Information Services

Structure Searching with Beilstein CrossFire

This guide to structure searching complements the basic Beilstein CrossFire guide.

Searching chemistry databases using a query defined as a chemical structure is a sophisticated and powerful technique, more precise and less open to ambiguity as a search and retrieve process than other types of query that you could use e.g. chemical name or chemical formula. It is usually easier to maximise exactness and precision in your search query by defining it as a pictorial structure, drawing out the atoms and bonds, as you would on paper.

What will a structure search give you?

The search will retrieve from the database all the information held on the substance you have defined in your search query. In many cases this is a very considerable list of reactions and data. The results data are hierarchically categorised with the hierarchy tree fanning out into several hundred individual categories, e.g. UV spectrum, dipole moment, conformation, triple point, critical pressure, enthalpies, refractive index, magnetic susceptibility, isoelectric point etc. The results will very often be a substantial set of data categories, but may sometimes be limited to only a few basic categories, according to what has been reported in the primary literature. Practically all searches will return basic data like melting and boiling points, molecular weight etc.

The results are presented in a separate window as one page, usually very long. You will therefore need to use the scroll bar on the right to bring the data of interest into view on the screen. At the top of each results page there will be a list, the **Field Availability List**, of all of the categories for which data has been retrieved and presented further down the screen.

Examine this list to see what is available and whether the particular piece of information you want is given. Use it as an index to the information your search has retrieved. The rest of the page expands the list, in the same order, citing the published work in which that item of data was reported, and often including the actual value of that piece of data.

As well as the usually wide range of data, the search result will contain details of all the chemical reactions known and reported for the substance you have specified in your query. The reactions are listed immediately following the Field Availability List and are in turn followed by the data categories.

The format for the search results is therefore:

- Substance identification details
- Field Availability List
- Reactions and citations
- Data and citations.

Starting your search

Set up and start the Beilstein CrossFire software as described in the companion to this guide, Beilstein CrossFire. Choose the database you require by clicking at upper left. Use Beilstein for organic chemistry; Gmelin for inorganic, organometallic and coordination chemistry.

How to define and execute your search as a structure query

The Beilstein Commander window is the master window through which you can enter and leave the various sub-windows e.g. a window for drawing/editing the structure query, another for viewing the results.

Open the **Structure Editor** window using the Structure button near the centre of the Beilstein Commander screen.

The structure must be drawn carefully and accurately, or copied, in the Structure Editor window, using the tools provided to the left and above. These are broadly similar to other chemistry drawing packages.

Use **Pencil** to draw atoms one by one, i.e. position the cursor and click; and then connect them together with bonds . The current element is chosen from the shortlist at the top left, the rest of the full set of elements being accessed through a pull-down menu. A click on **Element** will display a full periodic table. Click the element you want and then click OK.

Similarly, choose a current bond type (e.g. single, double etc.) from those at centre top, or others from the pull-down menu. Draw the bond by placing the cursor at the start atom, click and, holding the mouse button down, move the cursor to the other atom and release the button.

Mistakes can be reversed using **Undo**, in the Edit menu, or **Ctrl+Z**. Use **rubber** to remove anything. There is no display of the molecular formula of the structure that you generate. If you need this, you have to do it separately on paper.

When your drawn structure is complete, return to the commander window where it will be displayed. Initiate the search using the blue **Start Search** key. Small dialogue boxes will indicate the progress of the search and its results (nil is a possible result). Use the **Display Hits** key in this box to display the results window, which will appear, as described above.

Advanced tools and features

The basic pencil and rubber are supplemented with a range of more powerful and sophisticated tools.

Any part of the structure that is to be the subject of further editing (e.g. moving, copying, rotating, bulk deletion etc.) must first be selected.

Select tool

To select individual atoms or bonds, activate the Select tool (by clicking on the select icon, immediately below the pencil, on the left toolbar) then click on individual atoms or bonds. Double click anywhere on the structure to select the entire structure. When selected, single items (bonds or atoms) will appear highlighted. Larger parts will be enclosed in a double-lined box to indicate their selected status.

Lasso tool

Use the Lasso tool to select any portion of the structure. With the left mouse button held down, draw a loop around the part you wish to select and release the button. To de-select, click with the cursor positioned anywhere on the blank background

Rotate tool

The entire structure must be selected (i.e. enclosed in a double-lined box) before this tool is engaged from the left toolbar. Upon clicking on the rotate icon, a plain cross will appear in the centre of the selected/highlighted structure. This marks the centre of rotation. This cross mark can be moved to anywhere else using a click-drag. Note that repositioning it outside the structure will not result in the structure rotating upon itself. To perform the rotation, click on the structure and drag in an arc. The cross will remain until the rotate tool is disengaged with a further click on its icon, or until pencil is again used.

