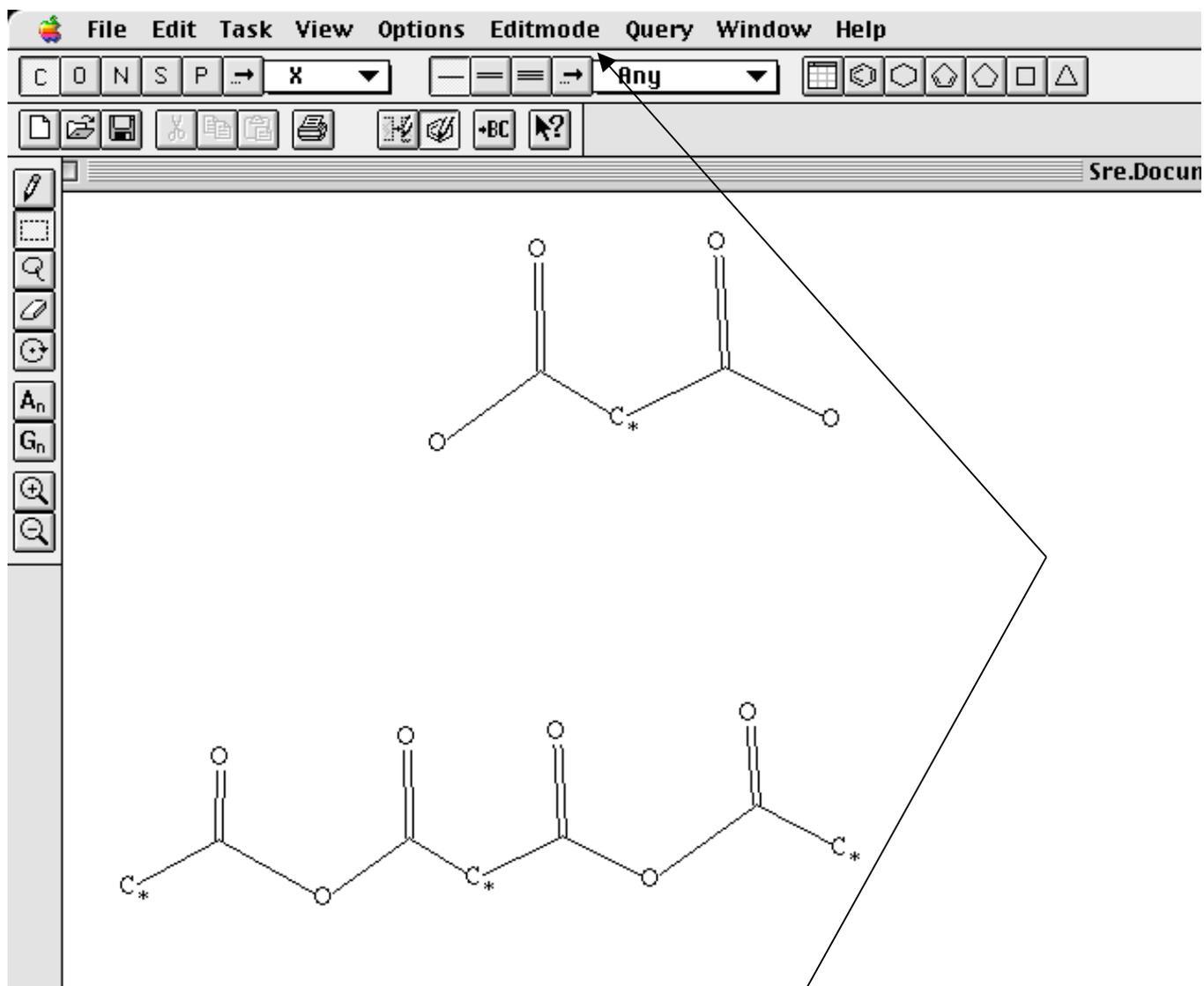


Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity
Prof. Joseph Fox

Chemical Database Searching- Handout 4

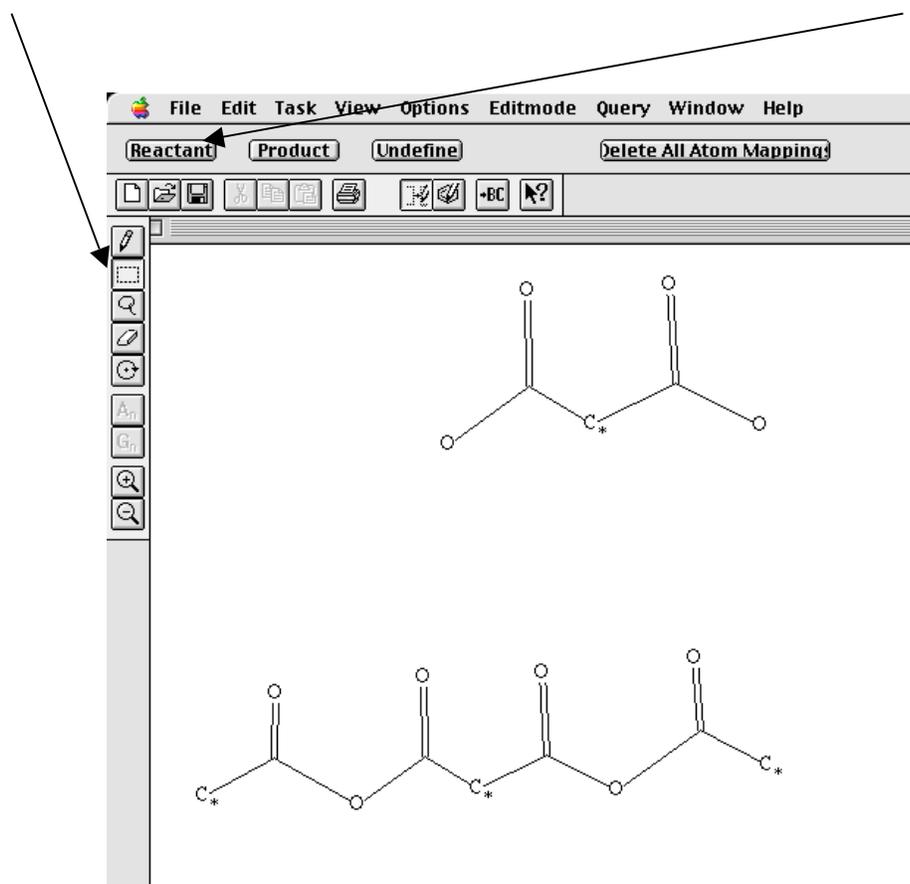
Handout 4: Introduction to Reaction searching with substructures
on Beilstein commander

1. Following the instructions from earlier tutorials, construct the following two structures. Remember that * stands for a 'free site'



