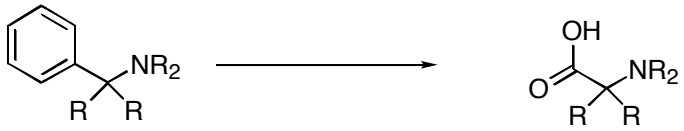
Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity
Prof. Joseph Fox

Chemical Database Searching- Handout 6

Handout 6: Functional Group mapping using Beilstein

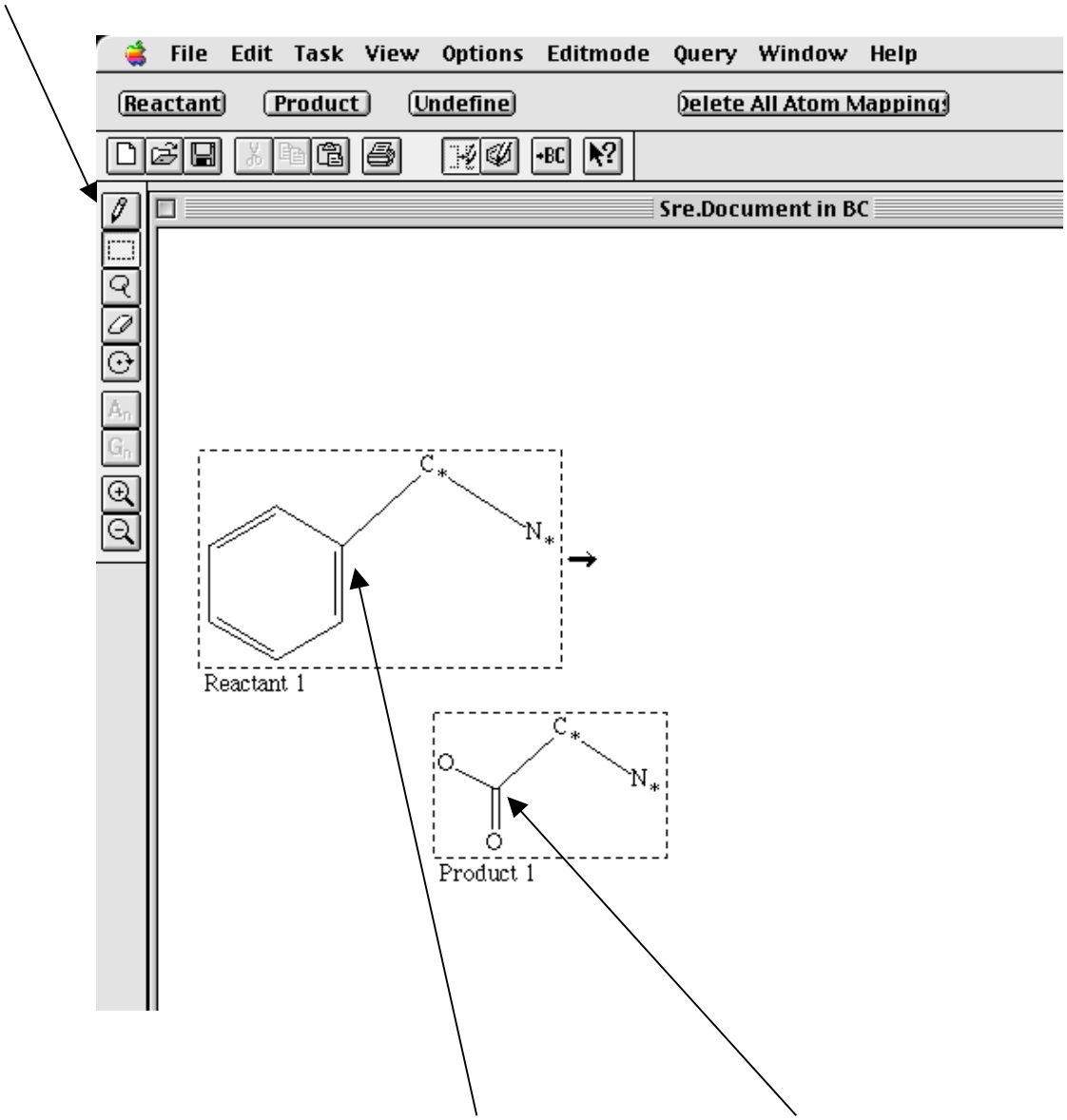
In this tutorial, we will demonstate how to use Beilstein to search with reaction mapping. For this specific search, we will search for reactions of the type below, to find if derivatives of amino acids can be prepared by oxidation of a phenyl group. We will proceed by telling the database that we want the quaternary carbon of the phenyl group to end up as the carbonyl carbon of the acid.



