

## Beilstein and Gmelin - Overview

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### I. Introduction

**BEILSTEIN** covers preparations and properties of organic compounds. Beilstein database is the world's largest compilation of chemical facts. It is searchable in multiple ways, including chemical structure, reaction, formula, and physical property parameters. It is worldwide in scope and indexes periodicals, books, dissertations, and patents.

- Over 10 million compounds;
- Over 10 million chemical reactions;
- Over 320 experimental property data;
- Over 960,000 abstracts and titles indexed from the primary organic chemical literature since 1980;
- Over 500,000 bioactive compounds.

<http://www.beilstein.com/features.shtml>. (Accessed 7/14/08)

**GMELIN** covers preparations, properties, and reactions in inorganic and organometallic chemistry and materials science. It is searchable in multiple ways, including chemical structure, formula, and physical property parameters. It is a scholarly bibliographic and property index based on the Gmelin Handbook of Inorganic and Organometallic Chemistry (1772-1975) and a core selection of chemistry journals.

- ~2 million compounds - coordination compounds, alloys, solid solutions, glasses and ceramics, polymers and minerals;
- 1.5 million reactions;
- 900,000 citations, including titles and abstracts from 1995.

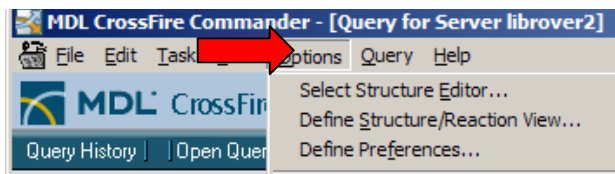
<http://info.crossfiregmelin.com/features.shtml> (Accessed 7/14/08)

**AutoNom** (AUTOMATIC NOMENCLATURE) is a program that generates IUPAC names directly from a structure. Clicking on the AutoNom icon button on the Beilstein commander window launches the application. Structures are input using the Beilstein Structure Editor or ISISDraw.

CrossFire is the search engine that ties all of this together.

#### Initial Set-up Options:

1. Install client: <http://minerva.library.wisc.edu/>  
ID and password available from Emily Wixson, Sharon Mulvey, or <http://chemistry.library.wisc.edu/askchem.html>.
2. Select preferred **STRUCTURE EDITOR**. CrossFire may be set to use two different structure editors: CrossFire Structure Editor and ISISDraw. All UW-Madison Libraries Beilstein Help pages use CrossFire Structure Editor.



## II. Database Organization

The screenshot displays the MDL CrossFire Commander interface. The main window is titled "MDL CrossFire Commander - [Query for Server default]". The menu bar includes File, Edit, Task, View, Options, Query, and Help. The toolbar contains buttons for Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search. The interface is divided into several panels:

- Search Field Name in Hierarchy:** A dropdown menu showing "dielectric constant" and a "Find" button.
- Predefined Search Forms:** A list of search forms including "Search Fields" and "Queries".
- Fact Editor:** A tree view showing a hierarchy of search fields. The "Dielectric Constant" field is highlighted.
- Query Builder:** A central panel for building queries. It includes a "Search in:" dropdown set to "Beilstein(2004/04)". Below this is a "Structure Editor" area with instructions: "Structure/Reaction Search. Double click to enter the Structure/Reaction editor. Right click to copy or paste the structure." To the right of the Structure Editor are "Structure Query Options" including "Free Sites" (hetero atoms, all atoms), "Stereo" (off), "Search" (as structure, as reactant, as product, as reagent/catalyst/solvent), and "Allow" (salts, addl. rings, isotopes, charges, radicals, mixtures, relat. Markush). Buttons for "Clear Structure" and "Extended Options" are also present.
- Search All Text:** A section with a dropdown menu set to "and", a "Search All Text" button, and "Truncate..." and "Clear Text" buttons.
- Search Fields:** A section with a dropdown menu set to "and", "Search Fields" button, "Enlarge...", "Advanced Search", and "Clear Table" buttons.
- Search Field Table:** A table with columns: Operator, Field name, Relation, Field content, List. The table contains three rows:

Operator	Field name	Relation	Field content	List
1	Dielectric Constant(DIC)	is		
2 and		is		
3 and		is		
- Start Search:** A large "Start Search" button at the bottom right, with a "Search Context" dropdown set to "Substances".