2. Under 'Editmode' select 'Reaction'

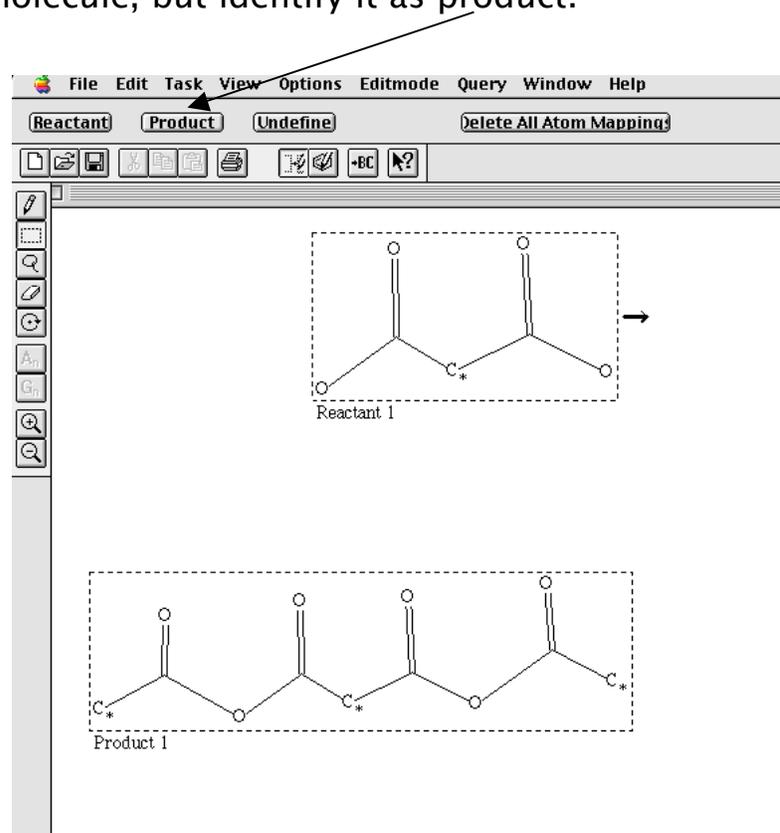
3. Use the box tool to select the first molecule. Identify this as reactant



4. Repeat for the second molecule, but identify it as product.

The screen should look like this:

You can return to the structure Editor if you wish (Editmode Pulldown). Otherwise, proceed To step 5



