

Lab 7

Online search of the chemical literature with Beilstein.

This lab will teach you how to use MDL CrossFire to search the Beilstein Chemical Database.

This weeks lab will consist of performing three basic searches on two chemical structures provided by your TA.

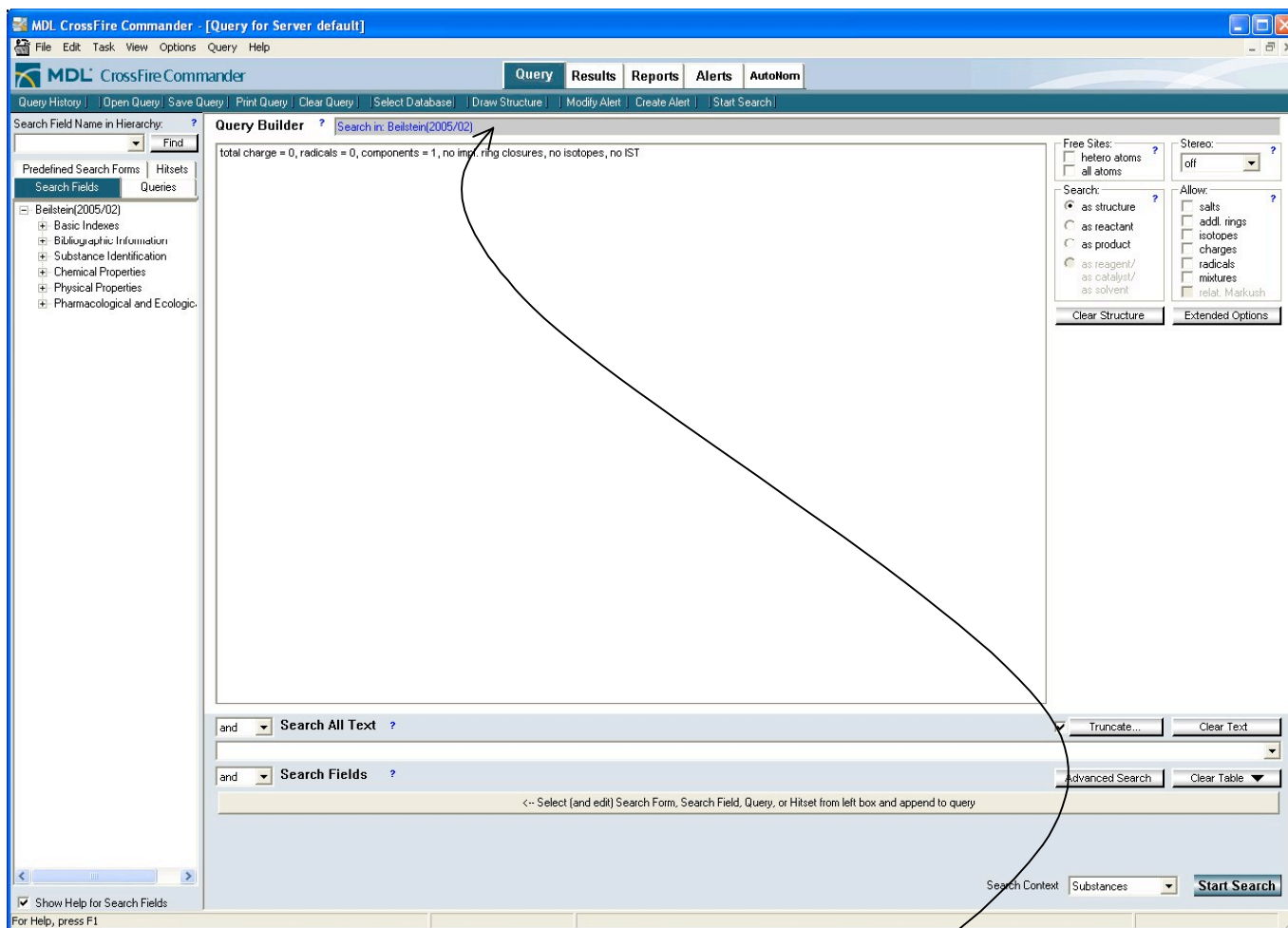
For each compound you will:

1. Perform an structure search (exact structure search).
 - a. write down how many “hits” your search revealed.
 - b. write down what information (mp. bp. ect.) that is available for the parent compound.
2. Perform a substructure search (using free sites) to see if compounds are known that contain your structure as part of a larger structure.
 - a. Write down the structure of the compound that contains your compound as a substructure.
 - b. Write down a citation for a paper for patent the references this larger structure. (just the reference - you do not need to get a copy of the paper)
3. Perform a search specifying your compound as a product (or a reactant if needed) in a synthetic reaction.
 - a. Write down the reaction including reagents used for the synthetic transformation.
 - b. Obtain a copy of an original research article citing this synthetic transformation. (This will involve looking up the citations for the compound and then seeing if our library carries that Journal. You only need to print the first page of the article and one other page that contains the structure of your compound.) Hint: Skip the references for patents or journals that are clearly not written in English, then look if UD has a subscripito in to this journal.

1. Open the application by clicking on “MDL CrossFire Commander” and select “Beilstein” if prompted to enter a database.

TIPS: The first time the program runs on a particular computer, you may be asked to enter a structure editor. Select “MDL CrossFire Structure Editor” (This will match the screen capture pictures below. You are welcome to try MDL ISIS/Draw as well but the pictures won't match those in the handout). If you get a message saying:” No Server is Connected”, press the connect button on the dark blue menu bar.

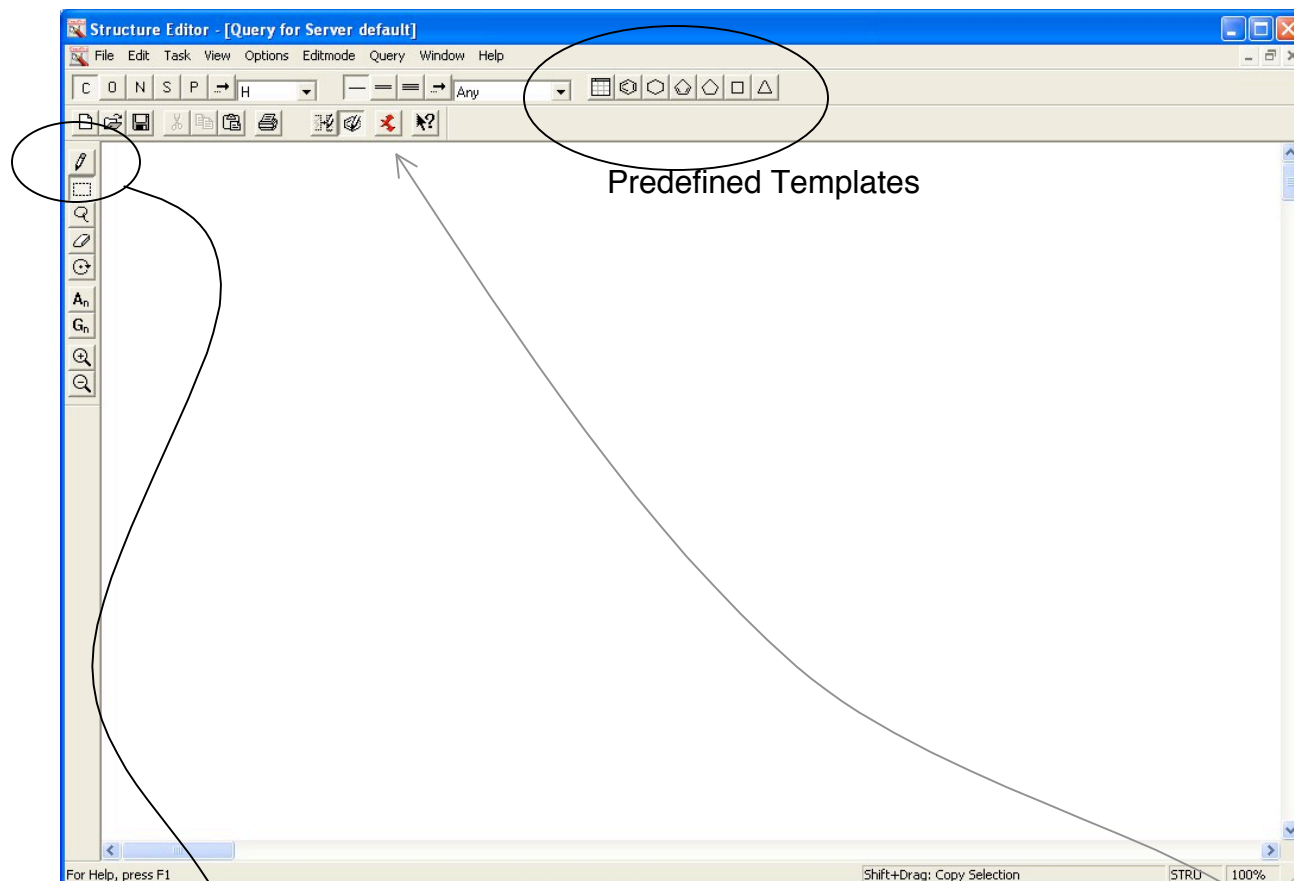
You will see the following window.