Three types of data (or "domains"):

- Substance: contains structural information with all associated facts and literature references, including chemical and physical properties and bioactivity data.
- Reaction: details the preparation of substances.
- Literature citations: author, title, and abstract (1980 - present), which are hyperlinked to substance and reaction records.

**Fact Editor** is often the best way to search **GMELIN** database.

**Structure Editor** is the best way to search **BEILSTEIN** database.

Note: Compounds of the type "biomolecule" (ctype=biomolecule), mixtures, and polymers do not have structure diagrams.

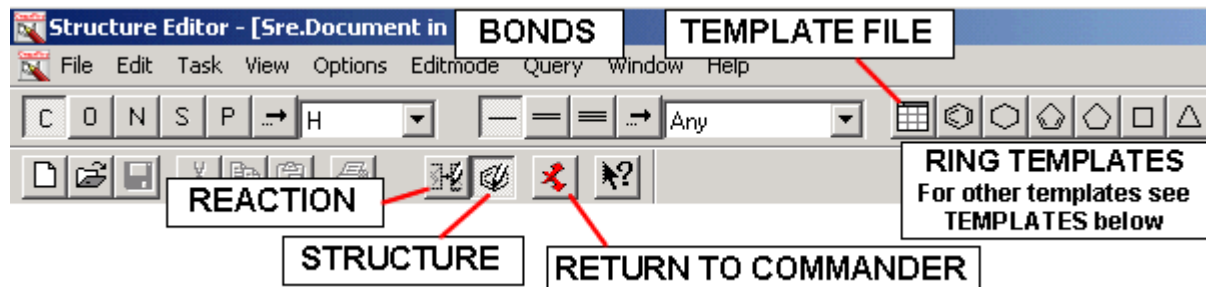
Sample Gmelin record: Water GRN 117

Sample Beilstein record: Acetic Acid BRN 506007

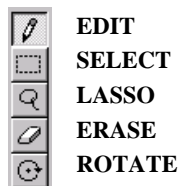
For comprehensive retrieval, conduct both structure and property searches.

Note: It is possible to search Beilstein and Gmelin simultaneously. If both databases are selected, only structure, text, and fields common to both databases may be searched.


### III. Structure/Substructure Searching



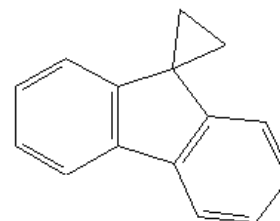
Toolbox:



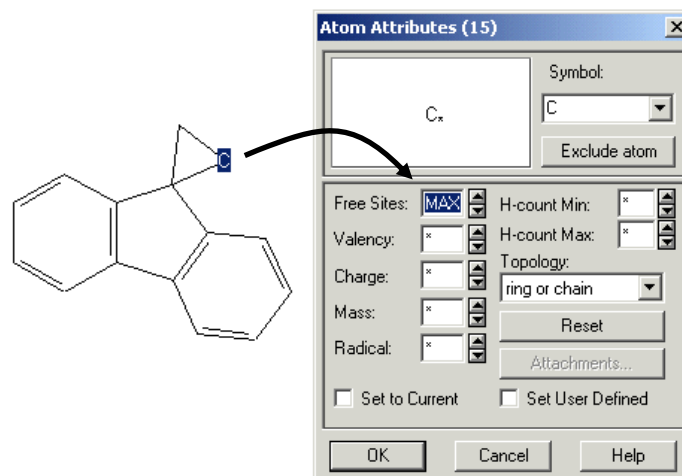
#### Basic Procedure

1. Double-click on **STRUCTURE EDITOR** in Commander window.
2. Click on **EDIT** in the Toolbox.
3. Draw the structure with the currently active atom (default is C) and bond (default is single), or select one of the ring templates.
4. Click on an existing atom to open the atom dialog box to modify it.
5. Set the number of free sites (default is none) and other specifications.
6. To merge individual structures, select the structure with **LASSO** or **SELECT**. Drag the square in the middle of the bond to the target bond or drag the square at the atom node to the target atom.
7. Click on  to return to Commander.
8. Select **STRUCTURE QUERY OPTIONS**.
9. Click on **START SEARCH**.

