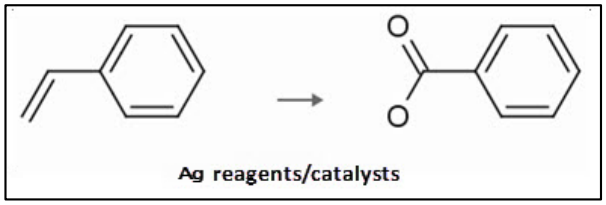
Reaction Searching

I would like to find information on the oxidative cleavage of c-c bonds (like those found in styrene) into carboxylic acids using silver-containing reagents/catalysts.



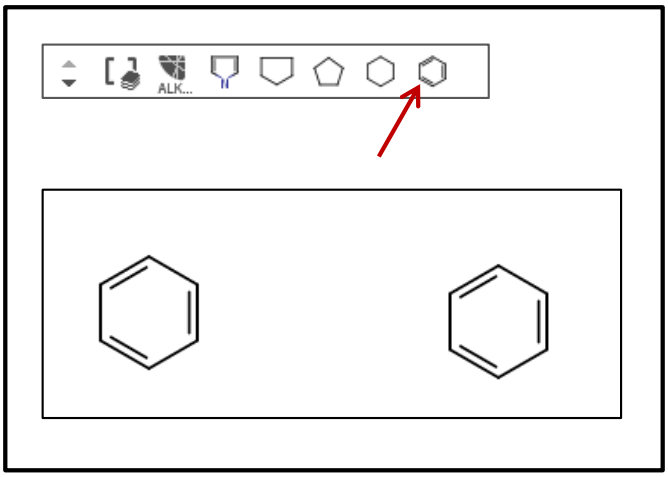
In this workflow we show examples that include:

- How to create a reaction query
- How to map atoms between starting materials and products
- How to change the bond defaults
- How to search for reactions "As substructure"
- How to narrow initial answers so that they contain only those with specific reagents/catalysts

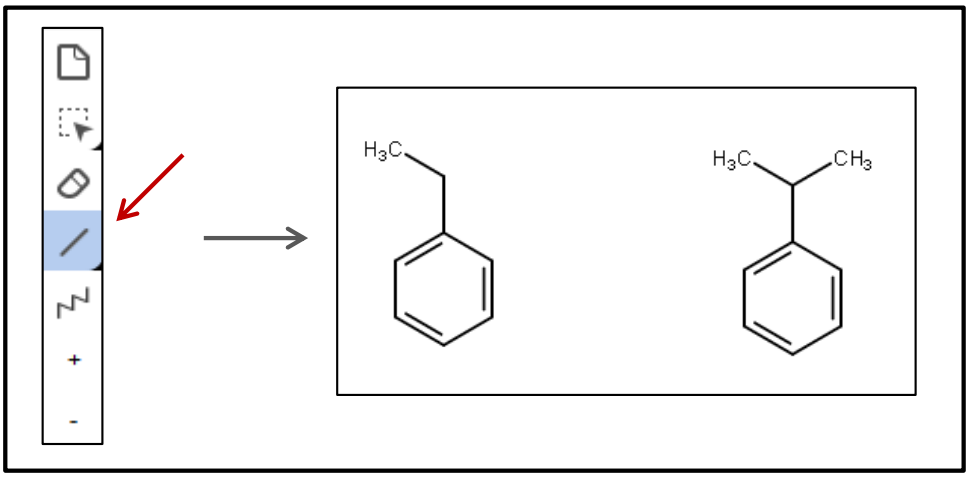
❖ Create a Structure Query

1. On the Reaxys home page click the ***Create Structure or Reaction Drawing*** box to open the structure editor (Marvin JS from ChemAxon).