2. Click on the “Draw Structure” button on the dark blue menu bar.

3. This brings us to the structure editor window. We will begin by doing a specific structure search. Construct the structure below.

Note: The structures should be considered in “bond-line” style where the hydrogens are implied unless otherwise specified (we will learn how to include a “Free Site” soon).



4. Draw the structure.

- Use the pencil or the predefined templates to draw the structure of the molecule you want to search.
- To add Nitrogen, oxygen or any other atom type, simply click on an existing atom with the pencil and a window will open that lets you specify the atom type. .

5. Return to the Crossfire commander window by pressing the Crossfire button



When you return to the commander window, your structure should be automatically imported.

6. Check the search type; In this case, we will be searching “as a structure.” In other words does this structure appear in the literature?

MDL CrossFire Commander - [Query for Server default]

File Edit Task View Options Query Help

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Query History Open Query Save Query Print Query Clear Query Select Database Draw Structure Modify Alert Create Alert Start Search

Search Field Name in Hierarchy: Find

Preddefined Search Forms Hitsets Search Fields Queries

Beilstein(2005/02)

Basic Indexes

Bibliographic Information

Substance Identification

Chemical Properties

Physical Properties

Pharmacological and Ecologic

total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST

Free Sites: hetero atoms all atoms Stereo: off

Search: as structure as reactant as product as reagent/ as catalyst/ as solvent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markush

Clear Structure Extended Options

and Search All Text Truncate... Clear Text

and Search Fields Advanced Search Clear Table

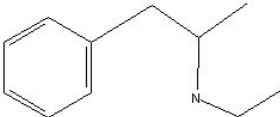
Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

