

# Beilstein & Gmelin

## MDL CrossFire V6/7




### Search For:

- ◆ **Substances:** Use the Fact and/or Structure Editor.
- ◆ **Reactions:** Use the Fact and/or Structure Editor.
  - ? → A "how do I make this type of compound"
  - A → ? "what do these starting materials give"
  - A → B "general or specific transformations"
- ◆ **Properties:** Use the Fact Editor.  
Electrical, Magnetic, Optical, Physical, Reaction, Solubility, Spectral, Thermal, etc.
- ◆ **Citations:** Use the Fact Editor.
- ◆ **Text:** Search keywords across both databases simultaneously.

### Fact Editor

- Predefined Search Forms for quick and simple searches by specific data fields.
- Double-click in table cells to view choice of field names, field values, and operators.
- Use \* to expand chemical name segments: **\*succinamid\*** will retrieve:  
**3-hydroxy-2-(4-phenylpiperidino)-5-succinamidotetralin**
- Enter molecular formulae in Hill order: carbon, hydrogen, followed by all other elements in alphabetical order.
- Phrases are not searchable, search each phrase element separately.

### Structure Editor

- Use the MDL CrossFire Structure Editor (under Options→Select Structure Editor).
- Specify attributes of atoms, bonds and molecules, including: charge, mass, valence, stereo formations, sub-structures, and Markush structures.
- In Reaction Editmode identify reaction roles, conserved atoms, bonds and reaction centers.
- Click on the Crossfire icon to send structure(s) to the Query Builder for searching. 
- Options box in the Query Builder allows further refinement of potential results (exact, free sites, stereochemistry, addl. rings, etc). 
- Always use the Structure Editor Icon to return to the editor (V6). 
- Structures can be searched across both databases simultaneously.

### Search Results

- Colored hyperlinks and white arrows move between related substance, reaction and citation records.
- Black arrows move between hits.
- Short Display view scans structures of multiple hits.
- Field Availability view displays selected fields.
- Use Hit Only view to see only fields specified in search.

### Printing / Exporting

- Display only desired fields before printing (default prints everything).
- Export desired factual and structure information into ASCII, HTML, or modeling program formats.

### Documentation – MIMAS Crossfire Service – [www.mimas.ac.uk/crossfire/docs.html](http://www.mimas.ac.uk/crossfire/docs.html)

For further assistance with Beilstein Crossfire, please contact a reference librarian at the Physical Sciences Library (pslref@cornell.edu, 255-4016).

# MDL CrossFire V6/7 – Database Contents

Database	Beilstein	Gmelin
Sources	<ul style="list-style-type: none"> <li>Beilstein Handbook 1771 – 1959</li> <li>Primary literature 1960 – present from 175 journals</li> </ul>	<ul style="list-style-type: none"> <li>Gmelin Handbook 1772 – 1975</li> <li>Primary literature 1975 – present from 62 journals</li> </ul>
Scope	<ul style="list-style-type: none"> <li>9.1 million compounds</li> <li>10 million reactions</li> <li>320 million experimental data facts in 425+ data fields</li> </ul>	<ul style="list-style-type: none"> <li>2.2 million compounds</li> <li>1.6 million reactions</li> <li>300+ million facts in 800+ data fields</li> </ul>
Content	<p><b>organic compounds</b></p> <ul style="list-style-type: none"> <li>Substances which contain carbon <b>and</b> the non-shaded elements in the periodic table below (and including Boron).</li> </ul> <p>Excluding:</p> <ul style="list-style-type: none"> <li>Substances which do not contain carbon.</li> <li>Pure elements</li> <li>CO, CS, CO<sub>2</sub>, CS<sub>2</sub>, COS, C<sub>3</sub>O<sub>2</sub>, C<sub>3</sub>S<sub>2</sub></li> <li>Carbonic acid and its thio analogs along with their salts with inorganic cations</li> <li>HCN, HOCN, HSCN and corresponding iso-acids together with all metal salts and complexes of these acids</li> <li>Dicyanogene</li> <li>Phosgene</li> <li>Metal carbides</li> <li>Metal salts of formic acid, acetic acid, and oxalic acid</li> <li>Fullerenes, which consist only of carbon</li> <li>Carboranes</li> </ul>	<p><b>inorganic and organometallic compounds</b></p> <ul style="list-style-type: none"> <li>All compounds containing no carbon.</li> <li>All compounds containing at least one "Gmelin Element" (shaded in the periodic table below).</li> <li>Additionally: elemental carbon, phosgene, alloys, carbides and carbide oxides, carbonic acid and its thio- and seleno analogues, CO, CS, CO<sub>2</sub>, CS<sub>2</sub>, COS and multicomponent systems with a carbon component</li> <li>Including: <ul style="list-style-type: none"> <li>Coordination compounds</li> <li>Alloys</li> <li>Solid solutions</li> <li>Glasses and ceramics</li> <li>Polymers</li> <li>Minerals</li> </ul> </li> </ul>

Periodic System of the Elements

Group \ Period	1a	2a	3a	4a	5a	6a	7a	8a or 0a	1b	2b	3b	4b	5b	6b	7b	8b		
1	H Hydrogen															He Helium		
2	Li Lithium	Be Beryllium					Au Gold			B Boron	C Carbon	N Nitrogen	O Oxygen	F Fluorine	Ne Neon			
3	Na Sodium	Mg Magnesium								Al Aluminum	Si Silicon	P Phosphorus	S Sulfur	Cl Chlorine	Ar Argon			
4	K Potassium	Ca Calcium	Sc Scandium	Ti Titanium	V Vanadium	Cr Chromium	Mn Manganese	Fe Iron	Co Cobalt	Ni Nickel	Cu Copper	Zn Zinc	Ga Gallium	Ge Germanium	As Arsenic	Se Selenium	Br Bromine	Kr Krypton
5	Rb Rubidium	Sr Strontium	Y Yttrium	Zr Zirconium	Nb Niobium	Mo Molybdenum	Tc Technetium	Ru Ruthenium	Rh Rhodium	Pd Palladium	Ag Silver	Cd Cadmium	In Indium	Sn Tin	Sb Antimony	Te Tellurium	I Iodine	Xe Xenon
6	Cs Cesium	Ba Barium	La* Lanthanum	Hf Hafnium	Ta Tantalum	W Tungsten	Re Rhenium	Os Osmium	Ir Iridium	Pt Platinum	Au Gold	Hg Mercury	Tl Thallium	Pb Lead	Bi Bismuth	Po Polonium	At Astatine	Rn Radon
7	Fr Francium	Ra Radium	Ac** Actinium															

*Lanthanides	Ce Cerium	Pr Praseodymium	Nd Neodymium	Pm Promethium	Sm Samarium	Eu Europium	Gd Gadolinium	Tb Terbium	Dy Dysprosium	Ho Holmium	Er Erbium	Tm Thulium	Yb Ytterbium	Lu Lutetium
**Actinides	Th Thorium	Pa Protactinium	U Uranium	Np Neptunium	Pu Plutonium	Am Americium	Cm Curium	Bk Berkelium	Cf Californium	Es Einsteinium	Fm Fermium	Md Mendelevium	No Nobelium	Lr Lawrencium