Structure Search: *Spiro[cyclopropane-1,9'-fluorene]spiro(1,9')-fluorenyl-cyclopropane*



Substructure Search with specified *Free Sites*:



Substructure Search using predefined **Atom Lists** and **Generic Groups**.

### Predefined Atom Lists and Generic Groups:

- All symbols ending with an "H" allow for hydrogen instead of the defined list or group.
- Atom Lists: A = any atom; Q = any atom except carbon or hydrogen; QH = any atom except carbon; M = any metal; X = any halogen.
- Predefined generic groups can only have one bond to the parent structure and setting explicit free sites is not allowed.
- Predefined atom lists and generic groups are entered into the structure like ordinary atom symbols.

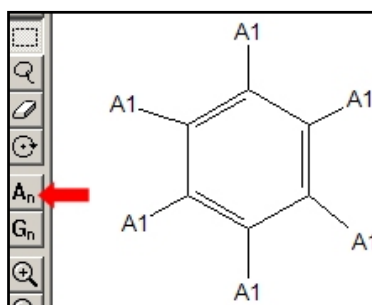
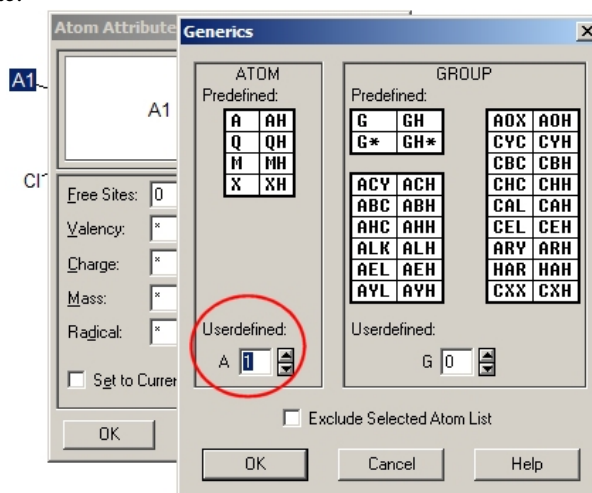
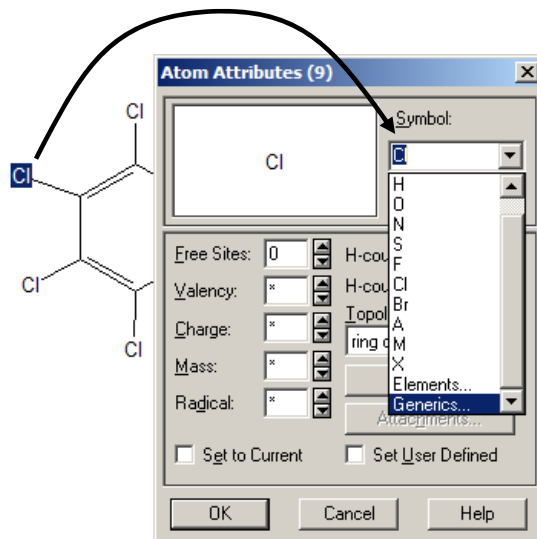
G or GH = Any arbitrary structure.

G\* or GH\* = Any arbitrary structure which can have any number of ring closures to any other G\* or GH\* group or free site.

### User defined Atom Lists (A1, etc) and Markush groups (G1, etc.)

1. Select **A1** in Generics Window.
2. Assign **A1** to atom nodes.

3. Click on **An** in the **Toolbox**.
4. Select the correct Atom List Number.
5. Click **OK** to open a periodic table.
6. Select the desired elements.
7. Click on **OK** to accept the chosen elements.