Show Help for Search Fields

Search Context Substances Start Search

7. Press Start Search.

8. In a moment, the following pop up appears- Wait for the search to complete and press “View”

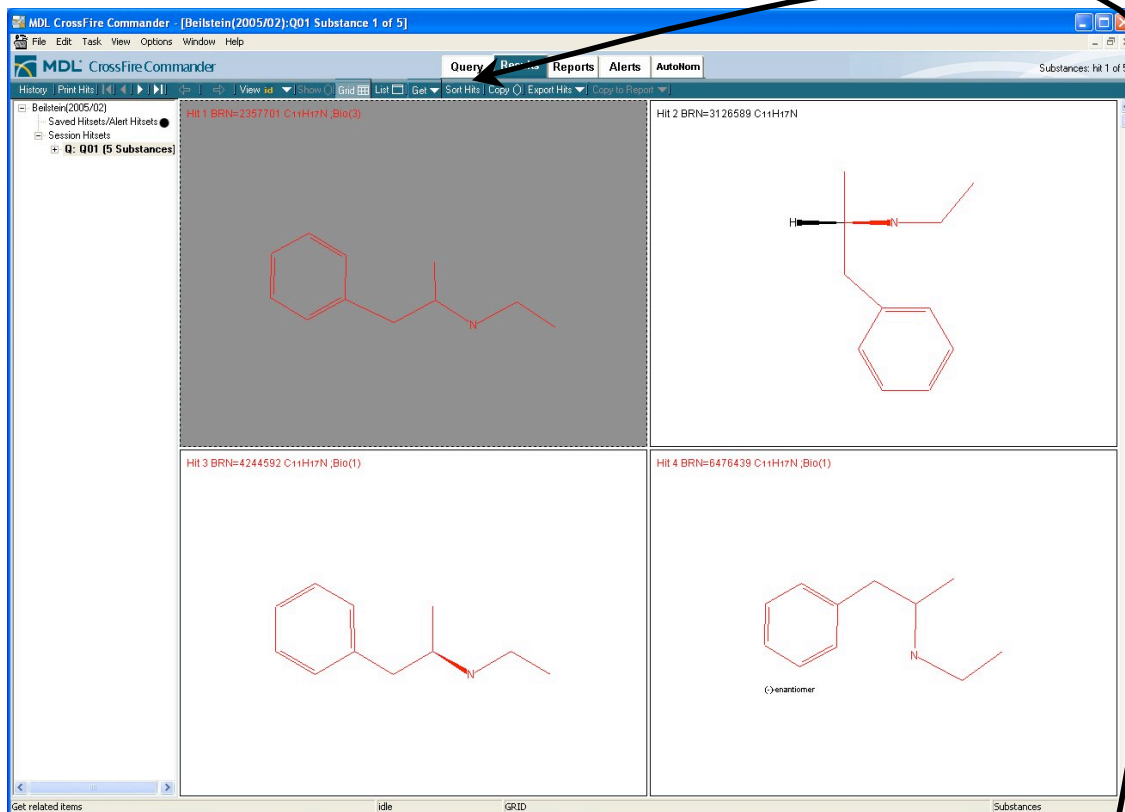
No.	Select	Hitset	Hits	Context	Database	Query	Options
1	<input checked="" type="checkbox"/>	Q01	5 Substances	Beilstein(2005/02)	total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST		original structure
2	<input type="checkbox"/>		stop after first result	Substances	Beilstein(2005/02)	same structure	free sites on hetero atoms
3	<input type="checkbox"/>		stop after first result	Substances	Beilstein(2005/02)	same structure	substructure search

Cancel

To Report

View

5. This will display a list of all of your hits in a grid format. Scroll down the window to see them all.



Double clicking on any of the structures gives you lots of exciting information about the compound. (Press the “grid button on the dark blue bar to return to this “grid display”

7. To find references for a specific compound, select “Get All Related Citations” from the “Get” Pull down menu: This will list citations to the literature (including patents). Many but certainly not all journals are available in our library.