NOTE: searches of this type, while useful, are far from perfect. Remember, this database is only as good as the person entering the information! These searches can also tend to be time consuming. Thus, for reaction mapping it is often more useful to conduct searches as demonstrated in Scheme 5 where we exercise a little patience in skimming through the hits.

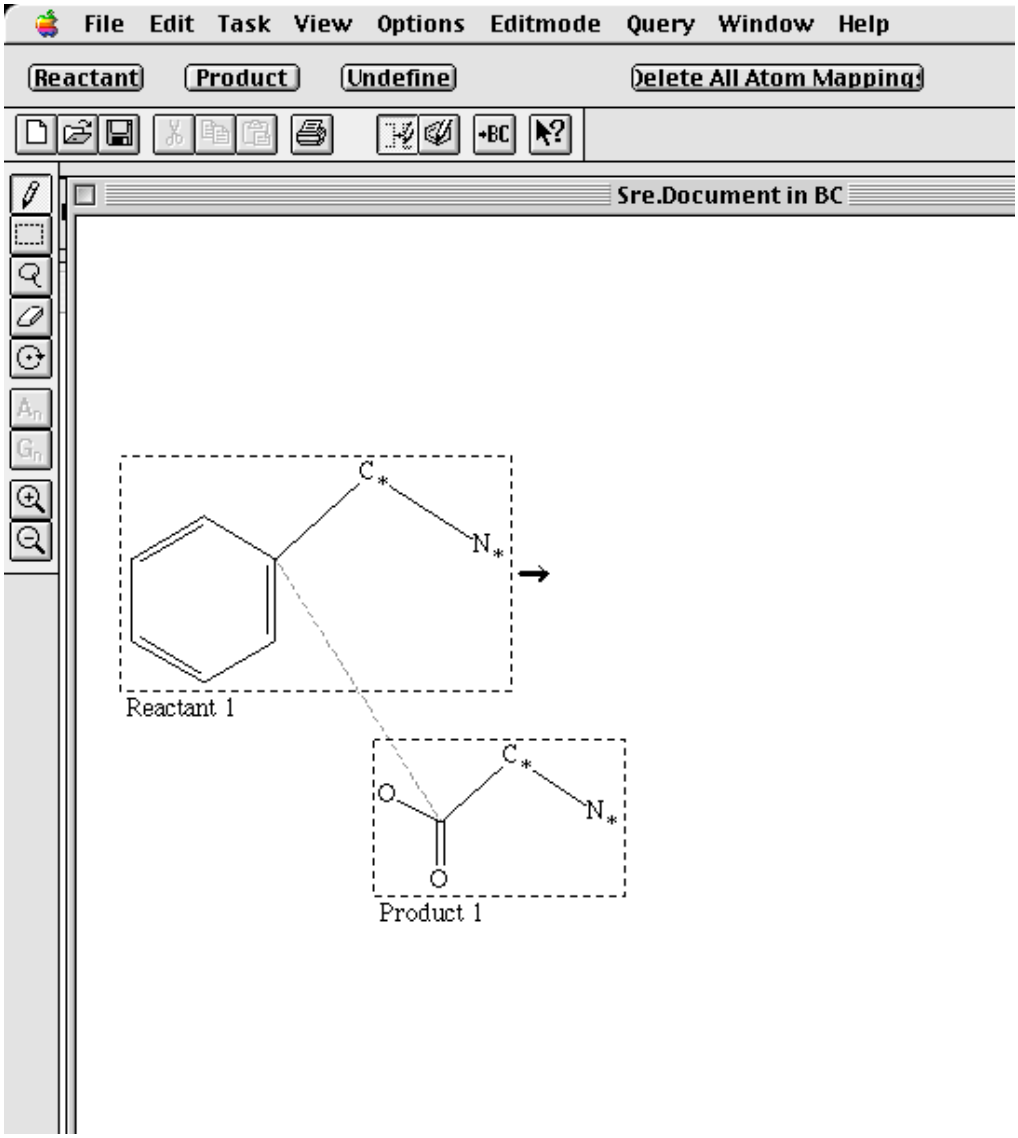
1. Begin by drawing the picture shown below, as we have done before

