

# SEARCHING BEILSTEIN CROSSFIRE USING MDL CrossFire Commander Version 7

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## I. LOGGING ONTO CROSSFIRE

Double click on the MDL CrossFire Commander 7.0 icon on your desktop. If the icon is not on the desktop, go to **Start: All Program** and find the MDL CrossFire Commander entry. Note that Beilstein CrossFire does NOT use standard web browsers. A special search program must be installed on the computer to access this database. Instructions are available at <http://ublib.buffalo.edu/libraries/e-resources/bc.html> (UB patrons only).

## II. MDL CROSSFIRE COMMANDER INTERFACE

The interface is both very powerful and very complex. Upon entering the program, the user is presented with 3 sets of tool bars on top, 3 main window areas with 12 panes (subwindows), and 8 buttons. And this is just the Query Building Screen!

### A. TOOLBARS

- 1) The topmost grey tool bar provides basic, standard program control and functions: *File, Edit, Task, View, Options, Query, and Help* commands.
- 2) The second from the top blue-grey tool bar starts with the icon of and title, *MDL CrossFire Commander*. In the center of this tool bar are a set of 5 Tabs that allows movement between the *Query* [Search criteria], *Results, Reports, and Autonom*, which is a separate program that generates IUPAC systematic names from structures drawn by the user. The *Alerts* Tab/feature is not available on our server. The currently active Tab is colored a dark blue-green.
- 3) The third from the top tool bar is a set of dark blue-green command buttons. The commands on this bar change depending on which Tab in the blue-grey tool bar is active. For example, when the *Query* Tab is active, all the displayed command buttons relate to Query operations. Some of the items on the toolbar duplicate functions available elsewhere on the screen while others are unique to this tool bar.

## B. MAIN WINDOWS

### 1) LEFT-SIDE COLUMN WINDOW

The tall, vertical window on the left-hand side (underneath the **Query History** button) has a text heading that varied based on which of the four Tabs below the text input box is active. Upon entering Beilstein CrossFire, the text heading “Search Field Name in Hierarchy” will normally be displayed. Underneath this are the four important Tabs (arranged in two layers with almost no visual divider, so they do not appear at first glance to be Tabs) that control what is displayed in the column below.

- The **Search Fields** Tab allows one to navigate and search the extensive hierarchical database structure, over 360 fields.
- The **Queries** Tab lists search queries created within the current session (and prior days if they have not been manually or automatically deleted).
- The **Hitsets** Tab lists the results (hits) created by queries within current session.
- The **Predefined Search Forms** Tab is a set of predefined query forms that greatly simplify searching many common substance, property, and bibliographical fields in the database. This Tab will frequently be used in the search examples in *Section III (Predefined Search Form Searches)*.

The **Query Builder** window takes up the rest of the screen.

### 2) QUERY BUILDER: STRUCTURE/REACTION SEARCH SECTION

The top section of the **Query Builder** window with a white background is the **Structure/Reaction Search** section. This section permits input of structure drawings and controls the parameters of the structure/substructure search. To create or modify a structure-based search query, note the instructions to double click anywhere inside the large white box. This action will open the Structure Editor. Use of the structure editor will be discussed in Section IV of this document.

### 3) **QUERY BUILDER: SEARCH ALL TEXT AND SEARCH FIELDS SECTIONS**

The bottom two sections with a blue/gray background are the **Search All Text** and **Search Fields** query (search) input areas.

The **Search All Text** searches keywords across all fields with English or German words in them. A detailed discussion of this feature is beyond the scope of this guide. Note however that there is no standardized controlled vocabulary (subject headings), and there is no guarantee that any particular record or field will have textual descriptions available.

In the very lower right-hand corner of this section is the all-important **Start Search** button. The system does not initiate any search until this button is clicked on. Simply hitting the **Enter** key will NOT start a search.

Note that it is important to clear the various areas, check boxes, radio buttons, and text boxes of the **Query Builder** window before beginning a new search. Any stray input left in place will be included in the search as you input new information in other parts of the **Query Builder**.

## **III. PREDEFINED SEARCH FORM SEARCHES**

This section will focus on frequently needed searches that can be done using various forms under the **Predefined Search Form** Tab located in the upper left-hand column underneath *Search Field Name in Hierarchy* text input box.

