




BEILSTEIN CROSSFIRE - VERSION 6

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 **Start**, then **MDL CrossFire Commander V6**. If the *Select database* field box (top left of screen) is empty, click on the red double arrow icon. 
3. In the lower left hand corner is a list of predefined forms. Highlight (click on) the **Ident. Data** entry. Click on the **Open** button below.
4. a) **Search by CASRN:** In the **Chemical Abstracts Registry Number** text input box, type in **xxxxx-xx-x**, where **xxxxx-xx-x** is the CAS RN. Do not use leading zeros at the very beginning of the number. Click on the **OK** button in the lower left-hand corner of the **Ident. Data** window. The 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 (**ID 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 **Magnify Glass Icon** 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 lower left-hand corner of the **Ident. Data** window. The window will close. To begin the search, proceed with Step 5 below.
5. Click on the bright blue **Start Search** button in the lower right hand corner. A **Query Result** window will pop up. Click on **Display Hits** button. If there are zero results, the **Display Hits** button will not be highlighted. See note at end of this guide for possible reasons.
6. The structure(s) for the retrieved records will display. Double click on the desired structure to display the full record. To make sure that you are viewing the entire record, click on **View** command on the top most (gray) tool bar. Make certain **All Fields** and **Include Field Availability** are both checked (active). The **Field Availability** table that appears after the basic substance information shows all the properties (fields) available for the displayed compound. Note the displayed record can be hundreds of pages long.

7. Click on any hyperlinked field code from the left-hand column of the **Field Availability** table 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 (or 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** and select for printing 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

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URL: <http://ublib.buffalo.edu/libraries/e-resources/bc-finding-prop-v6.pdf>