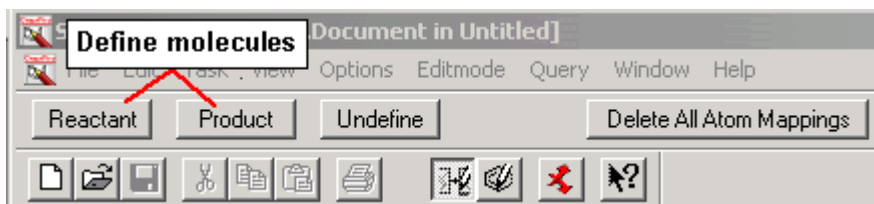



For more information, see Structure and Substructure Searching (<http://chemistry.library.wisc.edu/beilstein/structure-7.html>).

## IV. Reaction Searching

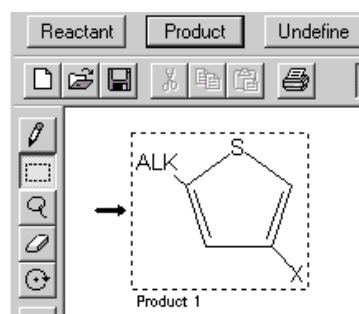
### Basic Procedure

1. Draw structure in **STRUCTURE EDITOR** as described above.
2. Click on **REACTION MODE** to open the Reaction window.



3. Use **SELECT** or **LASSO** to select the structure.
4. Click on **REACTANT** or **PRODUCT** to define each constituent.
5. Define Atom Attributes, Atom-Atom Mapping, and Query Options if necessary.
6. Click on  to return to Commander.
7. Click on **START SEARCH**.

*Half reaction search:*



For more information, see Reaction Searching (<http://chemistry.library.wisc.edu/beilstein/reaction-7.html>).

## V. Property Searching

### Basic Procedure

If a previous search is present in the **STRUCTURE** window or **FIELD TABLE**, click on **CLEAR**.

Enter a fact query in one of two ways:

For simple searches, use **Predefined Search** forms:

1. Click on **PREDEFINED SEARCH FORMS**.
2. Double-click on the appropriate form.
3. Enter search criteria.  
Note: Always click on **LIST** to preview field data format.
4. Click on **OK**.

	Operator	{	Field name	Relation	Field content	List	}	▲
1			Solubility(SLB)	<=	100	▼		
2	proximity		Solvent(SLB.SOL)	is	1,2-dichloro-ethane	▼		
3	and		NMR Spectroscopy(NMR)	exists		▼		

*Fact Editor search built from Beilstein Predefined Search Forms*

For complex searches involving many less common data fields, use the **SEARCH FIELDS** tab to identify appropriate fields or enter criteria directly in the **SEARCH FIELDS TABLE**.

1. Click on the **SEARCH FIELDS** tab.
2. Type a property name in the **SEARCH FIELD NAME IN HIERARCHY** search box.

3. Click on **FIND**.
4. Click on **FIND** again to view additional entries in the hierarchy.
5. Double-click on the desired field code to copy the code name to the **SEARCH FIELDS TABLE**.
6. Select appropriate operator from the **RELATION** drop-down menu.
7. Enter data value in **FIELD CONTENT** cell.
8. Click on **START SEARCH**.

	Operator	[	Field name	Relation	Field content	List	]	▲
1			Dielectric Constant(DIC)	is	28-31			
2	and		Description(ELE.KW)	is	electrical conductivity			
3	and			is				

*Fact Editor value range search combining field code and controlled term*

For more information, see Fact Searching (<http://chemistry.library.wisc.edu/beilstein/factsearching.htm>).

## VI. Displaying a Record

Crossfire retains the **VIEW** defined by the previous user. Therefore, you should set the initial display **VIEW** to the following settings:

- "ALL FIELDS"
- "ALL REACTIONS" or make the appropriate selection
- "HIGHLIGHT HITS" for ease of viewing substructure
- Use "INCLUDE FIELD AVAILABILITY" for quick display of record fields and to "jump" to specific fields in the record

1. Click on **VIEW** in the **SEARCH STATUS REPORT** window.
2. Click on **VIEW** in the top menu to customize the display.
3. Click on **GO TO NEXT HIT** or **GO TO PREVIOUS HIT** to move to the next or previous record.
4. Use **BACK** and **FORWARD** hyperlinks to move between links to substances, reactions and citations within the record.
5. Click on **GET** to get related substances, reactions or citations.
6. Click on **SORT BY** to sort or group the hitset by specified criteria.