- A) Any or all **physical property, spectra, and ecotox information on a particular substance**, if you know a fairly simply chemical name or CAS registry number.
- B) **All reactions involving a specific substance** as a product (preparation of), as a reactant, or as either one.
- C) **All reactions using a specified catalyst, reagent, or solvent.**
- D) A set of compounds based on **range searching of one or more physical properties.**
- E) All references by a given **author.**
- F) Substances with a specified **number and types of atoms.**

## To access the **Predefined Search Forms**:

1. Click on the **MDL CrossFire Commander 7.0** desktop icon. The program should automatically connect to the Beilstein database.
2. There is a long vertical pane on the left side of the Beilstein 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. All the instructions in the following sections start from the point that the **Predefined Search Form** Tab is the active tab (colored a dark blue-green).

### **III. A. Any or all physical property, spectra, and ecotox information on a particular substance, if you know a fairly simple chemical name or CAS registry number.**

1. The easiest way to find information on 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. Double click on the **Substance Identification Data** entry under the **Predefined Search Form** Tab. A **Query Form** window opens up.
3. 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 1<sup>st</sup> text box). Type in the chemical name. If you click on the link labeled **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.
4. 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.

5. The structure(s) for the retrieved compounds 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 **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.
6. 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.
7. **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]**. Make sure you know how many occurrences of a given field there are as this procedure will selected them all, even if there are 100 NMR spectra listings or 3,000 reactions. **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.

### III.B. All reactions involving a specific substance as a product (preparation of), as a reactant, or as either one.

1. **Important Note:** The procedure described below will reliably retrieve all reactions involving the precise substance as represented by the chemical name or CAS Registry Number. Be aware that any slight variation in stereochemistry, isotopes, charges, radicals, salts, etc. will be represented by a separate record under a different name and CAS registry number containing reactions related to that precise variation.
2. Follow Steps 1-5 of Section III.A.
3. Click on **View** command again on the top most (gray) tool bar. In the 4<sup>th</sup> section of the long drop down menu, check the option **Structure** included (unless one wants only the names of the products and reactants and not the reaction diagram. In the 5<sup>th</sup> section of this same long drop down **View** menu, check the desired option: **All Reactions** (if you wish to see all reactions regardless of whether the compound is a reactant or product), **Substance as Reactant only**, or **Substance as Product only**.
4. Note that the **Field Availability List** just below the substance information at the beginning of each record will show how many reactions there are. Note also that reaction view changes do not affect the property and spectra fields that are still displayed as part of the record after the reactions.
5. **Caution:** The record can still be hundreds of pages long. Be careful to print only the information you want.
6. *To select an individual reaction for printing, left click* on the **empty square box** in the blue shaded header line (*Reaction x of y*) just to the right of the **Home (Top)** icon. **Left click** on as many individual reactions 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 reactions you print is associated with.
7. *To print all reactions*, go to the first reaction and **RIGHT** click on the **empty square box** in the blue shaded field name header line (*Reaction 1 of y*) just to the right of the **Home (Top)** icon. Choose the option, **Select All the Facts: [Field Name]**. Up to the first 100 reactions will be selected (checked) for printing. If there are more than 100 reactions, move down to the 101<sup>st</sup> reaction (the first header line without a checkmark) and repeat the procedure above, 100 at a time. 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.

### III.C. All reactions using a specified catalyst, reagent, or solvent

1. **Important note:** It is important to search all possible name/formulas for a given substance. For example, if searching for methanol, search for *meoh*, *methyl alcohol*, *methanol*, and *CH<sub>3</sub>OH*. There is absolutely no standard format for catalysts, reagents, and solvents.
2. Double click on the **Reaction Data** entry under the **Predefined Search Form** Tab. A **Query Form** window opens up.
3. The last entry on the screen is labeled **Search in Reaction Basic Index**. Inside this entry, change the **starts with** to **contains** using the drop down menu arrow. . (If you click on the link labeled **list** just to the right of the text input box, you can browse a very long alphabetical list of designations/words present in the reaction fields.)
4. Type into the text input box the first possible variant of the name/formula, e.g. *methanol*. Hit the **Enter** key or click on the **OK** button in the upper right-hand corner of the **Query Form** window.
5. Repeat Steps 2-4 until all variant names, formulas, or other designations of the desired catalyst, reagent, or solvent are input. Note that as you input variants new lines are created in the **Search Fields** pane at the bottom of the **Query Builder** window on the main screen. The **Operator** column in the **Search Fields** pane must be changed to **or** from **and** for each line using the drop down menu arrow in the column.
6. Once all the variants are entered, click on the **Start Search** button in the lower right-hand corner of the main screen. A **Select Search Context** window will appear. Click on the **Search in Reactions** button. A **Search Status Report** window will appear showing the number of reactions retrieved by your query.
7. Click on **View**. Four reaction schematics per screen will display. **Double click** on any reaction schematic to see the full details of the reaction. To make sure that you are viewing the full record, click on **View** command on the top most (gray) tool bar. Make certain the entries for **All Fields**, **Highlight Hit Terms**, and **Structures Included** are all checked (active) and that **Structures in separate window** and **Field Availability included** are NOT checked.
8. **Caution:** There can be tens of thousands of reactions for a given catalyst, reagent, or solvent. Be careful to print only the information you want.