2. In reaction editor mode, select the pencil

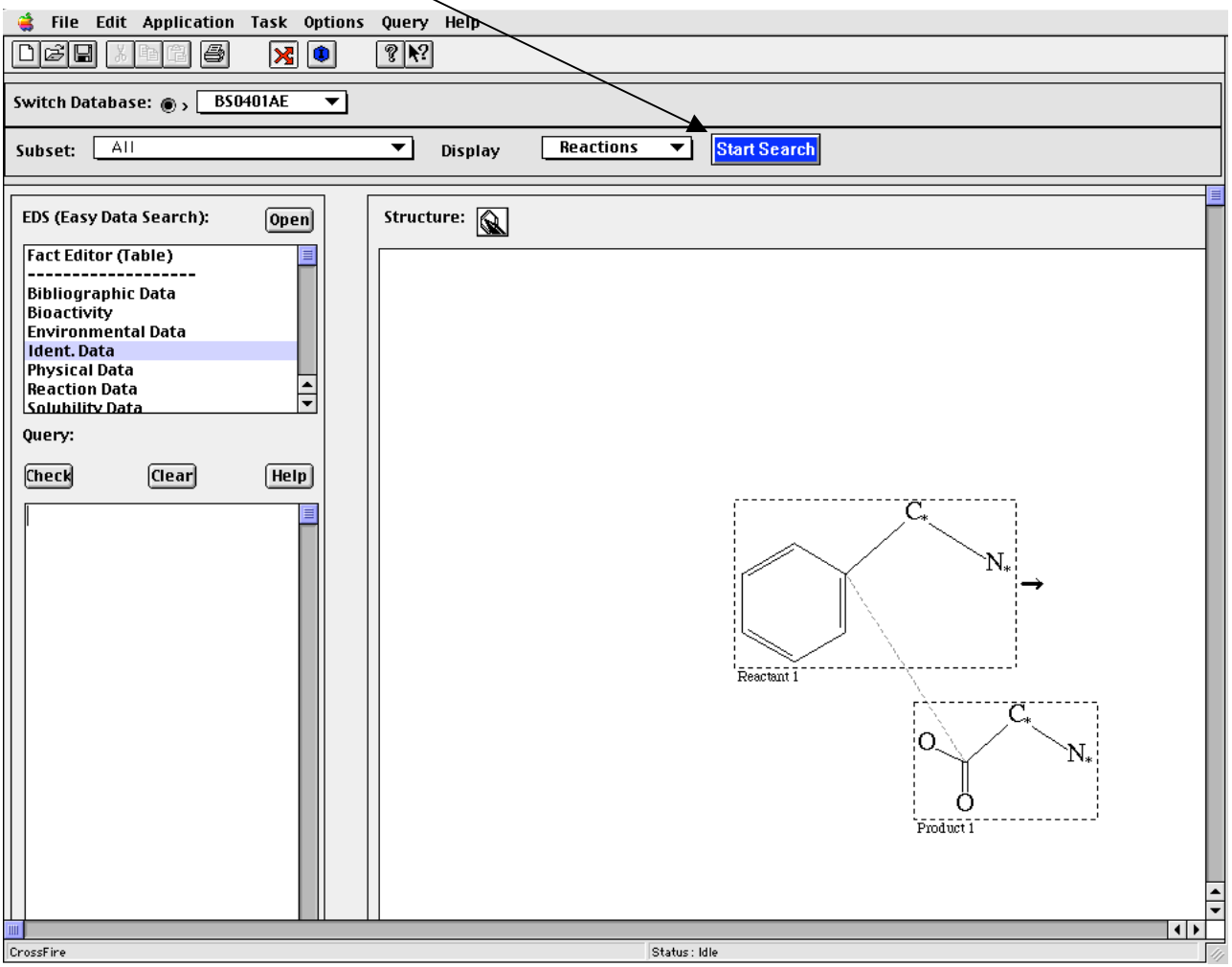


3. Draw a line that connects the quaternary phenyl carbon with the carbonyl carbon of the product.