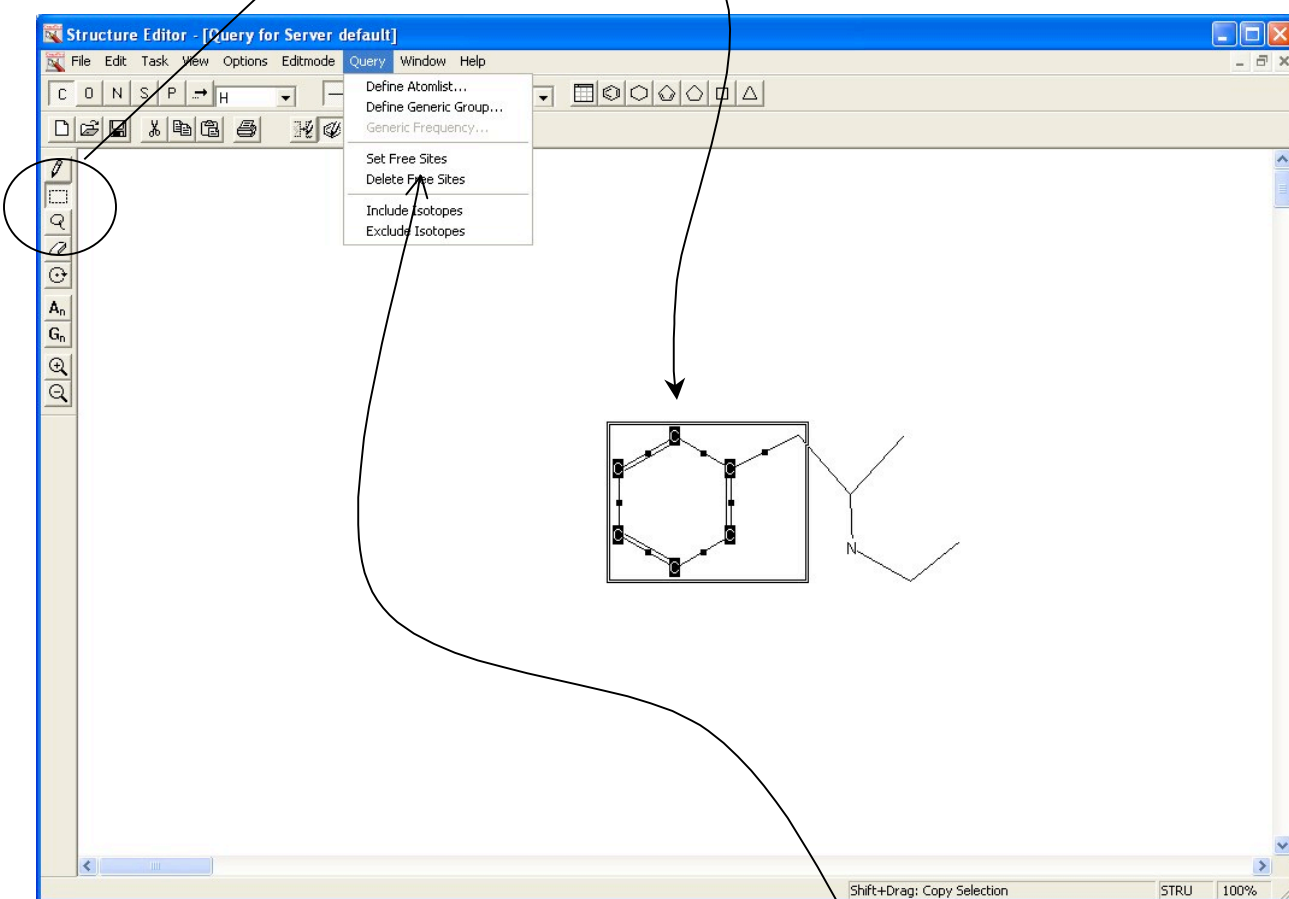
The screenshot shows the MDL CrossFire Commander interface. The title bar reads "MDL CrossFire Commander - [Beilstein(2005/02):Q02 Citation 1 of 2]". The menu bar includes File, Edit, Task, View, Options, Window, and Help. The toolbar has buttons for History, Print Hits, View, Show, Grid, List, Get, Sort Hits, Copy, Export Hits, and Copy to Report. The main window displays citation information. The top panel shows "Hit 1: 92595 Journal; Beckett,A.H. et al.; TETRAB; Tetrahedron; EN; 31; 1975; 1531-1535." The bottom panel shows "Hit 2: 1051256 Journal; Leonard et al.; JACSAT; J. Am. Chem. Soc.; 80; 1958; 4858,4859; JACSAT; J. Am. Chem. Soc.; 76; 1954; 5708,5709,5713." The left sidebar shows a tree view with "Beilstein(2005/02)" expanded, showing "Saved Hits/Alert Hitsets" and "Session Hitsets". Under "Session Hitsets", there are two items: "Q: Q01 (5 Substances)" and "L: Q02 (2 Citations)".

