties (crystallographic, mechanical, optical, magnetic, electrical), toxicity and hazards, economic and statistical data.

Caltech's annual subscription allows for UNLIMITED access and searching by faculty, staff or students at any time, from any location on campus.

MDL CROSSFIRE V6

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. A handout describing both the databases and search techniques is available at: <http://library.caltech.edu/publications/beilstein/BeilsteinGmelinV.6.pdf>

What is Beilstein?

- A database of over 35M property records for over 9M organic compounds (including salts, mixtures, peptides with <12 amino acids). Polymers are not indexed.
- Covers the scientific literature from 1771 to the present, with over 1.9M articles. Currently indexing 175 journals <http://www.mdl.com/products/pdfs/BSJournals.pdf>
- Reactions (9.5M) and properties are critically evaluated, with references to original articles.

What is Gmelin?

- -A database of property records for over 2.1M inorganic and organometallic compounds (including coordination compounds, alloys, ceramics, minerals, etc.).
- Covers the scientific literature from 1772 to the present, with over 1.1M articles. Currently indexing 62 journals <http://www.mdl.com/products/pdfs/GMJournals.pdf>
- Reactions (1.65M) and properties are critically evaluated, with references to original articles.

How can I access CrossFire V6?

- Workstations with the V6 client are available in the Millikan, SFL, Astro & Geology libraries, under the START MENU (as MDL Crossfire Commander v6).
- Macintosh or MS Windows versions are available for downloading to Caltech workstations from the library web page at: <http://library.caltech.edu/publications/beilstein/default.htm>

CrossFire features:

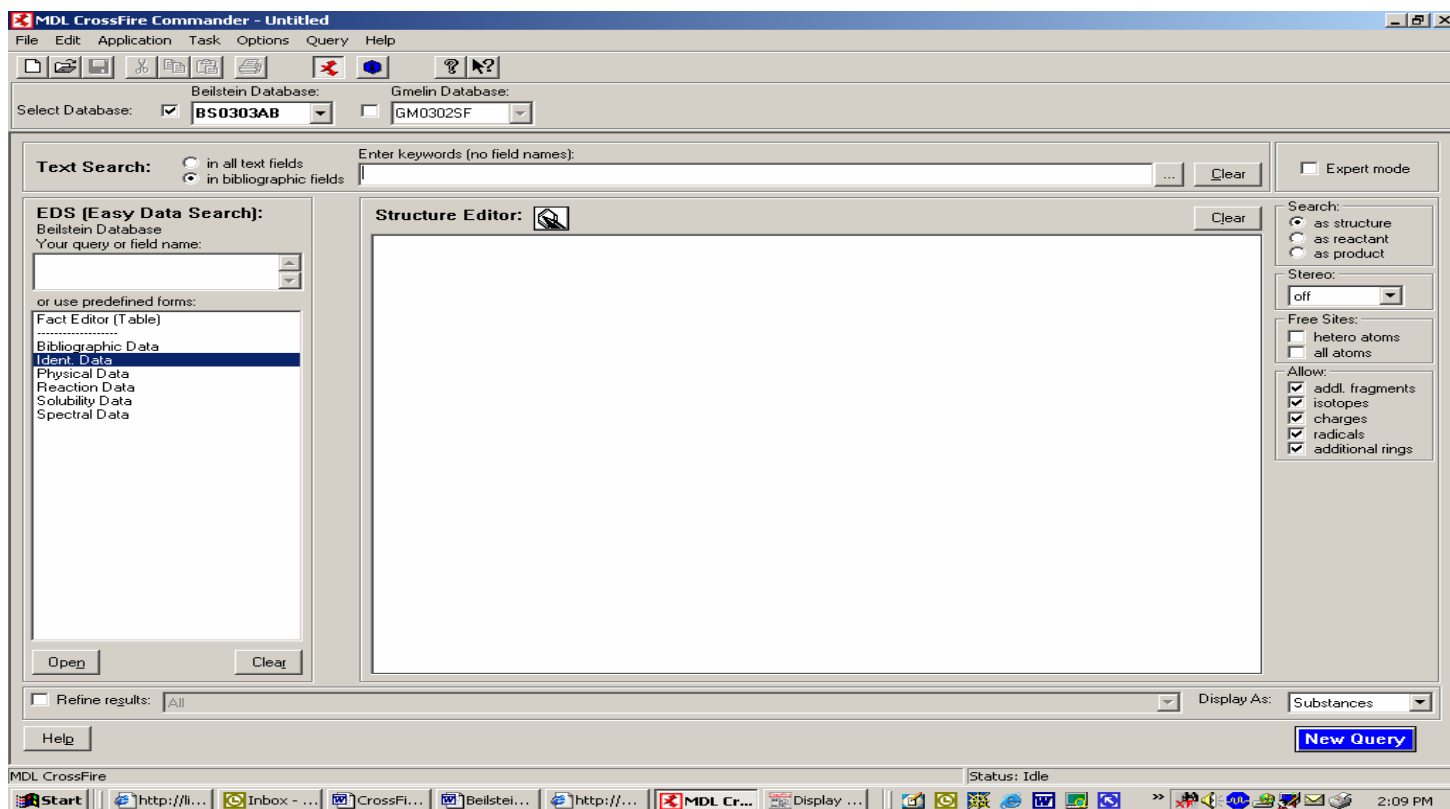
- Autonom - generates an IUPAC name from an organic structure.
- Text Searching - Search text words or author names (article titles/abstracts 1980+).
- Structure Searching - (Beilstein/Gmelin can be searched simultaneously).
Either draw a structure / sub-structure, modify a (Beilstein) template (under File menu), or search with a name and copy the structure from the 'short display'. Combine with property or text terms (e.g. NMR, malaria). Autosearch may provide additional retrieval.
- Reaction Searching (both Beilstein and Gmelin) by:
Specify the role (reactant and/or product) of a compound or sub-structure in a reaction.
- EDS (Easy Data Search) - Tables or predefined forms
Names or portion(s) of chemical names. CAS Registry numbers. Author names.
Property values and range searching (e.g. melting point between 100 and 102 degrees).
Reaction data, Solubility, Spectra.
- Combination Searching
Combine structures / substructures with property terms (e.g. NMR) in B or G (not both).
Search for text and/or structures in B & G simultaneously.