9. *To select an individual reaction for printing, left click* on the **empty square box** in the blue shaded header line (*Reaction*) just to the right of the *Hitset Family* button. **Left click** on as many individual reactions 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.
10. *To print a sequential range of reactions or all reactions*, simply click on the **Print Hits** button in the upper left-hand corner of the screen. Select the **Range of Hits** radio button and fill in the range (1 to nn) of records you wish to print.
11. The number of reactions for common catalysts, reagents, and solvents can be overwhelming. The easiest way to limit the number of hits is draw in a substructure in the **Structure/Reaction editor** (see *Section IV*). By default, the reaction hits must contain both the specified substructure and the specified information in the **Search Fields** query table. Alternately other search criteria can be entered using other **Predefined Search Forms**. Be sure to hit the **Start Search** button after inputting additional criteria.

### **III.D. A set of compounds based on range searching of one or more physical properties.**

There are scores of physical property data that can be range searched. This guide is limited to the four most common properties (mp, bp, density, and refractive index) searchable through the **Physical Data Predefined Search Form**. Searching other physical property ranges requires navigating the large field hierarchy under the **Search Fields** Tab near the top of the left-hand column of the main query screen. A detailed description of this technique is beyond the scope of this guide.

1. **Important Note:** The **units** used are the ones "commonly used in organic chemistry, not necessarily SI units" and are always the same for a given field.
2. Double click on the **Physical Data** entry under the **Predefined Search Form** Tab. A **Query Form** window opens up.
3. In the bottom portion of the form, enter the desired value or range of values (using hyphens) for the desired property (melting point, boiling point, density, or refractive index). Use the default '=' operator to search an exact value or range of values. One can also choose *greater than*, *greater or equal to*, *less than*, or *less than or equal to* operators using the drop down menu arrow just to the right of the '**value or range**' label. Melting point and boiling point are in degrees Celsius. Densities are in grams/cm<sup>3</sup>. Refractive Index, being a ratio, is unitless. Decimal values must be input with a leading zero, i.e. 0.85.
4. One can simultaneous search on any combination of these four properties by entering values in as many of the four fields as desired.

5. Once the desired value(s) are entered, click on the **OK** button in the upper right-hand corner of the **Query Form** window.
  6. 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 showing the number of substances matching the property ranges you input. 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.
  7. The structure(s) for the retrieved compounds 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 **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. If one wants only the substance identification and the physical property fields that were actually searched to display, simply click on **View** and check **Hit Only** entry (which will remove the **All Fields** checkmark).
  8. 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.
  9. **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]**. Make sure you know how many occurrences of a given field there are as this procedure will selected them all, even if there are 100 NMR spectra listings or 3,000 reactions. **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.

### III.E. All references by a given author

**Important Note:** Beilstein indexes no more than the first five authors of a paper. Names in the author field are NOT standardized. The same author's name may appear in a variety of formats. Sometimes only the last name of the author is given. In other cases, the last name is followed by a comma and then by any combination of initials and first/middle/hyphenated names. Format of names with connectives (e.g. van, von, d', de, etc.) are not formatted consistently, most likely matching the format of the name in the original publication. Browsing the alphabetical index of author's names is essential.

1. Double click on the **Bibliographic Data** entry under the **Predefined Search Form** Tab. A **Query Form** window opens up.
2. The author is the first field listed. Use the link labeled **list** to the extreme right of the author text input box to browse an alphabetical list of all author names, looking carefully for variations in format of the desired author (see *Important Note* above.).
3. Type into the text input box the first possible variant of the author's name. For unusual last names, one can simply type in the last name retaining the **starts with** option and retrieve all variant formats. Hit the **Enter** key or click on the **OK** button in the upper right-hand corner of the **Query Form** window.
4. Repeat Step 3 as needed until all variant names are input. Note that as you input variants, new lines are created in the **Search Fields** pane at the bottom of the **Query Builder** window on the main screen. The **Operator** column in the **Search Fields** pane must be changed to '**or**' from '**and**' for each line by using the drop down menu arrow in the column.
5. Once all the variants are entered, click on the **Start Search** button in the lower right-hand corner of the main screen. A **Select Search Context** window will appear. Click on the **Search in Citations** button. A **Search Status Report** window will appear showing the number of citations retrieved by your query.
6. 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.
7. The citations in brief format will display. Double click on any citation to display the 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 **Structures included** are both checked (active). The full record includes a listing of all substances indexed by Beilstein for that particular literature reference. Note a single record with the substances indexed displayed can be many pages. If one wants only the citation, change the View to **Hit only** option rather than **All Fields**.
8. **To print records**, be sure **View** is set to **Hit Only**, unless the lengthy display of substances indexed is desired (not generally recommended).