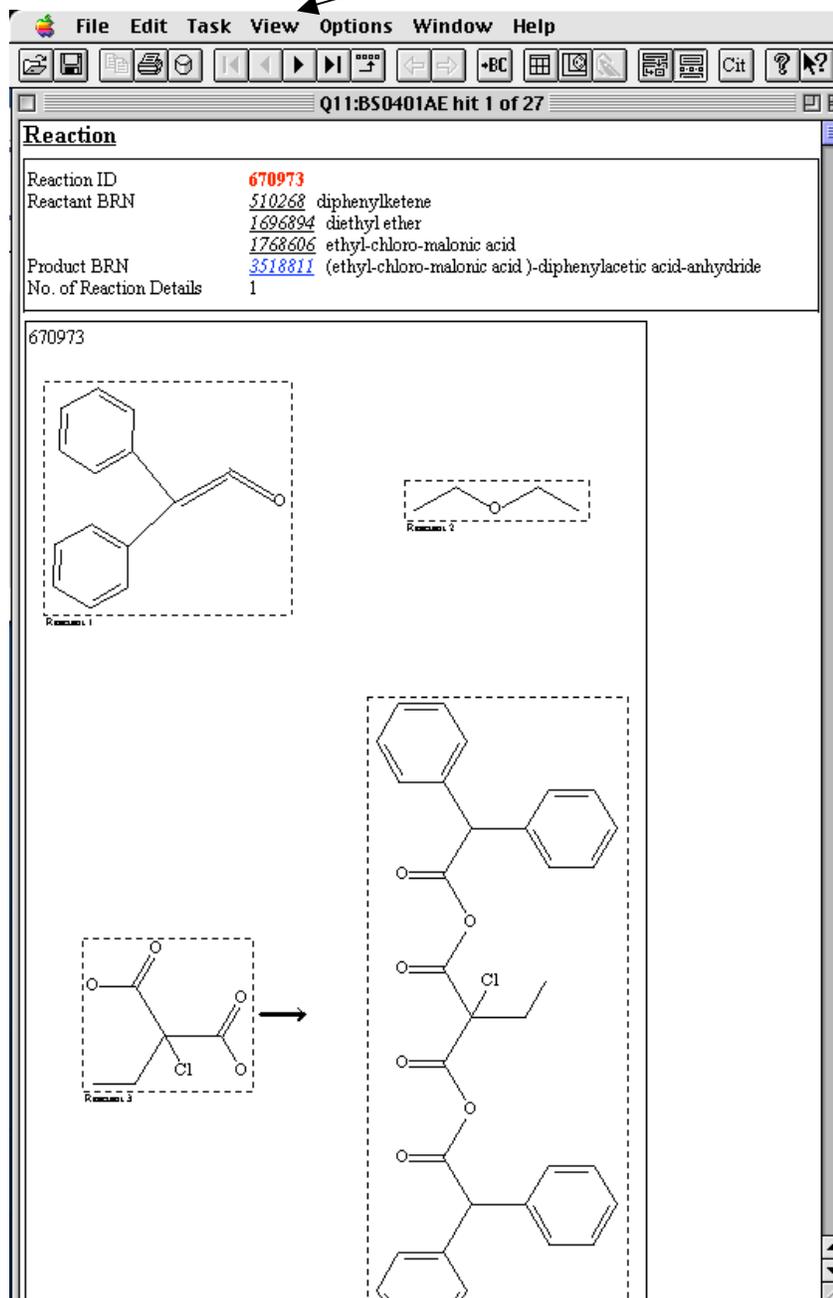
5. Return to the Beilstein commander window, and start the search

The screenshot shows the Beilstein Commander - BC window. At the top, there is a toolbar with various icons. Below the toolbar, the 'Switch Database:' dropdown is set to 'BS0401AE'. The 'Subset:' dropdown is set to 'All', and the 'Display:' dropdown is set to 'Reactions'. A blue 'Start Search' button is highlighted with a red arrow. The main window is divided into two panels. The left panel, titled 'EDS (Easy Data Search):', contains a list of data types: Fact Editor (Table), Bibliographic Data, Bioactivity, Environmental Data, Ident. Data, Physical Data, Reaction Data (highlighted), and Solubility Data. Below this list is a 'Query:' section with 'Check', 'Clear', and 'Help' buttons. The right panel, titled 'Structure:', shows a chemical reaction scheme. The reactant is a molecule with two carbonyl groups and a central carbon atom marked with an asterisk (*). The product is a chain of four carbonyl groups, also with a central carbon atom marked with an asterisk (*). The reaction is labeled 'Reactant 1' and 'Product 1'.

6. Display Hits

The screenshot shows the Commander window. The title bar reads 'Commander'. The main content area displays the following text: 'Query Result: 27 Reactions from BS0401AE stored in Q11'. Below this, it says 'Server Messages: CPU 5.39 sec' and 'ELA 6.00 sec'. At the bottom of the window, there are two buttons: 'Display Hits' and 'Close'. A red arrow points to the 'Display Hits' button.

7. This brings up the first hit. While you can scroll through each one Manually, it is usually more useful to view multiple reactions at a time. This can Be accomplished by selecting 'Short Display' under the View menu



8. This brings up the short display of your hits. Scroll through them until you Find reactions of interest. Double clicking on that hit brings up the full Display again.