Getting Started on a Library Workstation

From the **Start Menu** → **Programs** → **MDL CrossFire Commander V6** →



Structure or data searching: Click on the 'Crossed Red Arrows'. After connection, select either Beilstein (organic) or Gmelin (inorganic/organometallic), or both. The default is the last one used. Text (in substances, reactions or citations) and/or structures can be searched simultaneously.

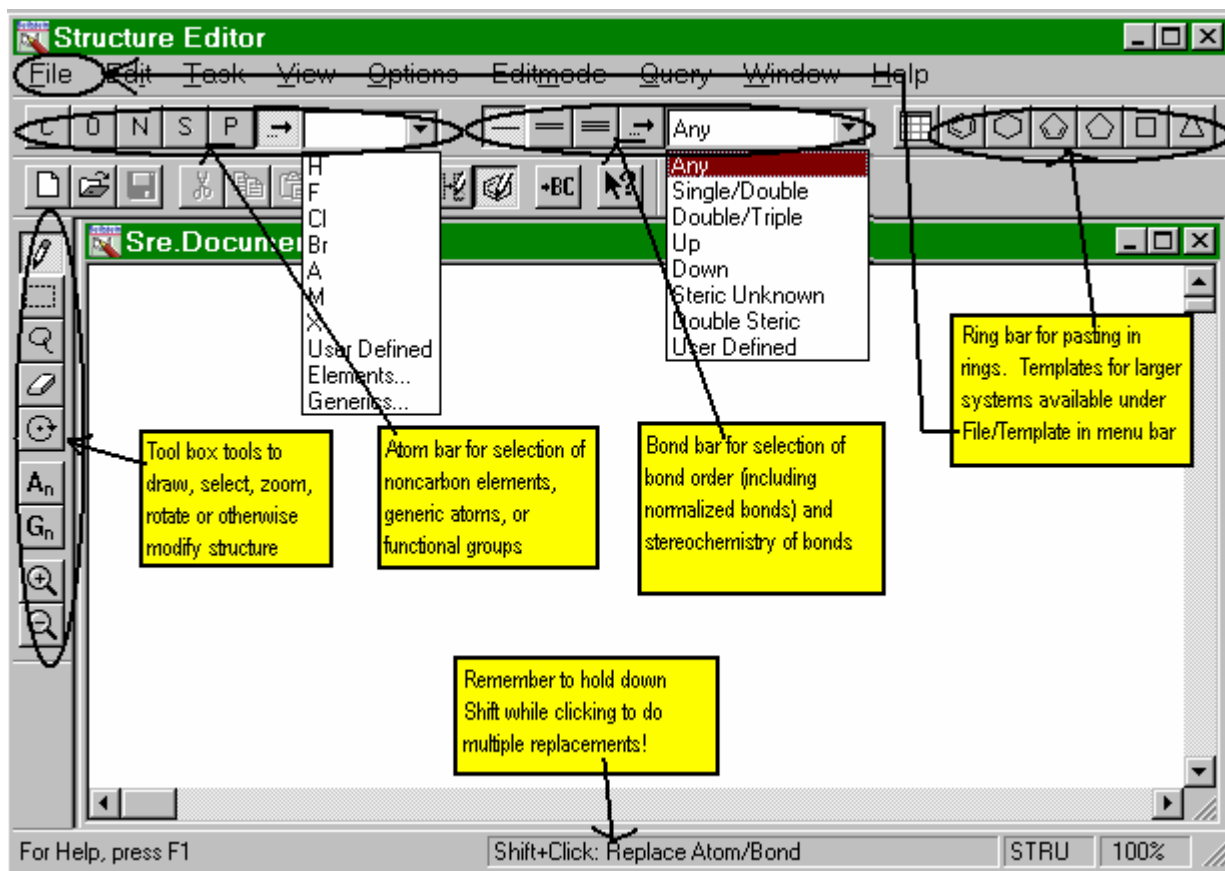


Structure Searching requires double clicking in the Structure Window, or clicking the Structure icon.

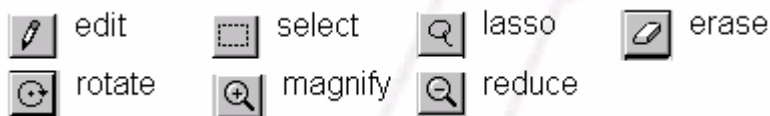
Drawing Chemical Structures -- (Crossfire or ISIS/Draw editors)

Commander screen → Options → Structure Editors → MDL ISIS or MDL Crossfire

The **Structure Editor** screen has a toolbox, and atom / bond / template / ring bars.



The **toolbox** along the left side of the screen provides a set of tools for drawing, selecting, activating, erasing, rotating or zooming structures.



The **atom/bond bars** offer a selection of default atoms and bond types for the **Edit** tool. Atoms or bond types not shown may be specified from either the Atom or Bond pull-down menus, although it is usually easier to draw a carbon skeleton and change atoms and bonds as necessary.

Click on the **Edit** (pencil) **icon** to draw a structure. The default atom and bond type are carbon and single. **Click and hold** down the left mouse button. **Drag** the mouse to the desired end point of the bond; **Release** the mouse button to terminate the bond and place the second atom. Repeat (**Click and hold, Drag, Release**) to continue drawing atoms and bonds.

Atoms and bonds already drawn can be changed by simply changing the default atom or bond (on the Atom Bar) and, while holding down the shift key, click on the atom or bond to be changed. Do **NOT** draw in hydrogen atoms.