Part II. Substructure Search:

Suppose you don't necessarily want to know if this exact compound was made before but rather want to know if any compound that contains this assembly of atoms as part of its structure has been reported before. You can search for a substructure by using free sites in your query.

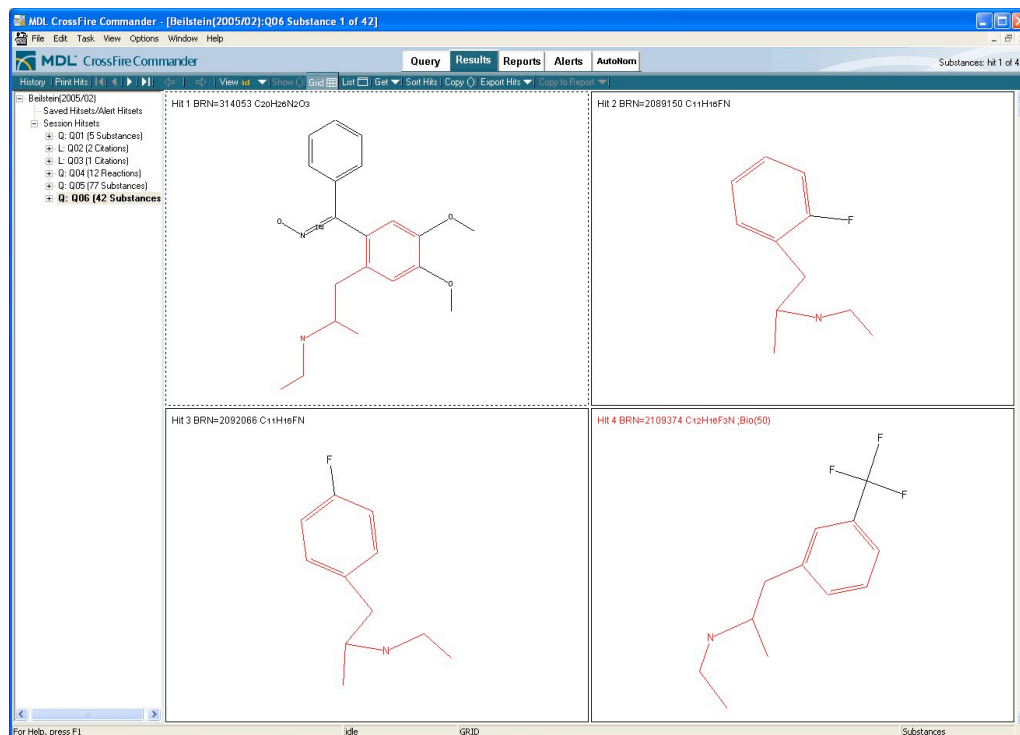
1. Go back to the Query window (by selecting the "Query" tab near the top of the window) and return to the structure editor by selecting "Draw Structure" button on the dark blue menu bar.

2. Use the lasso or the box tool to highlight the atom or atoms that you want to leave open for possible modification.



3. After highlighting the atoms you want to leave open, select "Set Free Sites" in the Query menu. These atoms will now appear with asterisks next to them. This means that the unspecified sites on these atoms can be something other than hydrogen.