*Click on Field Availability in separate window... (F5) to define custom user views.*

## VII. Printing/Saving/Exporting Records and Data

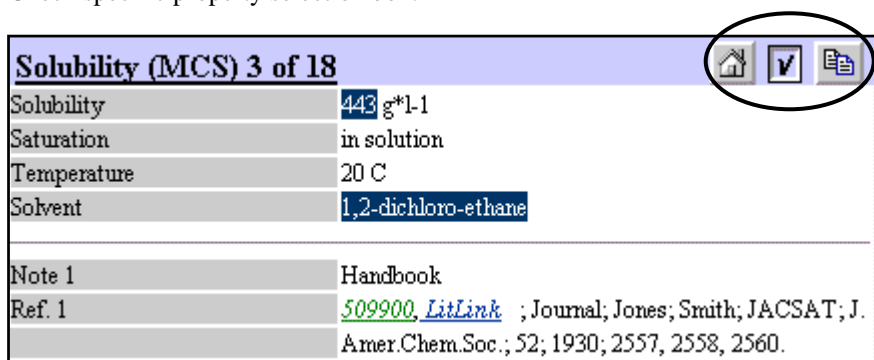
The **FILE** menu always applies to the task that is currently active. This includes **PRINT** and **SAVE**.

### Printing all or selected records in a hitset

1. **DISPLAY** the hitset and note the desired record numbers. (Caution: Some records are quite lengthy. Use **VIEW** to customize the display.)
2. Click on **PRINT HITS**.
3. Select **Range** choice.
4. Select **Options** choices.
5. Click on **OK**.

### Printing selected property data from all records

1. Display the hitset.
2. Check specific property selection box.



3. Click on **PRINT HITS**.
4. Select **Range** choice: **SELECTED FACTS**.
5. Select **Options** choices.
6. Click on **OK**.

### Saving records and data

Hitsets can be temporarily saved on the GLS server and opened for viewing later that day at an EL workstation or a personal workstation configured with the Beilstein client. Structures can be saved locally. Saved hitsets and structures drawn with the CrossFire Structure Editor can only be viewed within Beilstein. The **FILE** menu always applies to the task that is currently active. This includes **SAVE**.

1. Click on **DISPLAY HITS**.
2. Click on **FILE**.
3. Click on **SAVE HITSET AS**.
4. Type filename. (*Hitset is temporarily saved on the GLS server*)

### Saving a structure

1. Draw the structure in the Structure Editor.
2. Click on **FILE**.
3. Click on **SAVE COPY AS**.
4. [For library workstation] Change the drive to a: to save to a floppy disk or E: to save and email as an attachment using Internet Explorer.
5. Type **filename**. Beilstein automatically assigns the extension .bsd for CrossFire Structure Editor or .skc for ISISDraw.

## Exporting records

**EXPORT** permits export of structure, reaction and citation data in HTML, Excel or WORD formats. The available pre-defined export settings depend on the record "context". - substance, reaction, or citation. It is possible to create individual export settings for local installations.

1. Click on **EXPORT**.
2. Select type of information and file format to export.
3. Click on **START**.
4. Specify file location.
5. Click on **SAVE**.

For more information, see "Export Results" (<http://chemistry.library.wisc.edu/beilstein/export-7.html>).

## VII. Beilstein Help and Client Distribution

UW-Madison Beilstein web site: <http://chemistry.library.wisc.edu/beilstein/>

Search Help: <http://chemistry.library.wisc.edu/beilstein/search.html>

Client Distribution Page: <http://minerva.library.wisc.edu/>

Obtain the following information from Emily Wixson, Sharon Mulvey, or <http://chemistry.library.wisc.edu/askchem.html>.

User ID:

Password:

Group name:

Host IP Address: crossfire-acad.elsevier.com

v. 7.1 Article Resolver: <http://sfx.wisconsin.edu/wisc/>