- *To print selected, scattered citations for printing, left click* on the **empty square box** in the **Citation** blue shaded field name heading just to the right of the *Home (Top)* icon. Also click on the same empty box in the **Citation Number** field heading if you wish to print the Beilstein citation number with the citation. **Left click** on as many citations 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.
- *To print a sequential range or the entire set of citations*, simply click on the **Print Hits** button. Select the **Range of Hits** radio button and fill in the range (1 to nn) of records you wish to print.

### III.F. Substances with a specified number and types of atoms.

A little used, but extremely powerful, feature of Beilstein is the ability to search elements counts and number of elements derived from the molecular formula. The **Molecular Formula Search Predefined Search Form** permits the input of up to 3 individual elements counts (e.g. Br<sub>2</sub>, F<sub>3</sub>, C<sub>12</sub>) and a specified total, 'greater than', or 'less than' number of elements.

As many element counts, number of atoms, number of elements, molecular formula ranges, number of fragments, and molecular weights can be searched in any combination by navigating the large **Molecular Formula** fields hierarchy under the **Search Fields** Tab near the top of the left-hand column of the main query screen. A detailed description of this technique is beyond the scope of this guide.

1. Double click on the **Molecular Formula Search** entry under the **Predefined Search Form** Tab. A **Query Form** window opens up.
2. Input values for as many fields as you wish in order to define the desired substances.
  - **Element Counts** – are entered with the standard chemical symbol and a number (no spaces). Examples: F<sub>5</sub>, Be<sub>2</sub>, S<sub>3</sub>. Up to three element counts can be entered, one in each of the three input boxes. All small case or an initial cap for two-letter elements will work. All caps (e.g. CL<sub>5</sub>) will give zero hits.
  - **Number of elements** – is the total number of elements (NOT atoms) in the molecular formula. Hence, C<sub>7</sub>H<sub>5</sub>F<sub>3</sub> has three elements. Note that the *operator* can be changed from 'equal to' to 'less than', 'less than or equal to', 'greater than', or 'greater than or equal to' using the drop down menu arrow to the right of the field name.
  - **Search Formula** – either the exact formula or formulas with ranges (like C<sub>9-12</sub>) can be searched. Follow the format as given in the examples below the text input box.
3. Once the desired value(s) are entered, click on the **OK** button in the upper right-hand corner of the **Query Form** window.

4. 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 showing the number of substances matching the criteria you input. 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.

5. The structure(s) for the retrieved compounds 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 **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. If one wants only the substance identification information, simply click on **View** and check **Hit Only** entry (which will remove the **All Fields** checkmark).

6. 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.

**7. 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]**. Make sure you know how many occurrences of a given field there are as this procedure will selected them all, even if there are 100 NMR spectra listings or 3,000 reactions. **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.

## IV. STRUCTURE/REACTION EDITOR

Types of searches appropriate for the *Structure/Reaction Editor* include finding:

**A)** Any or all **information** (structural, reaction, physical properties, spectra, etc.) **on a particular substance** where only the **structure** is known (no name or CAS registry no.).

**B)** All substance records in the database containing a given **substructure**.

**C)** Structure-based **reaction transformations** (A → B).

The procedure for each type of *Structure/Reaction Editor* search is described in the following sections. The *Structure/Reaction Editor* is reasonably easy to use. Detailed instructions are beyond the scope of this pathfinder, click on **Help** command while inside the *Structure/Reaction Editor* for more help. If you have done other searching using the predefined search forms, text, or field searching, be sure to clear this information from the query screen or it will be used as part of the criteria for the search (at times, this is a great benefit as one can use field searching to limit an overly broad substructure).