4. Return to the Commander (by pressing the crisscross arrow button) and press the start search button.

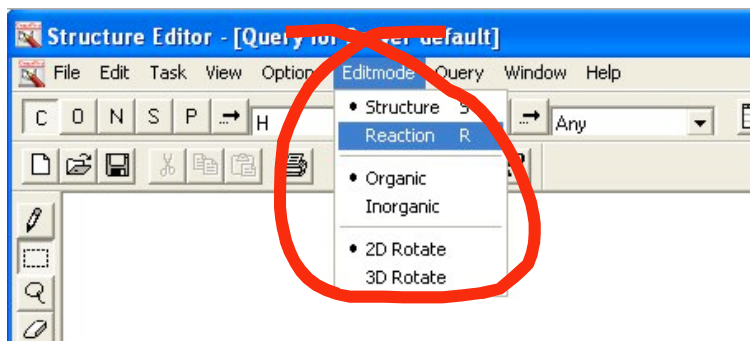


Now your structures will include any molecule that has your structure as a part of its structure but only with variation at the specified sites.

Part III.

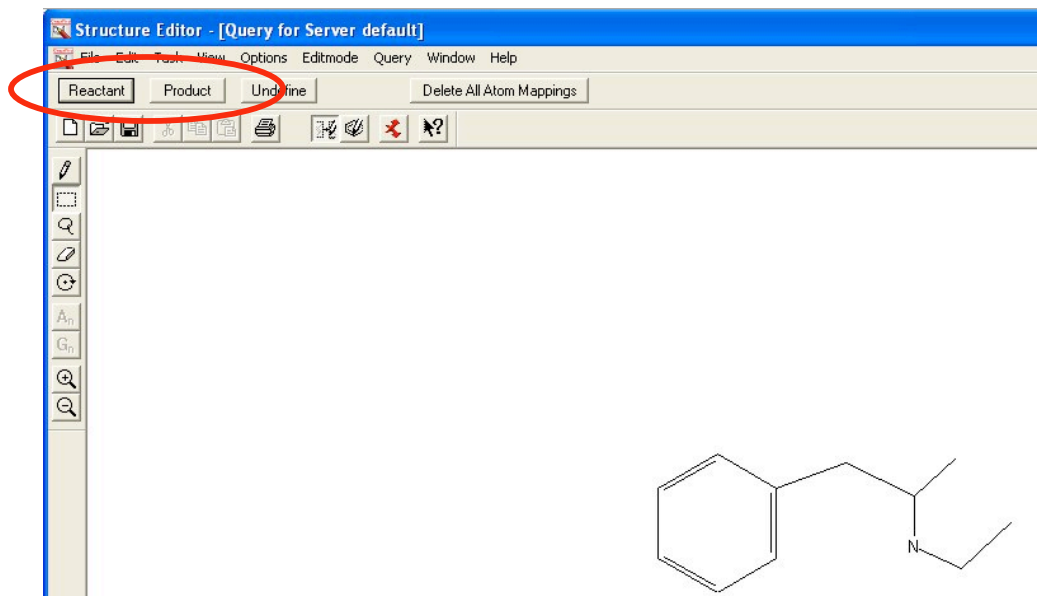
Basic Reaction Searching

1. Go back to the Query window (by selecting the “Query” tab near the top of the window) and return to the structure editor by selecting “Draw Structure” button on the dark blue menu bar.
2. In the top menu bar select “Reaction” under the Editmode pull-down.