To erase a portion of a structure that has been drawn, select the **Eraser** tool from the tool bar. Position the eraser (the tool shows a "B" or "A" when positioned correctly) and click on each atom/bond as needed. To erase a larger portion of a molecule, use the **Lasso** tool to circle the area to be erased and click on the **Scissors Icon**. The screen can be cleared by clicking **Delete All** under the edit menu. **Undo** under the edit menu will undo the last operation.

To move or rotate a molecule, first **activate** it (by double clicking one of the atoms or bonds) with the **Select** tool.

To access the full range of options for atoms and bonds, use the **Edit** tool (pencil) to click on a bond or atom (the tool shows a "B" or "A" when positioned correctly). Clicking on an atom displays the **Atom Attributes** box (see figure below, right side), which allows changing the element, free sites, hydrogen counts, etc. Clicking on a bond displays the **Bond Attributes** box (see figure below), which allows changing the bond type, topology, etc.

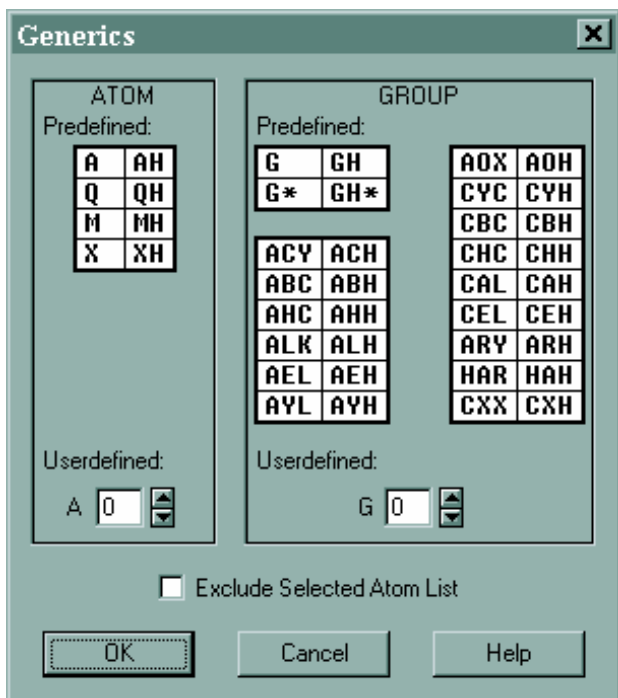
The screenshot displays the **Structure Editor** software interface. The main window shows a chemical structure of a complex molecule with a pencil tool (labeled 'A') and an eraser tool (labeled 'B') positioned over it. The interface includes a menu bar (File, Edit, Task, View, Options, Editmode, Query, Window, Help) and a toolbar with various icons. Two dialog boxes are open:

- Bond Attributes (16 - 17)**: This dialog box is in the foreground. It features a preview window showing a dashed bond. The bond type is set to **Any** (selected with a radio button). Other options include Single, Double, Triple, Single / Double, Double / Triple, Up, Down, Steric Unknown, and Double Steric. The Topology is set to "ring or chain". There are checkboxes for "Set to Current" and "Set User Defined".
- Atom Attributes**: This dialog box is partially visible behind the Bond Attributes dialog. It shows the symbol **C_{x1}** and a list of elements (C, H, O, N, S, F, Cl, Br, A, M, X) with **S** selected. It also includes fields for Free Sites (1), Valency (*), Charge (*), Mass (*), and Radical (*). There are checkboxes for "Set to Current" and "Set User Defined".

At the bottom left of the interface, there is a note: "For Help, press F".

Pre-defined Generic Groups and Atom Lists

Pre-defined Atom Lists (e.g. Any Halogen, Alkali Metals, etc.) and Generic Groups (e.g. Alkyl, Aryl, etc.) may be added to a structure by clicking the 'down arrow' in the atom box on the function bar and selecting '**Generics**'. This displays the Generics menu shown below. Selecting one of the pre-defined atom lists or generic groups, changes the **Edit** tool (pencil) default to that atom list or generic group. This is particularly useful for repeatedly adding the same atom list or generic group.



Alternatively, for adding a single group, you can double click an atom with the **Edit** tool, then click the down arrow in the Atom Attributes Symbol Box and select '**Generics...**' from the menu. This also displays the Generics menu shown above. Click on one of the pre-defined atom lists or generic groups. Click OK on the Generics menu and click OK again on the Atom Attributes box. This changes the selected atom.

