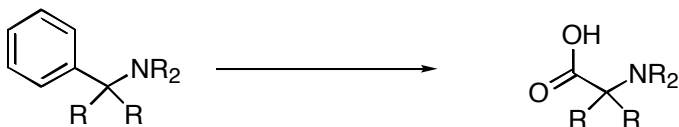


Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity
Prof. Joseph Fox

Chemical Database Searching- Handout 6

Handout 6: Functional Group mapping using Beilstein

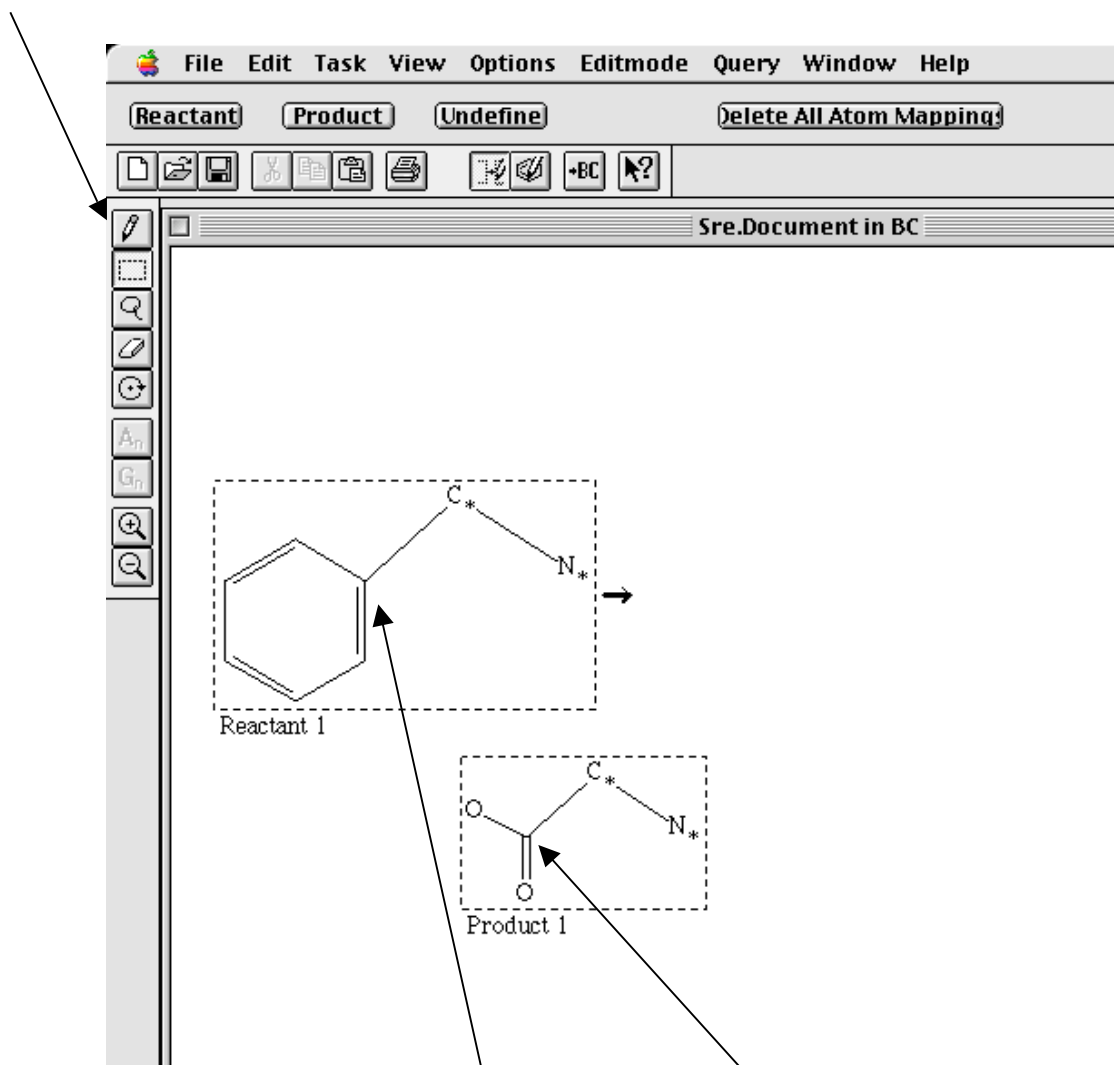
In this tutorial, we will demonstrate how to use Beilstein to search with reaction mapping. For this specific search, we will search for reactions of the type below, to find if derivatives of amino acids can be prepared by oxidation of a phenyl group. We will proceed by telling the database that we want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