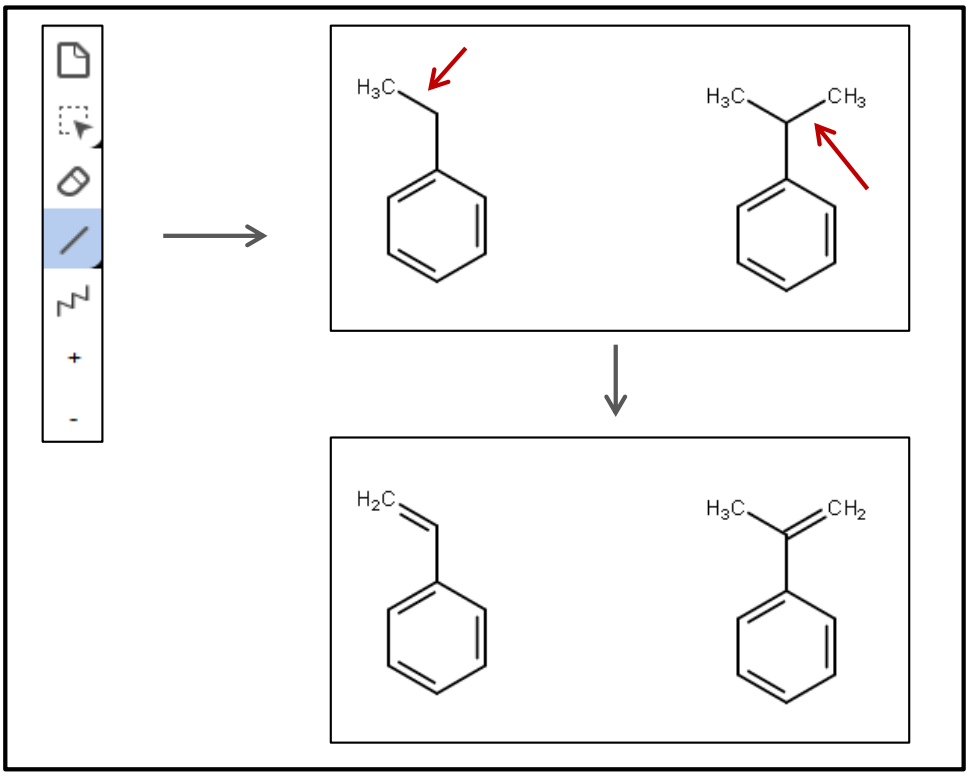
2. Draw an aromatic system.
   a. Select the ***Benzene*** tool
   b. Create two benzene rings as shown



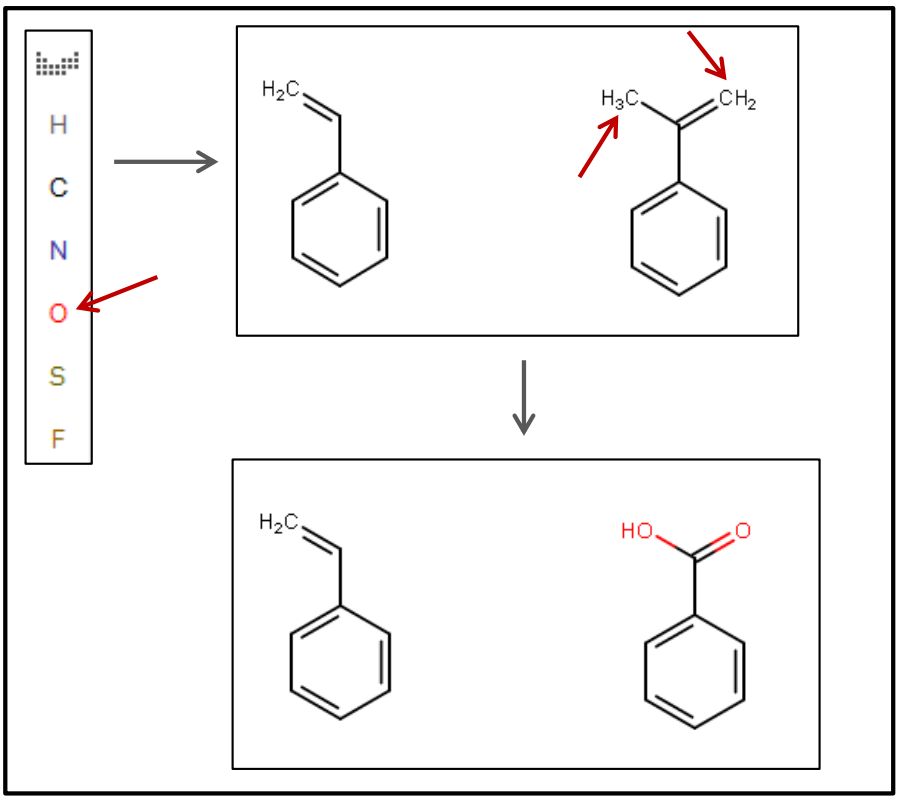
3. Select the ***Single bond*** tool
   a. Add bonds as shown



