

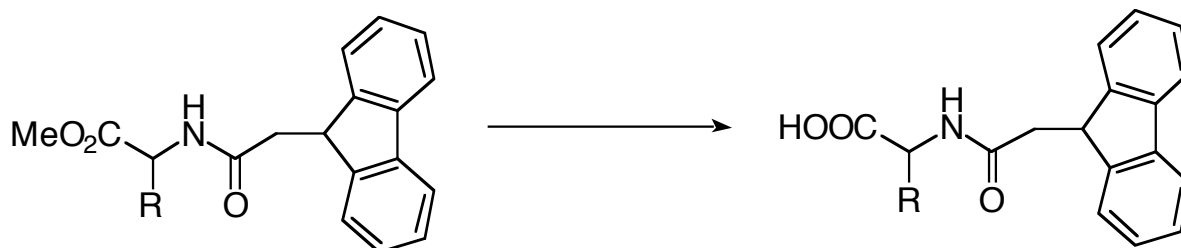
Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity

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Chemical Database Searching- Handout 5

Handout 5: Introduction to Reaction searching for functional group tolerance on Beilstein commander

In this tutorial, we will demonstrate how to use Beilstein to search for functional group tolerance. For this specific search, we will use the example of cleaving a methyl ester preferentially in the presence of a Fmoc protected amine. The type of reaction that we are interested in is shown below.

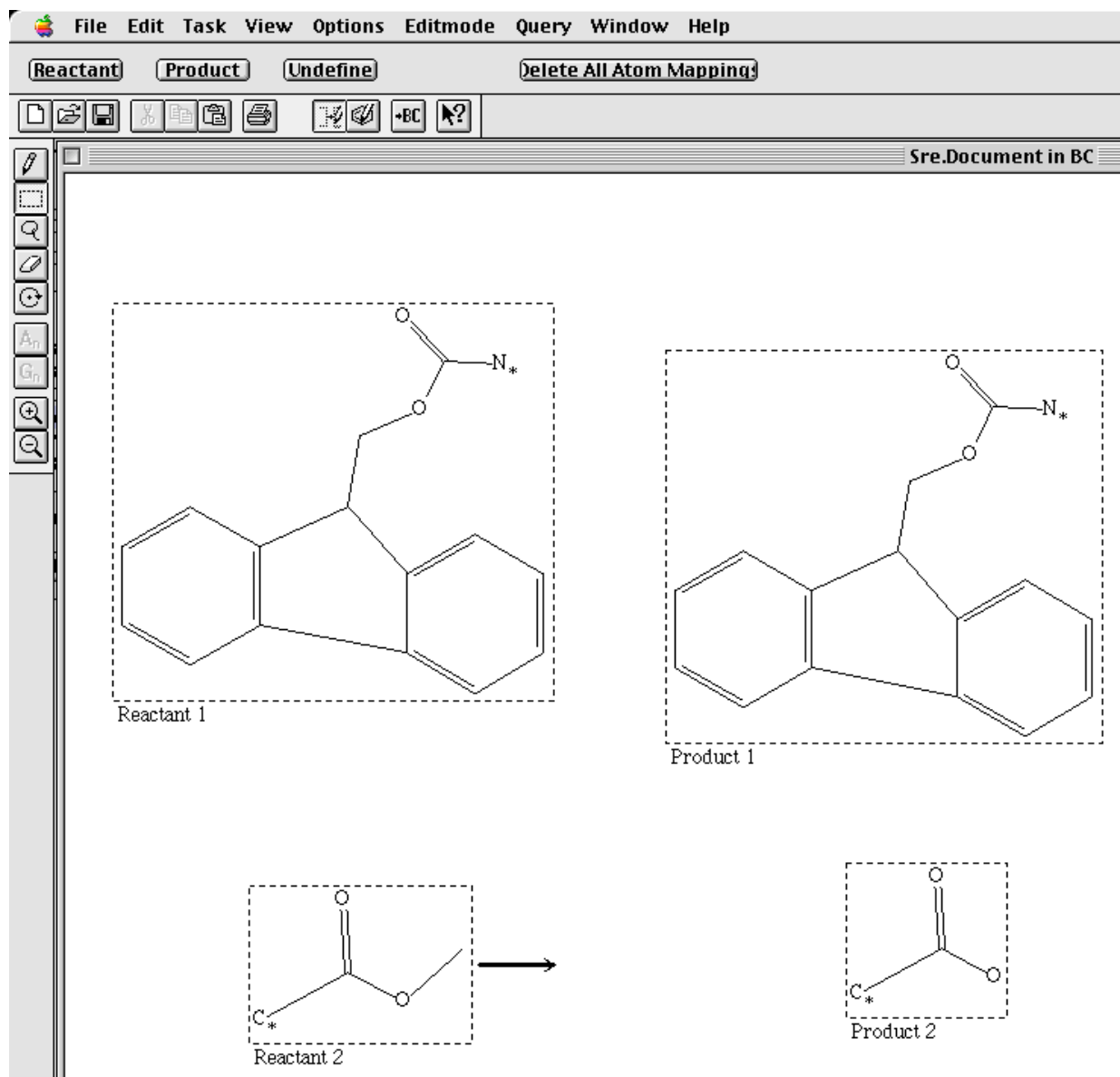


As an example, we will say that we are interested in precedents for removing the ester in the presence of Fmoc under basic conditions. This is not trivial, since both groups are cleaved by base-- we are going to see if it can be done selectively.

Note that we are not going to limit our search to alpha amino acids. Rather, we will begin by searching broadly. As long as we get less than 500 hits for the reaction search, it will be easy to scan for desirable precedents in a short (<30 min) amount of time.

Draw the four structures below, and identify them as reactants and products in the Reaction Editor. Be sure to put the free sites in as shown. Note what we are doing here: we are specifying that both the product and the starting material have an Fmoc protected amine. We are then specifying that the starting material contains a methyl ester, and the product contains an acid.

Begin the search



This search should bring up at least 139 hits. The first thing that you will notice is that reactions 1 through 4 have nothing to do with the reaction we want. That's OK, our idea was to conduct a very open ended search-- we are willing to sort through these examples in order to find ones we want. Scroll through and find some useful precedents.