The *Structure/Reaction Editor* can be entered by **double clicking** anywhere inside the large **Structure/Reaction Search** window in the very center of the **Query Builder** screen. If you get the error message, “Cannot connect to ISIS/Draw. It is not installed correctly.”, click **OK** to close the error window. Then click on the **Options** command on the topmost toolbar and choose the **Select Structure Editor...** entry. Change the **Structure Editor** radio button to the last entry, **MDL CrossFire Structure Editor**, and click the **OK** button.

### IV.A. Information (structural, reaction, physical properties, spectra, etc.) on a particular substance where only the structure is known

Draw the entire structure in the structure editor. Do not include hydrogens as all free sites can automatically be filled with hydrogen. Return to the **Query** screen by clicking on the **red double-arrow icon** below the **Query** command in top tool bar. Your structure will automatically be inserted into the Structure Window. Simply hit the **START SEARCH** button. By default, an exact structure search is performed.

Remember that even a single substance record can be very lengthy. See the display printing instructions in **Section III. A. Step 4-7**.

### IV.B. All substance records in the database containing a given substructure

1. Draw the desired substructure in the structure editor. Bonds and atoms default to ring or chain. To check specifications of any atom or bond, left click on an existing atom or bond. A pop-up window permits specifications of charges, numbers of connections, hydrogen counts, etc. It is far safer to specify hydrogens with hydrogen counts rather than explicitly drawing in hydrogens. Generic groups (e.g. alkyl) and variable atoms may be specified.
2. Return to the **Query** screen by clicking on the **red double-arrow icon** below the **Query** command in top tool bar. Your structure will automatically be inserted into the *Structure Window*.

3. To the right of the *Structure Windows*, choose the desired **Free Sites:** and **Allow:** by checking the appropriate entries.
4. Choosing the **Free Sites: Hetero atoms** will allow additional non-hydrogen attachments only at heteroatoms. **Free Sites: all atoms** allows non-hydrogen attachments anywhere it is chemically possible.
5. The **Allow:** options retrieve various variations of the base structure such as salts and radicals. These are mostly self-explanatory, except for the **Allow: addl. rings**. The **Allow: addl. rings** permits the possibility of ring closures between atoms that are part of the user-drawn substructure. Leaving this option unchecked will still allow additional rings in the retrieved substance that are apart from the atoms that have been drawn in, assuming at least one free site is specified.
6. Hit the **START SEARCH** button. Follow the display and print instructions in **Section III.A. Steps 4-7**.

#### IV.C. Structure-based reaction transformations (A → B)

If a specific reactant or product is known, follow the instructions in *Section III.C*. The following technique retrieves reactions based on more generic substructures.

##### 1) Draw and specify reactant and product structures

Using the *Structure/Reaction Editor*, draw the relevant reaction site(s) and the structural context for the reactant or the product or both. Once the substructure drawing is complete, specify all reaction information by clicking on **Editmode** command on the top toolbar, then **Reaction**. Draw a box around each reactant one at a time and hit the **Reactant** button. Do the same for products, hitting the **Product** button.

##### 2) Map common atoms

Mapping atoms helps the computer understand how the reactant and product are related. Change the drawing tool from the dotted box tool to the **pencil** on the left side of the drawing screen. Map atoms by clicking on an atom in the reactant and holding the left mouse button down. Then move the cursor over the corresponding atom in the product and release the mouse button. A dotted line linking the two atoms will appear.

##### 3) Specify reaction sites

For each bond broken or formed in the reaction, position the mouse cursor over the bond and left click. The pop up window permits detailed specification of what happens to that bond. It is usually sufficient just to check the box that says **Break/Make Bond**.

##### 4) Perform search

Return to the **Query** screen by clicking on the **red double-arrow icon** below the **Query** command in top tool bar. Your reaction structure(s) will automatically be inserted into the *Structure Window*. Specify the appropriate options in the **Free Sites:** and **Allow:** boxes. See *Section IV.B. Steps 4-5* for details on these options. Note that if no Free Sites are specified, the structures used in the reaction will exactly match the user input.

Click on **START SEARCH** button. It is possible to receive an overwhelming number of hits. In that case, provide more structural details in the *Structure/Reaction Editor* or use *Predefined Search Forms* to specify catalysts, solvents, reagents, or any other type of information. Note that although all reactions

have fully described reactant and product structures, not all reactions have catalysts, solvent, reagent, yield, etc. information available (See *Section III*). In other words, limiting a reaction to a particular catalyst will eliminate all reactions where catalyst information is not available, i.e. not input by Beilstein.

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URL: <http://ublib.buffalo.edu/libraries/e-resources/BeilsteinGuide.pdf>