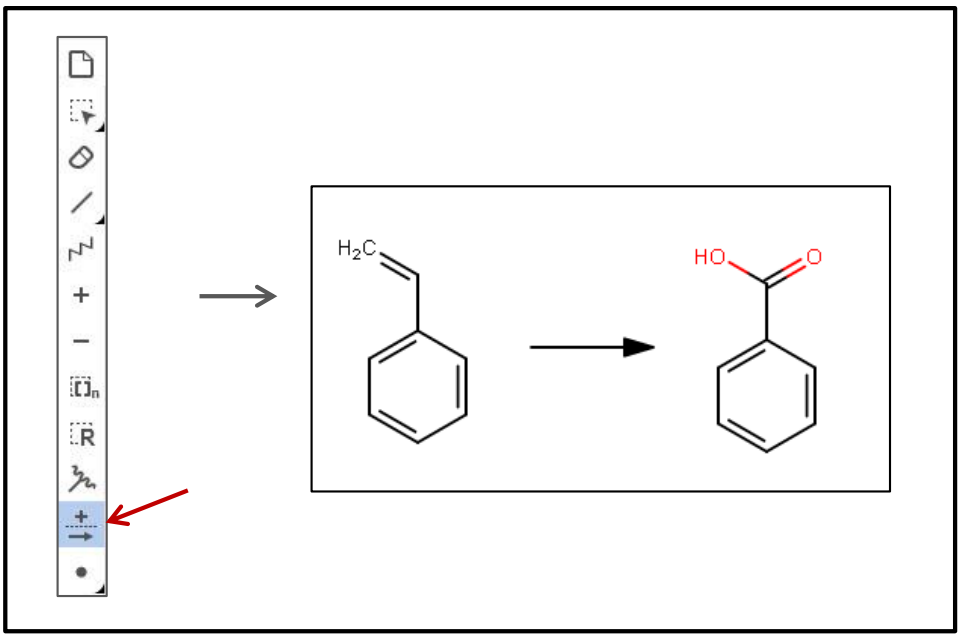
4. Define two double bonds:
   a. With the ***Single bond*** tool still selected, click the two bonds as shown



5. Change atoms as necessary:
   a. Click '***O***' in the atom toolbar, click the '***CH_2***' atom
   b. Click the '***H_3C***' atom