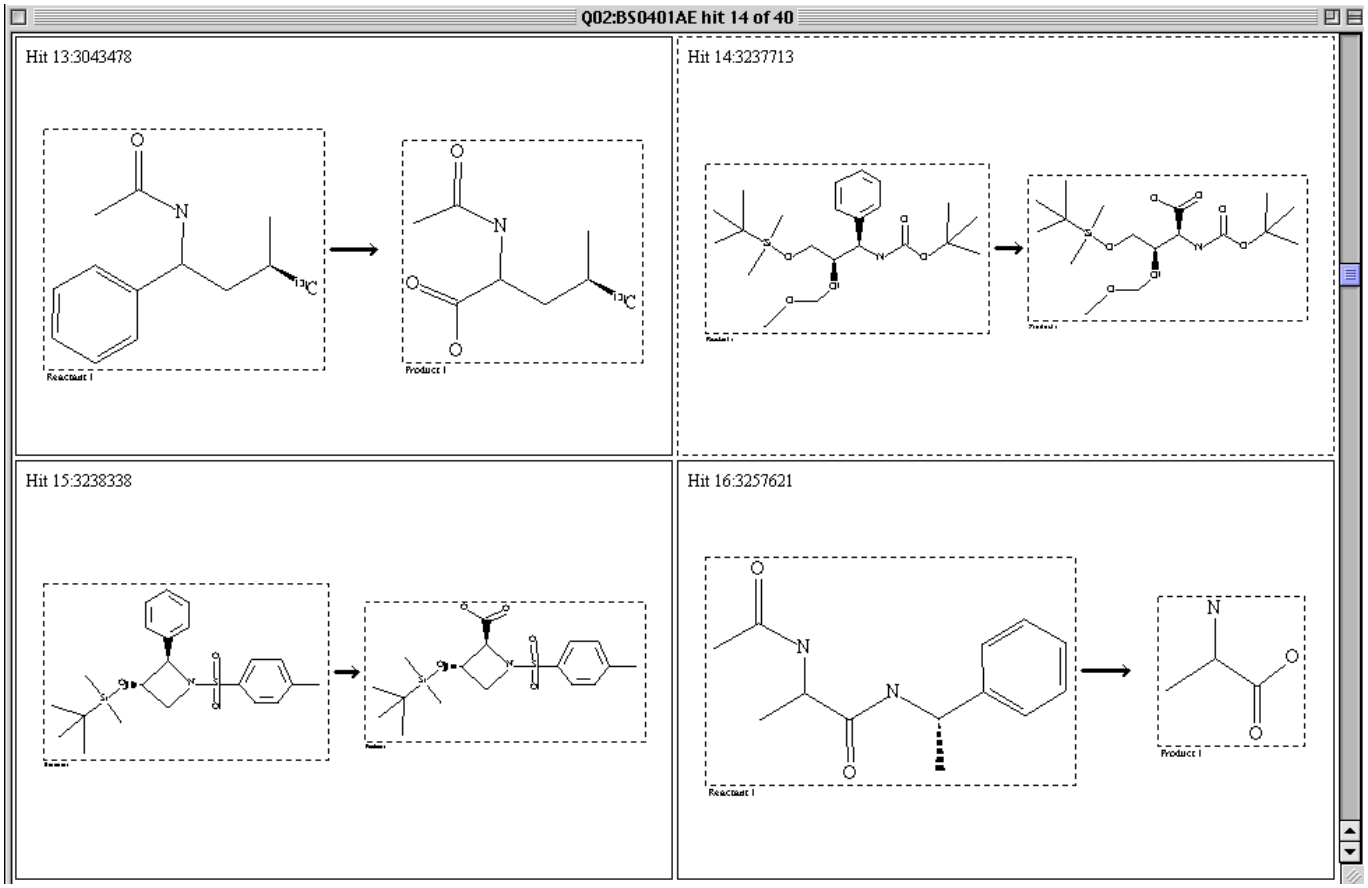
4. You should see a dashed line connecting these atoms. This tells the database that this carbon of the reactant is that same carbon atom in the product