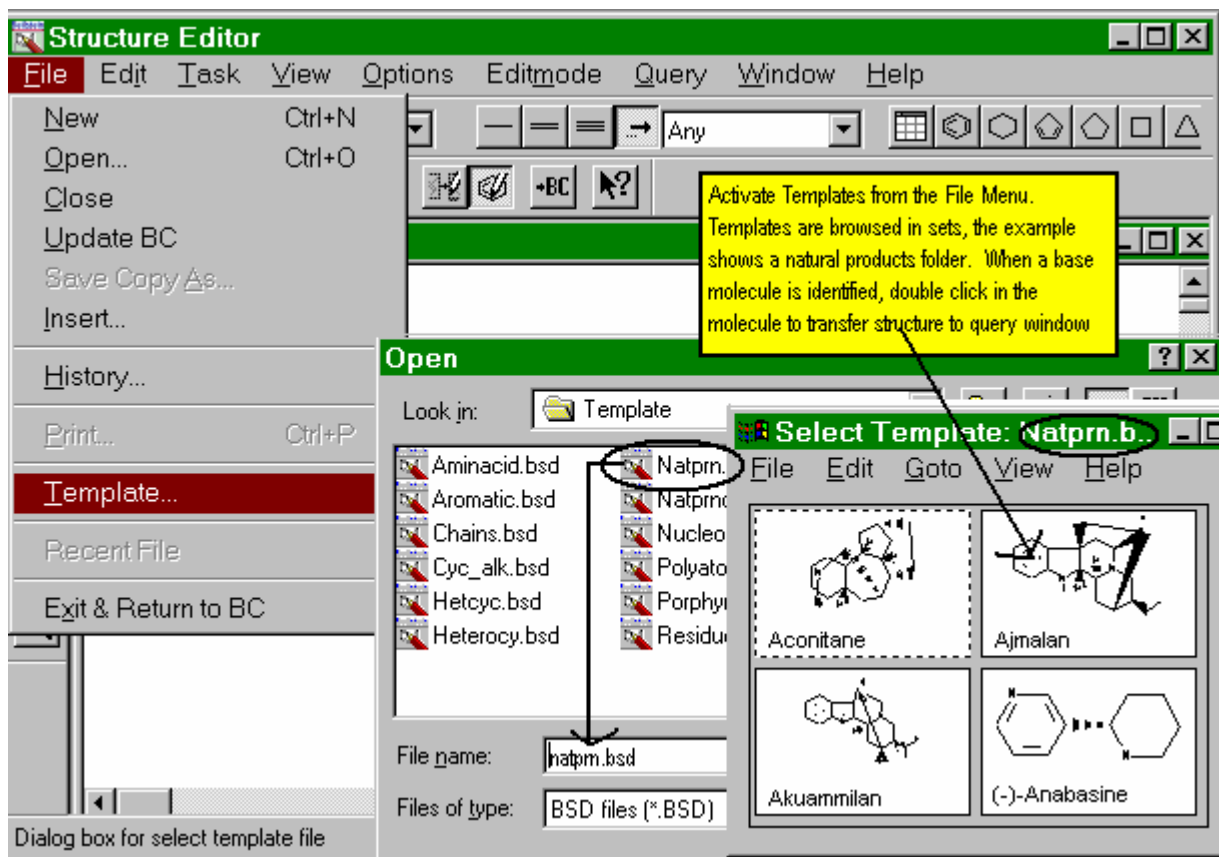
Creating User Defined Groups and Atom Lists

Atoms: Click the atom in the structure, which needs to be variable. Type '**A1**' in the Atom Box and click OK to make the change. Next, click the '**An**' button in the **Tool** Box (left side), and the 'Atom List Number' box will appear. Click OK to display a 'Define Atom List A1' periodic table. Click as many elements or element groups as needed and click OK. A list of the all the selected atoms will appear in the Structure Editor window.

Groups: Click the atom, which will be the variable group in the structure. Type '**G1**' in the Atom Box and click OK to effect the change. Next, draw a group in the Structure Editor window, '**Select**' a group structure (i.e. by double clicking an atom or bond with the **select tool**) and click the '**Gn**' button in the **tool box**. Set **G=1** and click OK. Repeat for additional groups. One atom in each group must be designated as the attachment point. Click on this atom (with the **Edit** tool), to display the 'Atom Attributes box. Click '**Set User Defined**' and then click '**Attachments**'. Click '**1**' in the 'Attachment Points' box and click OK (in that box). Then click OK in the 'Atom Attributes' box.

TEMPLATES (Both Beilstein & Gmelin)

Clicking on a **menu ring**, or clicking on one of the structures in the **Group Templates** folder, transfers an '**active**' structure to the Structure Editor window. This 'active' structure may be moved, resized or rotated. Click outside the 'box' to 'deactivate' the structure. The resulting structure may be further edited (**after clicking on the edit tool**).



Templates for Complex Structures (BC2000 has Group and User Template files)

The following group template files are available:

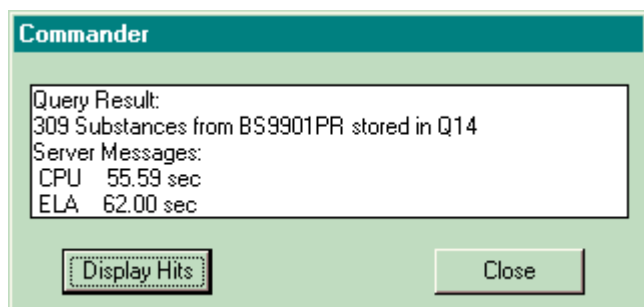
AMINACID.BSD	Amino Acids	POLYATOM.BSD	Coordination Types
AROMATIC.BSD	Aromatics	PORPHYR.BSD	Porphyryns
CHAINS.BSD	Chains	RESIDUE.BSD	-NO ₂ , -COOH, -SO ₃
CYC_ALK.BSD	Cycloalkanes	STEROIDS.BSD	Steroids
HETEROCY.BSD	Heterocyclics	SUG_OPEN.BSD	Sugars (open)
NATPRN.BSD	Cyclic N-containing	SUG_RING.BSD	Sugars (cyclic)
NATPRNOS.BSD	Cyclic N-, O-, S-containing	TERPEN.BSD	Terpenes
NUCLEOSI.BSD	Nucleosides		

After drawing a structure, click on the Crossed Red Arrows → Beilstein Commander.

Next, under the **Query** Menu, click 'Structure Query Options'. This gives options for adding isotopic variants, radicals, ions, etc. A structure search can be combined a physical property data search (e.g. click Spectral Data (under Easy Data Search menu) and check NMR), in either Beilstein or Gmelin (not both).

Searching and Displaying ...

Click the **Start Search** button. CrossFire will search the database and report how many compounds match the search criteria (i.e., how many "hits").



Search Results

Click the **Display Hits** button to review the substances.

The Display Hits window shows a list of substances with a sidebar menu and a main display area. Annotations highlight key features:

- Toggle between full molecule display and text display:** Points to the 'Short Display' menu option.
- Toggle between a text display and all full molecule displays:** Points to the 'Hit only' and 'User View' options.
- Choosing Identification and Include Field Availability gives a good display for reviewing records quickly:** Points to the 'Identification' and 'Include Field Availability' options.