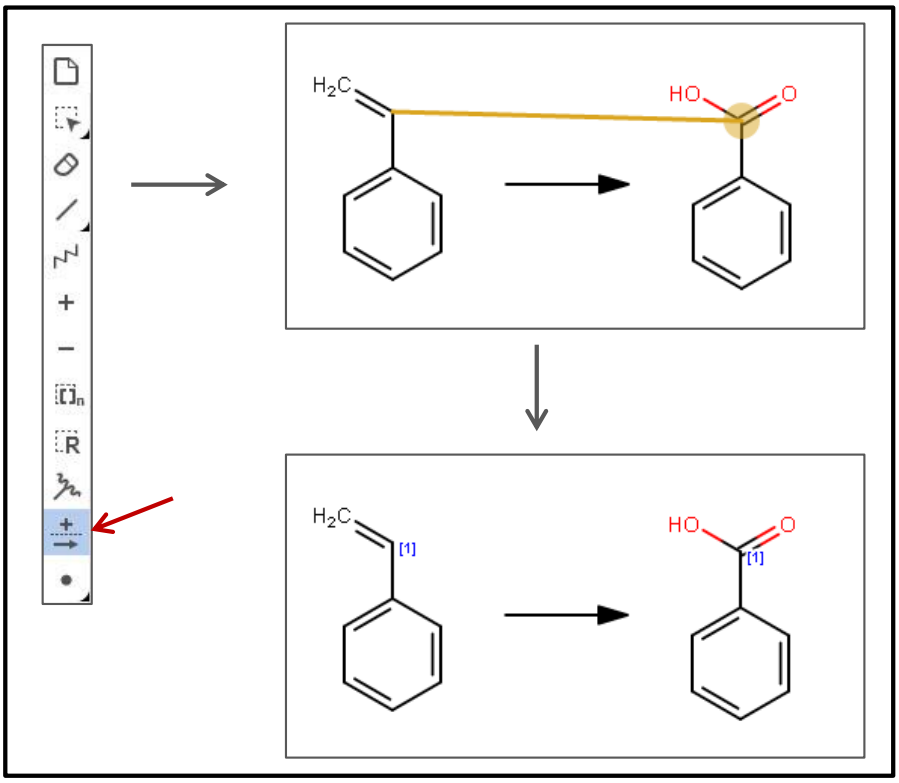


6. Create a **reaction**:
   a. Click and drag to draw the arrow using the ***Straight arrow / Reaction*** tool.

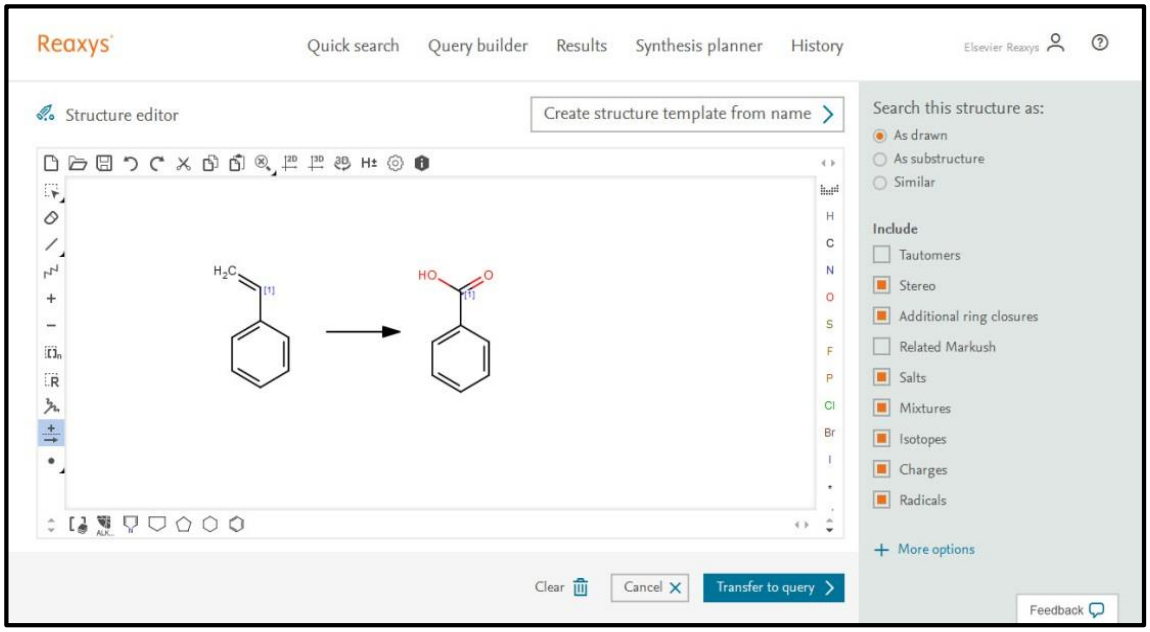


7. **Atom Mapping**
   a. Using the same ***Straight arrow / Reaction*** tool, click and drag to define the atom mapping between the carbon atom on the reactant and the analogous carbon atom on the product.

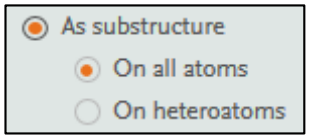
      This will map the two atoms (alternatively right-click the carbon atom on the reactant and add a 1 in the Map field of the Atom properties dialog. Do the same for the analogous carbon atom on the product).



The final query looks like this:



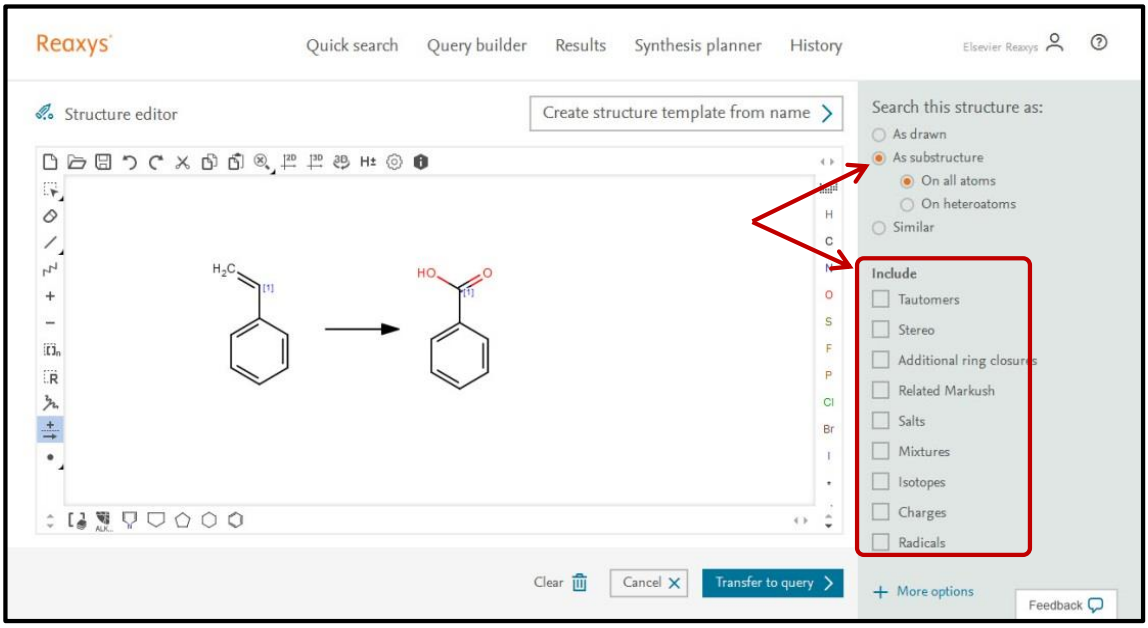
8. In the ***Search this structure as:*** panel, there are three options.
   - **As drawn**: Reaxys will find results for the query as drawn
   - **As substructure**: Reaxys offers two sub-options:



     - **On all atoms** will substitute any explicit or implicit hydrogen with any other atom or group
     - **On heteroatoms** will do the same but only on heteroatoms
   - **Similar**: Reaxys will find results for a similarity search based on the drawn query

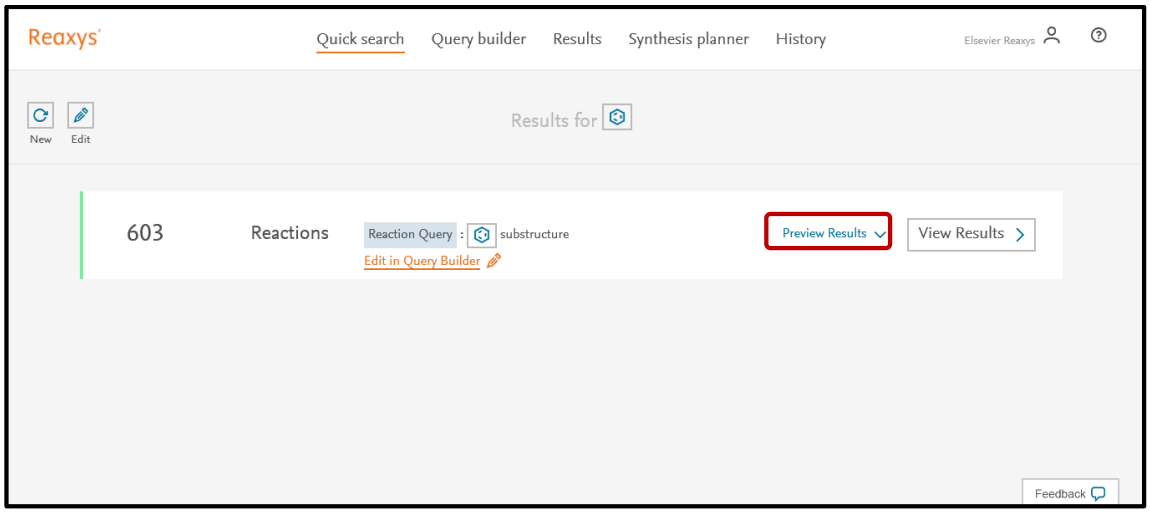
Since this is a substructure search and we want substitutions on all the atoms:

a. Click ***As substructure*** + ***On all atoms***
b. Turn off all ***Include*** features