Templates

Various common structural themes/motifs/ fragments are available to use as basic building blocks, and the one you choose will draw itself instantly on the screen e.g. chains , rings etc. All of these can be used as is, or used as a starting point for another structure, with subsequent editing . Simple ring forms, C_3 to benzene, are obtained with a single click on the appropriate icon in the toolbar at upper right.
A vast range of some 530 more complex templates are available through **File** menu **Group Template**

This will produce a dialogue box setting out the classes of templates available. Choosing one will then show all the individual templates in that family. You may have to use the scroll bar to see them all. Double click on the one you want and the structure window will return, with the chosen structure displayed, ready for you to use. As a short-cut to these several steps, a click on the icon next to benzene on the top toolbar, will show one of the family sets of templates, usually the last used set. If you want a different set, use the **File** menu route to obtain it.

How atoms and structures appear on the screen

The default structural representation does not show carbon atoms as explicit atoms, i.e. there is no "C" symbol shown at the junction of the bonds. Other options are available e.g. showing all atoms as sequential numbers, or as their proper chemical element symbol.

Use the **Molecule View** dialogue box, obtained through the **Options** pull-down menu, to change the way the atoms actually appear on the screen. It is not possible to show element symbols and position numbers simultaneously. Please note that, by convention, Hydrogen atoms and their bonds are not shown. You can however, for clarity and your own peace of mind, include them in the structure you draw.

Saving result sets

Within the current session, all of the result sets that your queries have retrieved are available for redisplay, at any point. They are given, by default, sequential numbers starting with Q to identify them e.g. Q01, Q02 etc. You will lose all these result sets when you terminate the session, unless you take specific action to save them.

You can save individual result sets for further use. They are saved at the Beilstein server end, not on your computer, disk, or the University network. They cannot be downloaded or saved onto a disk.

To initiate the save instructions you must be in the Display Hits window. **File menu**, **Save Hitset as** will produce a dialogue box where you enter a file name of your choice. The box will also list the other result sets being stored for you.

The query itself, i.e. the structure you have drawn (or a fact-based query) can be saved to any disk destination, in the ordinary way. The saved query file will have the name of your choice, and the file extension .BSD You will find there is already a sub-directory titled BSD in your network filespace, or you can direct the file to your own disk in drive A: You must be in the Commander window to save a query. **File** pull-down menu **Save As** will produce a dialogue box. Enter file name and path details, then use the **Save** button.

Reusing saved items

To display a hitset that you saved in a previous session, you must be in the Display Hits window. In the **File** pull-down menu click on **Open Hitset**. A dialogue box will appear showing what you have previously saved, plus the hitsets of the current session. Double click on the set that you want. It is possible to open more than one hitset at a time.

To reload and reuse a previously saved query (structure or fact), you must be in the commander window. Use the **File** pull-down menu and click on **Open** A dialogue box listing the queries you have previously saved will appear. This lists the files that have been saved to (by default) your network filespace. If the file you want is elsewhere, e.g. on your own disk in the A: drive, you will have to set up the correct path details in the box. Choose the file you want i.e. it will become highlighted, and use the **Open** button in the dialogue box.

Some general points

- Tools remain selected and active until replaced by another.
- Notice that the cursor will show an A or B when positioned on an Atom or Bond. Use this cue to help in accurate positioning of the cursor, and avoid mistakes.
- For most of the commands, operations, and processes , there are other ways or routes to the same end, which can sometimes be quicker. You will discover these with familiarity and regular use.

- Co-ordination compounds are not handled in the way you usually see them printed in books etc. Retrieve and examine e.g. ferrocene, tris(acelylacetonato) Cobalt (III) , or chlorophyll a to see how they are different from what you will see in print.

- When in any of the subsidiary windows, use the ? **BC** button to return to the main window.

- It is possible to define a query and search using specific stereochemistry, i.e. showing “up” and “down” bonds in the structure. You are recommended to first become familiar with the exact conventions used by Beilstein CrossFire for representing stereochemistry by, for example, exploring compounds whose stereochemistry you are familiar with and using the relevant sections of the online manuals.

- Beilstein Commander is a very powerful and sophisticated search and retrieve tool. It has many more features and facilities than the basic ones described here. If you expect to use Beilstein CrossFire a lot, a good investment will be some of your time spent with the online manuals and tutors that are available.

Some common errors

- Failure to click OK in a dialogue box.
- Lack of precision in cursor control in drawing structures.
- Attempting operations whilst in the wrong window.

Manuals and tutors

Comprehensive written manuals, describing in detail all its features and how to use them support Beilstein CrossFire. These are available online at the Mimas website
www.mimas.ac.uk/crossfire/docs.html
The manual listed, near the bottom of the page, as “NEW Beilstein Database Reference Guide” covers everything and has a very comprehensive index. The other manuals shown cover more limited topics.

Also excellent, and new, is the online interactive tutor called Firepower,
www.mimas.ac.uk/crossfire/firepower
It contains both introductory and advanced levels. You need to enter your Athens username and password to use Firepower.

For further information or assistance contact the Science Library
Tel: 029 2087 4085 Email: SciLiby@Cardiff.ac.uk

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