Field Availability List 1-2 of 2

Code	Field Name	Occ.
RXB	Non-Graphical Reaction	1
MP	Melting Point	2

Display Hits Screen Basic Information

First (under the **View Menu**) click 'Short Display', to identify compounds of interest among a large set. Clicking the 'Field Availability' icon, or from under the **View Menu**, provides a quick display of available properties.

The 'All Fields'/'Field Availability' mode provides a convenient display for compounds with extensive properties. The 'Field Availability' display provides a scrollable property list that can be clicked to quickly display specific data fields.

To sequentially view the text records, use the center two arrows on the menu bar at the top of the screen. Use the outer two arrow buttons (the ones pointing to a vertical line) to move to either the first or the last hit.



Underlined numbers in various colors seen in the text records are hyperlinks to the Beilstein record for another compound, reaction or citation. To move to the linked record, click on the highlighted number. Moving back and forth between the original and linked records is done with the back and forward buttons (shown below).



'Reaction View' under the **View Menu** provides for display of 'substance as a reactant' or 'substance as a product'. To quickly search for preparations of a specific organic compound, do a compound search, go to the 'View' menu and click on 'Reaction View' and 'Substance as a Product'.

Reaction Searching

There are currently about 8.7 million structure searchable reactions in Beilstein and 1.5M reactions in Gmelin allowing you to build complete reactions or half reactions and search for them.

First draw the reactant and/or product molecules, in the Structure Editor. Then switch to 'Reaction Editmode' by clicking the '**Reaction Attr.**' Button on the tool bar.



The function bar then changes to allow reaction roles to be set. **Select** the appropriate molecule (with the select tool) and click either the Reactant or Product button to define that molecule's role in the reaction. Half-reactions can also be defined by drawing and defining only a reactant or a product.

The structure of a molecule can be changed by switching back to the Structure Editor, after **Selecting** the molecule, and using the **Undefine** button, to delete product and reactant assignments.

Click on the **BC** button to transfer the structure to Beilstein Commander, and click **'Start Search'**.

Search Tips:

Preparative reactions can be quickly displayed, after a compound search, from the 'View' menu → Reaction View → Substance as a Product.

Structures can also be copied into the Structure Editor from the **Short Display** under the **View** menu. First search for a model compound by name (e.g. Ferrocene). Highlight the 'short display' structure by clicking once and then from the **Edit** menu, select 'copy structure to SE'.

To move a structure -- **Select** the structure / drag the small black square

To expand or contract a structure -- **Select** the structure / drag the side of the 'box'.

To copy a structure -- select structure / shift key / drag

Beilstein Lawson Numbers define a structural similarity. After finding the Lawson Number for a model compound and then using it as a search term, results are restricted to substance classes without actually drawing a structure and searching for it.

CUSTOM DISPLAYS AND PRINTING

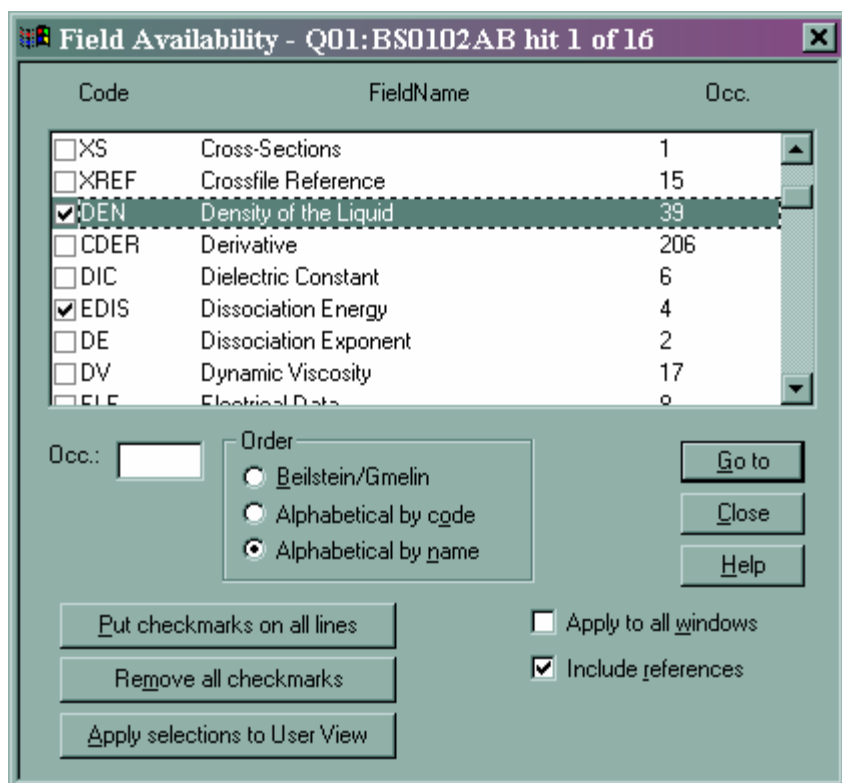
Records in the database can be hundreds of pages long. To avoid printing unwanted information, you can:

1. Use the **check boxes** to designate specific 'fields' in a record, and click on the **print icon**



Reaction 1 of 2	
Reaction ID	8713044
Reactant BRN	8687490 1-hydroxy-2,3-dihydro-1H-3,4a,5-triaza-fluoren-4-one
Product BRN	8682045 3H-3,4a,5-triaza-fluoren-4-one

2. Under the **View Menu** click both **All Fields** and **Field Availability**. The **Field Availability** list can be alphabetized (in Gmelin, however, the order is case sensitive). The default order corresponds to the print volumes (chemical properties, physical properties, etc.). For printing selected fields, click **Remove all checkmarks** and check off fields (as shown) and click **Apply selections to User View**



