Science & Engineering Library
Searching Guide
Capen Hall

BEILSTEIN CROSSFIRE - VERSION 7

FINDING PROPERTIES & SPECTRA FOR SPECIFIC COMPOUNDS

1. The easiest way to find compounds in Beilstein is to search by a simple chemical name or by Chemical Abstracts Service Registry Number (CASRN). Use of the CASRN is recommended since chemical names are easy to misspell and can have many variations in punctuation and format. If possible, identify the CASRN from a standard source, such as *SciFinder Scholar* database, the *Dictionary of Chemical Names and Synonyms* (UGL/SEL Reference TP 9.H65 1992) or the *Merck Index* (UGL/SEL Reference RS356 .M524).

2. Click on the **MDL CrossFire Commander 7.0** desktop icon**.** The program should automatically connect to the Beilstein database.

3. There is a long vertical pane on the left side of the complex search interface. Towards the top of this pane, click on the **Predefined Search Form** Tab directly under the **Search Field Name in Hierarchy** search box. Double click on the **Substance Identification Data** entry that appears. A **Query Form** window opens up.

4. a) **Search by CASRN:** In the **Chemical Abstracts Registry Number** text input box (NOT the *Compound Registry Number* box), type in **xxxxx-xx-x**, where **xxxxx-xx-x** is the CAS registry number. Do not use leading zeros at the very beginning of the number. Click on the **OK** button in the very top right-hand corner of the **Query Form.** The **Query Form** window will close. To begin the search, proceed with Step 5 below.

   b) **Search by Simple Chemical Name:** In the second set of text input boxes (**Identification Properties)**, locate the second text box labeled **Chemical Name** (NOT the *Chemical Name Segments box* which is the 1st text box). Type in the chemical name. If you click on the link list just to the right of the **Chemical Name** text box, you can browse a very long alphabetical list of all chemical names in the database. Click on the **OK** button in the very top right-hand corner of the **Query Form.** The **Query Form** window will close. To begin the search, proceed with Step 5 below.

5. Click on the dark **Start Search** button in the very lower right-hand corner of the screen. A **Search Status Report** window will pop up. There may be more than one hit. Click on the **View** button in the very right-hand corner of the window.. If there are zero hits, the **View** button will not be highlighted. See the **Note** at end of this guide for possible reasons for zero hits..

6. The structure(s) for the retrieved compounds will display. Double click on the desired structure to display the full record. To make sure that your are viewing the entire record, click on **View** command on the top most (gray) tool bar. Make certain **All Fields** and **Field Availability included** are both checked (active). The **Field Availability List** that appears after the basic substance information shows all the properties (fields) available for the displayed compound including reactions and spectra.. Note the entire record can be hundreds of pages long.

7. Click on any hyperlinked field code from the left-hand column of the **Field Availability List** to jump down to that point in the record.

8. **Extreme care must be used in printing records since all information for a given compound is in a single record that can be hundreds of pages long.**

- ***If the record is short***, the entire record can be printed using the **Print Hits** button in the upper left-hand corner of the screen (below the MDL CrossFire Commander Header Line).

- ***To select an individual fact for printing*** (a single table or occurrence of a field), **left click** on the **empty square box** in the blue shaded field name heading just to the right of the ***Home*** *(Top)* icon. **Left click** on as many individual facts (tables) as you wish, and then click on the **Print Hits** button in the upper left-hand corner of the screen. Note that **Selected Facts** radio button is automatically selected in the **Print** window. Remember to select the first field for printing, **Substance**, so you know which compound the information you print is associated with.

- ***To print all occurrences (or tables) of a given field***, **RIGHT** click on the **empty square box** in the blue shaded field name heading just to the right of the ***Home*** *(Top)* icon. Choose the option, **Select All the Facts: [*Field Name*].** Up to the first 100 occurrences (values) of a given field will be selected (checked) for printing. If there are more than 100 occurrences and you want to print the remainder, move down to the 101st occurrence (the first blue header line without a checkmark) and repeat the procedure above, 100 at a time. **RIGHT click** on as many different fields as you wish; and then click on the **Print Hits** button in the upper left-hand corner of the screen. Note that the **Selected Facts** radio button is automatically selected in the **Print** window. Remember to select the first field for printing, **Substance**, so you know which compound the information you print is associated with.

Note: Reasons for zero results (in order of likelihood)

- Substance is not an organic compound (check with a reference librarian).

- ***If a chemical name was searched:***
  - the name is misspelled, punctuated, or formatted differently in the list of synonyms.
  - the name searched is not listed in the database. Try a different name or identify the CASRN.

- ***If a registry number was searched:***
  - Registry number was mistyped. Check your transcription and input.
  - Registry number in error in source. Check SciFinder Scholar (Chemical Abstracts).
  - Substance is in Beilstein CrossFire database, but does not have CASRN field entry. A structure search is the only definitive approach to find a Beilstein compound record.

- Substance is novel or not covered by Beilstein. This is unlikely. A check of SciFinder Scholar would normally confirm or contradict this.

by A. Ben Wagner, Sciences Librarian
Document: 29 December 2004
URL: http://ublib.buffalo.edu/libraries/e-resources/bc-finding-prop-v7.pdf