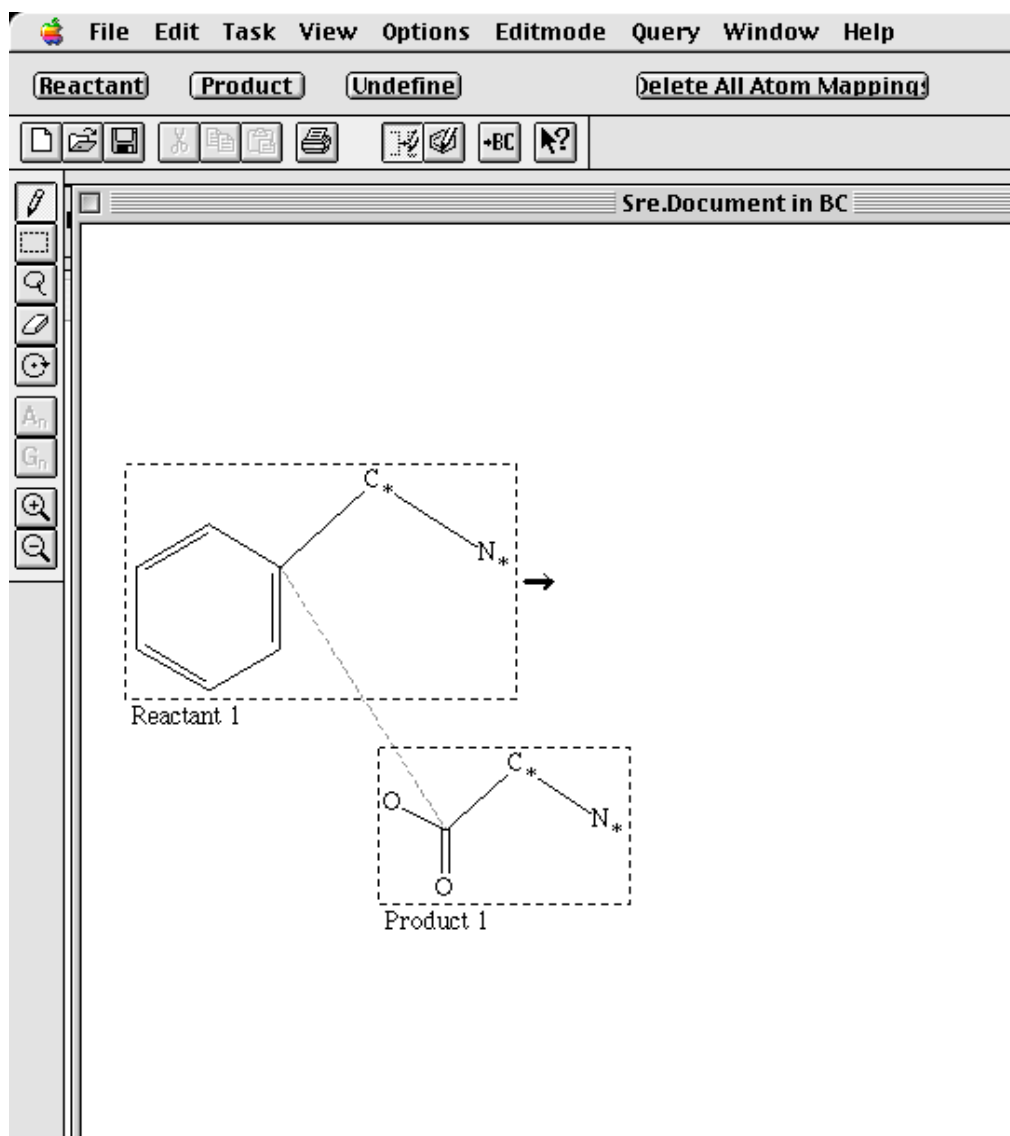
1. Begin by drawing the picture shown below, as we have done before

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

The screenshot displays the CrossFire software interface. At the top, a menu bar includes File, Edit, Application, Task, Options, Query, and Help. Below the menu bar is a toolbar with various icons. The main interface is divided into several sections:

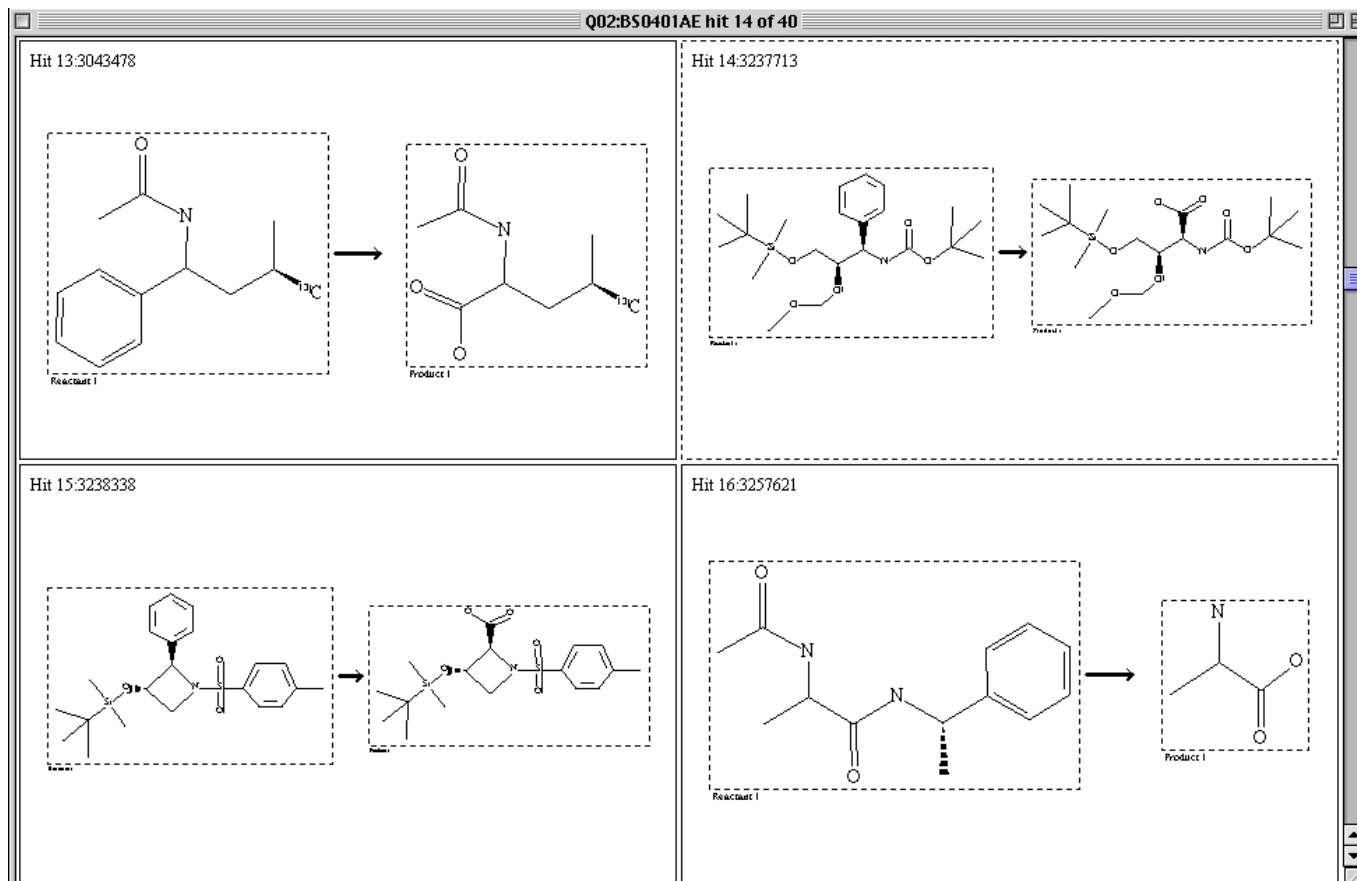
- Switch Database:** A dropdown menu showing "BS0401AE".
- Subset:** A dropdown menu showing "All".
- Display:** A dropdown menu showing "Reactions".
- Start Search:** A blue button with the text "Start Search".

On the left side, there is a panel titled "EDS (Easy Data Search):" with an "Open" button. Below this, a list of data categories is shown, with "Ident. Data" selected. Other categories include Fact Editor (Table), Bibliographic Data, Bioactivity, Environmental Data, Physical Data, Reaction Data, and Solubility Data. Below the list are buttons for "Check", "Clear", and "Help".

The main area is titled "Structure:" and contains a chemical reaction diagram. The reactant, labeled "Reactant 1", is a benzene ring attached to a carbon atom (C*) which is also bonded to a nitrogen atom (N*). The product, labeled "Product 1", is a benzamide derivative where the benzene ring is attached to a carbonyl group (C=O) which is also bonded to a carbon atom (C*) and a nitrogen atom (N*). A dashed arrow indicates the transformation from the reactant to the product.

At the bottom left, the text "CrossFire" is visible. At the bottom right, the text "Status: Idle" is visible.

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-butyltrimethylsilyloxy-2-methoxymethoxy-3-phenylpropane
 Product BRN [5880411](#) (2S,3R)-2-tert-butoxycarbonylamino-4-tert-butyltrimethylsilyloxy-3-methoxymethoxybutanoic acid
 No. of Reaction Details 2

3237713

Reactant 1 → Product 1

Field Availability List [Home](#)

Code	Field Name	Occ.
RX	Reaction Details	2

Reaction Details 1 of 2 [Home](#)

Reaction Classification	Preparation
Reagent	NaIO ₄ , RuCl ₃
Solvent	CCl ₄ acetonitrile H ₂ O

Ref. 1 [5719546](#) ; Journal; Matsuura, Fumiyoishi; Hamada, Yasumasa; Shioiri, Takayuki; TELEAY; Tetrahedron Lett.; EN; 33; 51; 1992; 7917-7920.

Reaction Details 2 of 2 [Home](#)

Reaction Classification	Preparation
Reagent	RuCl ₃ , NaIO ₄
Solvent	CCl ₄ acetonitrile H ₂ O
Time	48 hour(s)
Other Conditions	Ambient temperature

Note 1 Yield given

Ref. 1 [5808247](#) ; Journal; Matsuura, Fumiyoishi; Hamada, Yasumasa; Shioiri, Takayuki; TETRAB; Tetrahedron; EN; 49; 36; 1993; 8211-8222.