Code	FieldName	Occ.
<input type="checkbox"/>	XS Cross-Sections	1
<input type="checkbox"/>	XREF Crossfile Reference	15
<input checked="" type="checkbox"/>	DEN Density of the Liquid	39
<input type="checkbox"/>	CDER Derivative	206
<input type="checkbox"/>	DIC Dielectric Constant	6
<input checked="" type="checkbox"/>	EDIS Dissociation Energy	4
<input type="checkbox"/>	DE Dissociation Exponent	2
<input type="checkbox"/>	DV Dynamic Viscosity	17
<input type="checkbox"/>	ELE Electrical Data	0

Occ.:

Order

Beilstein/Gmelin

Alphabetical by code

Alphabetical by name

Go to

Close

Help

Put checkmarks on all lines

Remove all checkmarks

Apply selections to User View

Apply to all windows

Include references

This limits the Display Hits window to just the desired fields, which can then be printed. The full display is regenerated by clicking **All Fields** under the **View Menu**.

3. Text can easily be copied and pasted into e-mail messages, MS Word and Excel documents. Structure images must be first transferred to the **Structure Editor**, and from the **Edit Menu**, click **Copy All** and in MS Word, paste special **Picture**.

AUTONOM

AutoNom (which is included in the client software) automatically generates IUPAC names from organic chemical structures, using the Beilstein Structure Editor.

The screenshot shows the MDL CrossFire Commander software window. The main area is titled "AutoNom Name" and contains a "Structure:" field with a chemical structure of 2-bromo-6-chloro-4-fluorobenzoic acid. Below the structure, the text reads: "total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST". To the left of the structure field, there are input fields for "Enter your comment:" and "Notes:". Below the structure field, the "AutoNom Name:" field displays the generated name: "2-Bromo-6-chloro-4-fluoro-benzoic acid". The status bar at the bottom indicates "Status: Idle".

DATA (NAME / PROPERTY) SEARCHING

Data searching requires double clicking the Fact Editor or one of the quick search options (e.g. Physical Data). Beilstein display is shown. Gmelin offers additional options. The magnifier button opens a dictionary to check spelling, etc.

The screenshot shows the "Physical Data" search dialog box. It contains the following options and input fields:

- Find all compounds, which have:
 - Melting or Decomposition Point values
 - Boiling Point values
 - Dissociation Exponents (pK value) given
 - Density values
- Or search for detailed values:
 - Melting Point: value or range: [=] [] [magnifier] from sol.: [] [magnifier]
 - Boiling Point: value or range: [=] [] [magnifier] at pt.: [=] [] [magnifier]
 - Density: value or range: [=] [] [magnifier]

Buttons for "OK", "Help", and "Cancel" are located at the bottom.

BEILSTEIN NOTES:

Some of the original print database was not translated into English. The 'Other Conditions' line in the Reaction Field, for example, is in German. A Beilstein German-English dictionary is available at:

<http://www-sul.stanford.edu/depts/swain/beilstein/bedict1.html>

In the creation of Beilstein CrossFire, the algorithm used to update the very cryptic abbreviations, used in the early years, assigned the current abbreviation to journals that have changed title over the years. For example, 'chem.ber.' is given as the abbreviation for Ber. Dtsch. Chem. Ges.(1868-1946)

Beilstein discontinued coverage of patents in 1980. Although a few scattered 19th and early 20th century patents were covered, the strength of Beilstein's patent coverage begins in 1925. About 2K patents were indexed in 1930, steadily increasing to 5000 in 1956 and to 15K in 1966. Coverage began to slowly decrease dropping to about 10K patents in 1979.

Chemical names in Beilstein generally reflect usage in the article. Since 1992, Chemical Abstracts Registry Numbers are not assigned, unless they appear in the article. It is advisable to rename a compound according to IUPAC rules (e.g. tert-butyl-methyl ether → 2-methoxy-2-methyl-propane) or, better yet, do a structure search.

Simply drawing a cis or trans structure will NOT define it for a structure search. The results will include both cis and trans compounds (the bonds are labeled E and Z in the Short Display). The wavy bonds refer to mixtures of E & Z isomers or a compound of unknown configuration.

Range searching is allowed. For example, you can search for compounds with melting points greater than 500 degrees (mp>500 in a Tabular Query). Searching for a melting point of 134 degrees will retrieve compounds with a melting point listed as 133-135 degrees.

Coverage of the literature is somewhat inconsistent in Beilstein. For example, Organic Syntheses has not been covered since 1979 (since it is not a journal). Coverage of SynLett did not begin until 1997, and coverage of Organic Letters did not begin until mid-2000. In general, articles are not indexed until about one year after publication.

In the mid-seventies, there was a new definition of "inorganic" and "organic" compounds. Beilstein currently indexes compounds that contain carbon and the yellow-shaded elements in the periodic table at: <http://www.library.wisc.edu/libraries/chemistry/beilstein/beilsteinelements.htm>
The remainder are indexed by Gmelin.

The following are NO LONGER Beilstein compounds: CO, CS, CO₂, CS₂, COS, C₃O₂, C₃S₂, H₂CO₃, HCN, HOCN -- their sulfur analogs and metal salts/complexes, Dicyanogen (C₂N₂), Phosgene (CCl₂O), Metal Carbides, Metal salts of formic, acetic and oxalic acid, Fullerene and Carboranes. 'Gmelin' compounds included in Beilstein are organometallic compounds known before 1980, such as Ferrocene, Dimethyl Mercury, etc. Searching both databases is strongly recommended for complete retrieval.