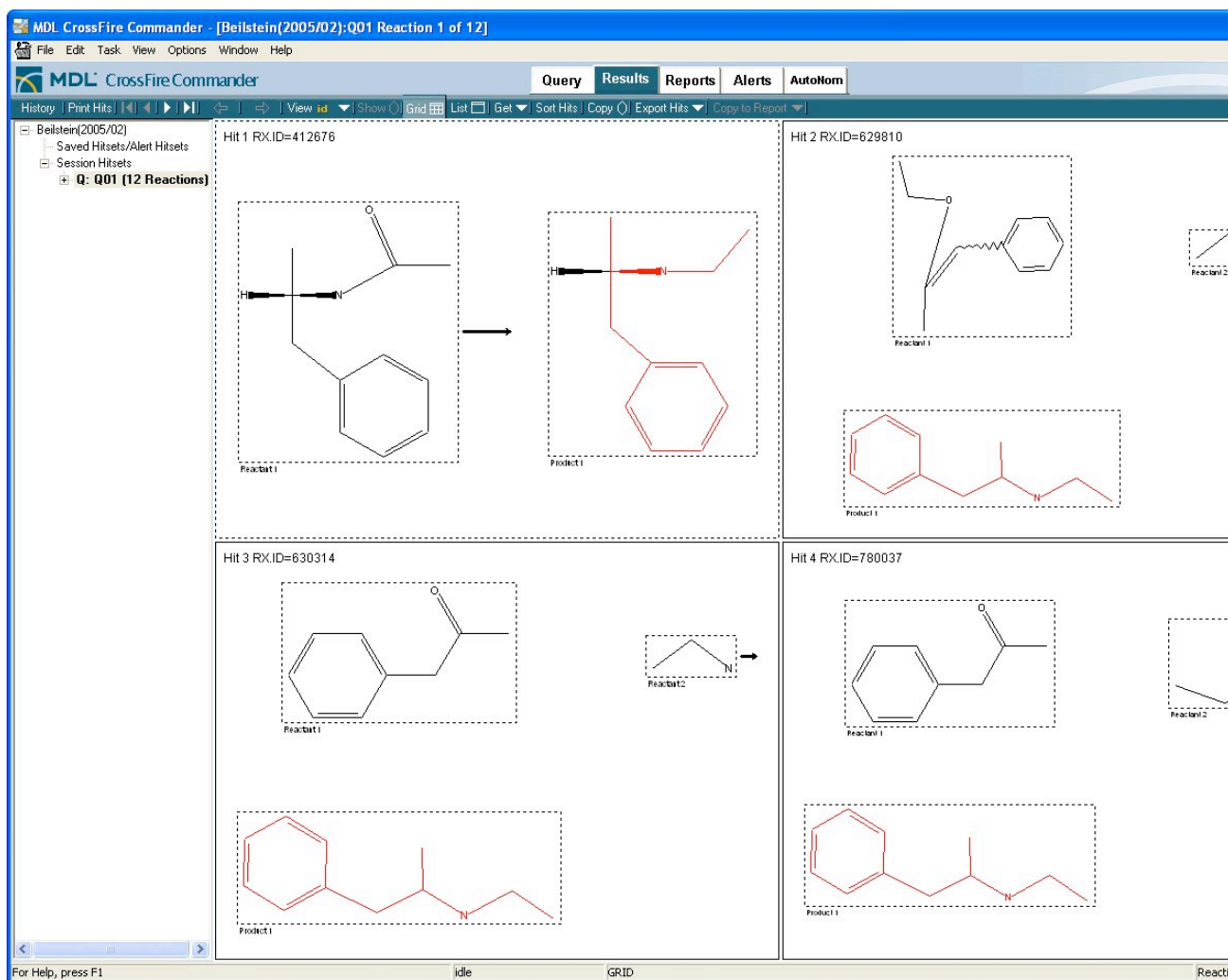


3. In the Reaction mode use the box or lasso tool to select the compound you want to define as product (or reactant) in a reaction and click on the “Product” (or Reactant) button.

(Note Beilstein is quite sophisticated and will let you define both a reactant and a product if there was a very specific reaction you wanted to search. Here we will only define one. If you really want to get fancy, you can even specify exactly how atoms of the reactant map to atoms in the product)



4. Return to the commander (clicking the crisscross arrow button) and select start search. (It will ask you to confirm that you want to search in reaction mode - just click ok) and when the search is done select “view”



5. This window now shows you reactions (chemical transformations) that list your selected compound as a product. You can find more information about reaction conditions by double clicking on one of the squares or get the reference(s) from the “get” menu.