5. Begin the search



6. This search produces 40 hits. Try selecting hit #14



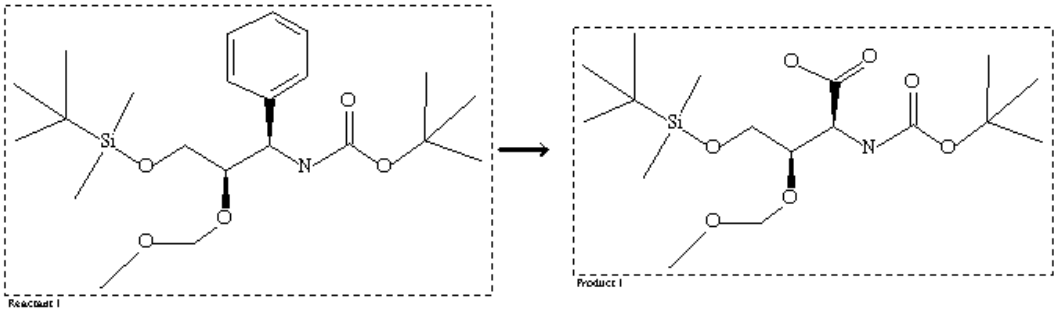
7. Here we see an example of using RuCl3, NaIO4 to oxidize a phenyl to a carboxylic acid to produce a protected amino acid derivative.

Q02:BS0401AE hit 14 of 40

Reaction

Reaction ID	3237713
Reactant BRN	5885576 (2R,3R)-3-tert-butoxycarbonylamino-1-tert-butyldimethylsilyloxy-2-methoxymethyloxy-3-phenylpropane
Product BRN	5880411 (2S,3R)-2-tert-butoxycarbonylamino-4-tert-butyldimethylsilyloxy-3-methoxymethyloxybutanoic acid
No. of Reaction Details	2

3237713



Field Availability List

Home

Code	Field Name	Occ.
RX	Reaction Details	2

Reaction Details 1 of 2

Home

Reaction Classification	Preparation
Reagent	NaIO4, RuCl3
Solvent	CCl4
	acetonitrile
	H2O

Ref. 1 5719546 ; Journal; Matsuura, Fumiyoshi; Hamada, Yasumasa; Shioiri, Takayuki; TELEAY; Tetrahedron Lett.; EN; 33; 51; 1992; 7917-7920.

Reaction Details 2 of 2

Home

Reaction Classification	Preparation
Reagent	RuCl3, NaIO4
Solvent	CCl4
	acetonitrile
	H2O
Time	48 hour(s)
Other Conditions	Ambient temperature

Note 1 Yield given

Ref. 1 5808247 ; Journal; Matsuura, Fumiyoshi; Hamada, Yasumasa; Shioiri, Takayuki; TETRAB; Tetrahedron; EN; 49; 36; 1993; 8211-8222.