GMELIN NOTES:

1. For all compounds with molecular units (e.g. small molecules like H₂O and coordination compounds) a structure search or substructure search is recommended. If the connectivity of ligands is not unique, coordination compounds may only be searched as fragments (e.g. a substructure of the ligand in combination with complexed metal).
2. For compounds without molecular units, e.g. solid state materials, salts (like NaCl), formula searching is the preferred. Note that H₂O is included in component MF for hydrates. To reduce the hits, restrictions can be set, e.g. number of components. `nc=1` is a single phase compound -- K4Fe(CN)6. number of fragments. `nfrag=2` -- K and Fe(CN)6. number of elements. `ne=4` -- K, Fe, C, and N.
3. Searching for chemical names is another possibility. However, not every compound has a systematic name, since only names given in the article text are entered. Furthermore, since chemical names of inorganic compounds are less standardized than organic ones, structure or formula searching is recommended. Searching with chemical names can be useful if a ligand is very complex to draw. Search for the ligand by name (with asterisks, e.g. **ferrocene**) to retrieve compounds containing this sub-structure. The desired structure can then be loaded into the structure editor, and altered as needed.
4. In contrast to Beilstein, Gmelin indexes polymeric compounds. These may be searched as structures, with the structure editor. For example, enter a Ge atom (with max free sites). Return to Commander and (in the fact editor) enter `[type=polymer]`. This will retrieve all Germanium polymers. Alternatively, you can attach two generic groups (e.g. Aryl or Acyl) to retrieve, for example, compounds with a `[Aryl--Ge--Aryl]` repeating structure (with a Ge backbone).
5. Polymers can also be searched by monomer molecular formula (e.g. C12H10Ge will retrieve polydiphenylgermane. In SFS, this would be searched as `(C12H10Ge)x`.
6. More than 99% of the original Gmelin Handbook thru 1975 is indexed in CrossFire Gmelin. Some material was added to Beilstein (a matter of re-definition) and some volumes (e.g. Geology of Iron) were omitted. Handbook volumes published after 1975 were not indexed for CrossFire Gmelin.

Beginning in 1976, Gmelin began indexing the 120 most important journals in inorganic and organometallic chemistry. There is currently a major effort to bring the database up to date, by adding material from 1995-2001. The GDCh is responsible for excerpting articles from 1995-2000 by the end of 2004. Coverage of new journals is problematic. Inorg. Chem. Commun. (1998+) will be indexed from 2003+ . Both Z. Kristallogr. New Cryst. Struct. and Acta Crystallogr. Sect. E are under evaluation.

BEILSTEIN & GMELIN'S RELATIONSHIP TO SCIFINDER SCHOLAR

SciFinder Scholar (Chemical Abstracts plus) and Beilstein/Gmelin have different criteria for indexing articles that describe preparative reactions and their products. Beilstein & Gmelin, while currently indexing a much smaller number of journals, are much more comprehensive in their coverage of the synthetic chemistry literature, since their primary focus is on chemical compounds, their physical properties and reactions. CAS, per its stated policy, focuses on 'new' information and the main point of the article.

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 or patent, etc. This differs significantly from B/G and the CCD which index a small subset of chemical journals, focusing on the synthetic chemistry literature. Their primary focus is on compounds, physical properties and reactions.

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 & Gmelin dropped after 1979, and the CCD covers very selectively) strongly suggests that compound searches should be performed in all three databases.

SciFinder Scholar's Registry File contains over 43M substances, while Beilstein/Gmelin have indexed 9.2M organic and 1.5M inorganic/organometallic compounds respectively. The CCD only lists 486K organic compounds and natural products and 102K inorganic/organometallic compounds. A comparison of results from the four databases highlights the need to search all three databases. For example:

**Lithium, [2-(dimethylamino)phenyl]-(SFS) [2-(Dimethylaminophenyl)] lithium (SFS,CCD)
2-Dimethylaminophenyllithium (B) 2-(dimethylamino)phenyllithium (G)
C₈H₁₀LiN -- 22608-37-3**

Beilstein: 5 references (4 as a reactant and 1 preparation) from 1977-1997.
The preparation reference is unique to Beilstein.

Gmelin: 14 references as a reactant (including a German patent) from 1943-1990

CCD: 6 references (5 preparation and 1 use) from 1966-1990, including a book chapter.
3 of the preparation references are unique to the CCD.

SFS(CA): 31 references, from 1969-2001, of which 7 describe preparation. The 1977 Beilstein synthesis reference is not included in SFS, since the main point of the article was the reactivity of the starting materials. 4 of the preparation references are unique to SFS.

Brian M. Stoltz (as an author)

Beilstein: 20 references (including 2 with Stoltz misspelled at Stolz. The most recent being Angew. Chem. Int. Ed.; 2003, 42(9). Beilstein didn't index (TL 1999, 40, 2061).

Gmelin: 5 references (all in Beilstein). The most recent being JACS; 2002; 124(42)

SFS(CA): 56 references (including all the references in Beilstein and Gmelin). In addition, there are references to his thesis, a patent, ACS Abstracts -- as well as a recent Tetrahedron article (2003; 59(45) article. There was also a synthesis article indexed in SFS that should have been indexed in Beilstein

CrossFire Documentation and Help:

[MDL CrossFire Commander Version 6 \(2002\)](#) (Caltech Splash Page)

[MDL CrossFire Commander V6 -- Quick Reference Guide](#)

[CrossFire Beilstein Brochure](#)

[CrossFire Beilstein Data Fields Reference Guide \(v.6\)](#)

[CrossFire Beilstein Tips and Hints on Certain Fields](#)

[CrossFire Beilstein Tutorial](#)

[List of ... journals covered in the Beilstein Database](#)

[CrossFire Gmelin Brochure](#)

[CrossFire Gmelin Database Reference Guide](#)

[List of ... journals covered in the Gmelin Database](#)

[Autonom Brochure](#)

For searching tips, consult these guides:

[Beilstein and Gmelin Databases](#) (UW-Madison)

[Structure Searching: Quick Review - 2002](#) (Caltech)

[University of Chicago Web Guides for Beilstein CrossFire](#)

[Other Web Guides for Beilstein CrossFire](#)

Predefined Atom Lists

- A Any atom
- AH Any atom or Hydrogen
- Q Any atom except Carbon or Hydrogen
- QH Any atom except Carbon
- M Any metal atom
- MH Any metal atom or Hydrogen
- X Any Halogen
- XH Any Halogen or Hydrogen

Workshop Exercises

1. Work thru exercises given at:

<http://chemistry.library.wisc.edu/beilstein/exercises.htm>

http://www.mimas.ac.uk/crossfire/examples/examples_bs_structure.html

2. Find Pharmacological information on the Chinese herb Quinghaosu (Artemisia Annua) which has been used in the treatment of malaria.

The search requires finding compounds isolated from a natural product (INP field) that mention malaria or antimalarial in the (PHARM.COM field).

Introduction

Ask group : Who knows what Beilstein means? Generally I've found that no one knows. So that's the introduction to explaining that Beilstein is the last name of German chemistry professor of the 19th century who personally compiled and edited the first three editions of the Handbook of Organic Chemistry. Essentially his surname, Beilstein, has become synonymous with his life's work.

Show picture...

Biographical on Friedrich Konrad Beilstein: .b 1838 in St. Petersburg, Russia of German parents. Educated in Germany and recieved his doctorate at University of Goettingen where he began his professional career. He relocated to the Technical Institute in St. Petersburg in 1866 where in remained until his death in 1906.

First edition of the Handbook published in 1881 including 15,000 compounds documented in the literature back into the 1700's (1789). By the 1990's there were 7.5 M compounds and 10M reactions documented. The fourth edition of 1938 published by the German Chemical Society appeared after his death and covered the literature up to 1910. F. K. Beilstein devised the organization of the compounds into 27 logical volumes by compound class (e.g. Acyclics,

Isocyclics, Heterocyclics)... Here I usually ask if anyone has used the print Handbook - I haven't found anybody yet! To add data - supplements were published. Supplements to the fourth edition cover the literature up through 1979 but took into the 1990's to publish. Adding physical print supplements to the logical arrangement made use very cumbersome. This hurdle and time lag and cost - most individual volumes cost \$1000 dollars or more - caused most research libraries to suspend their subscription. For the literature after 1979, Beilstein coverage was limited to 120 core or significant organic chemistry journals. Beilstein focuses on structure, properties, reactions and does not cover all uses and applications. Therefore, depending on need, it may be necessary to search BOTH Beilstein and CAS.

I use the scenario of what happened to the publishing of this Handbook to illustrate the general problem of cost/access/ scholarly communication.

Current statistics: [LOGIN FIRST](#) [dzrlib ...](#)

Home > Support > Knowledge Base > Product Release Information >

Select **<CrossFire Beilstein and Gmelin Databases>** from Select Product drop-down Menu.

Then Download .PDF file.

dzrlib@library.caltech.edu <http://library.caltech.edu/collections/chemistry.htm>

BEILSTEIN CrossFire Beilstein

BS0303 BS0304 4 Microsoft Windows 2000

BRN: 9259 K *

RxID: 8773 K †

CNR: 1875 K ‡

GMELIN CrossFire Gmelin

GM0302 GM0303 4 Microsoft Windows 2000

GRN: 1501 K *

RxID: 1897 K †

CNR: 1007 K ‡

Version 6, you can disable LitLink. In the xf.ini file change the LITLINK=Yes to LITLINK=No. This ini file is located at c:\program files\mdl crossfire commander v6\xf.ini

From the original Gmelin Handbook up to the year 1975 more than 99 % is in CrossFire Gmelin. The only parts we did not add are what went into CrossFire Beilstein (a matter of definition) and some volumes that do not deal with chemistry, like the one about Geology of Iron.

The handbooks published after 1975 are not included in CrossFire Gmelin, however the excerpts of the 120 most important journals (Year 1976 to 1995) are in the database. This would be the source of the handbooks that would have made their way into CrossFire Gmelin anyway, so there is no loss.

The time between 1995 and 2001 is handled by our partner GDCh.

Since 2001 MDL Information System GmbH is responsible for the data.

Dr. Jochen Tannemann
Product Manager
MDL Information Systems GmbH
mail: j.tannemann@mdl.com

As you might know MDL started to maintain the Gmelin Database in the beginning of the year 2000 in close cooperation with the Gesellschaft Deutscher Chemiker. The closing of the Gmelin Institute as a Governmentally funded institution in the year 1995 left a gap of nearly 5 years in the abstraction of the literature. The Gesellschaft Deutscher Chemiker will close this gap very soon. To keep continuity we started in 2000 to abstract the journals which were already abstracted before by the Gmelin Institute. Unfortunately the start of Inorganic Chemistry Communications in 1998 does lie in between the five-year gap. However we are constantly evaluating new journals concerning their necessity for improvement of the Gmelin Database for the benefit of our users. We will evaluate this journal as soon as possible.

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eMail: C.Druckenbrodt@mdl.com

I just noticed that Gmelin isn't covering Acta Cryst. E (the new Structure > >Reports Online) nor Inorganic Chemistry Communications. Since Inorg. Chem. > >Commun. is a twig that "Aims to replace the (Preliminary) Communication > >section of Inorganica chimica acta, Polyhedron and the Journal of > >organometallic chemistry" this would seem like an obvious and highly > >necessary addition to the Gmelin database.

Therefore, if you search for ANY preparation of B, do a compound search for B filter all reactions "... as product(this, again, works only on the "reactions", NOT on the "non-graphical" reactions that are left alone by this filter !) and in addition, check for the "preparations" in the NON-graphical recations - they may contain important information

BS0501

Highest BRN: 9.844.397

No. of compounds: 9.218.418

Highest Rx.Id: 9.711.590

No. of reactions: 9.677.538

Highest CNR: 6.465.790

No. of citations: 1.949.390