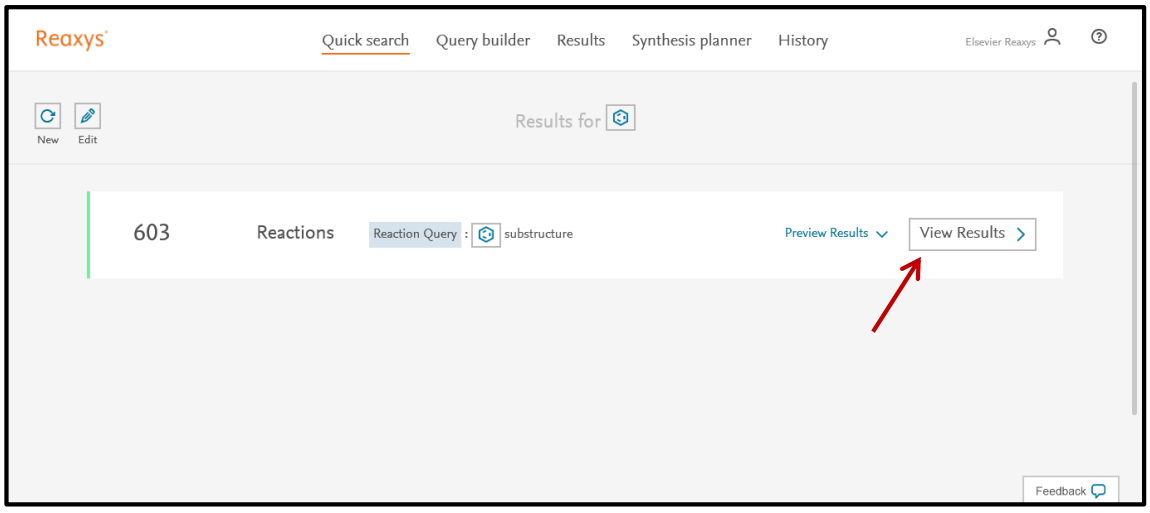


9. Click ***Transfer to query*** and click ***Find***.

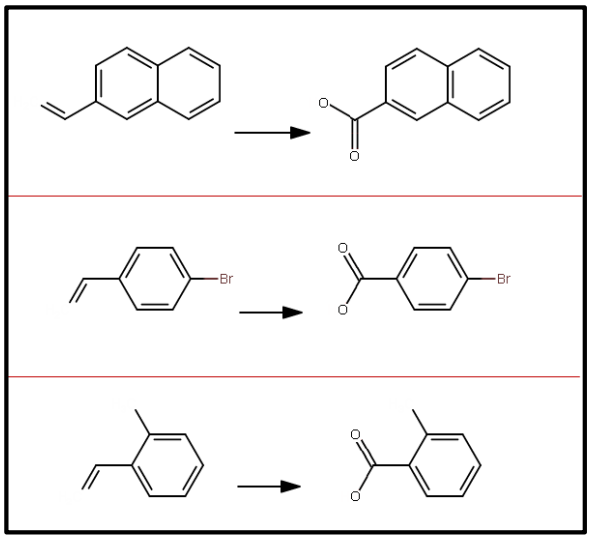
   The **Results Preview** is displayed. Each result option has a ***Preview Results*** feature that presents the top 3 results for the given query. You can check the results of your query before continuing to the full result set.



10. Click ***View Results*** for the result set.



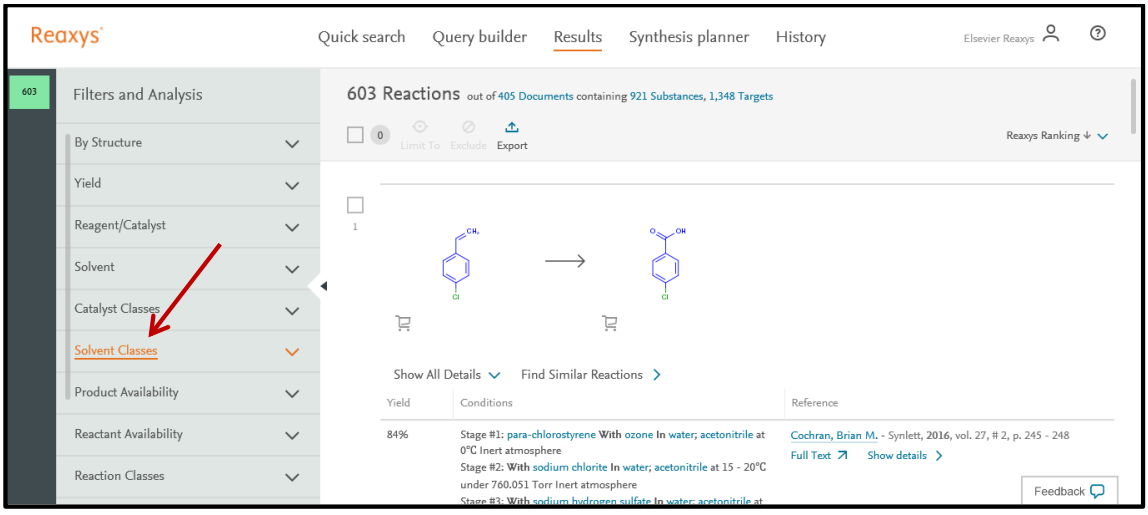
Several hundred reactions, like these, are retrieved:



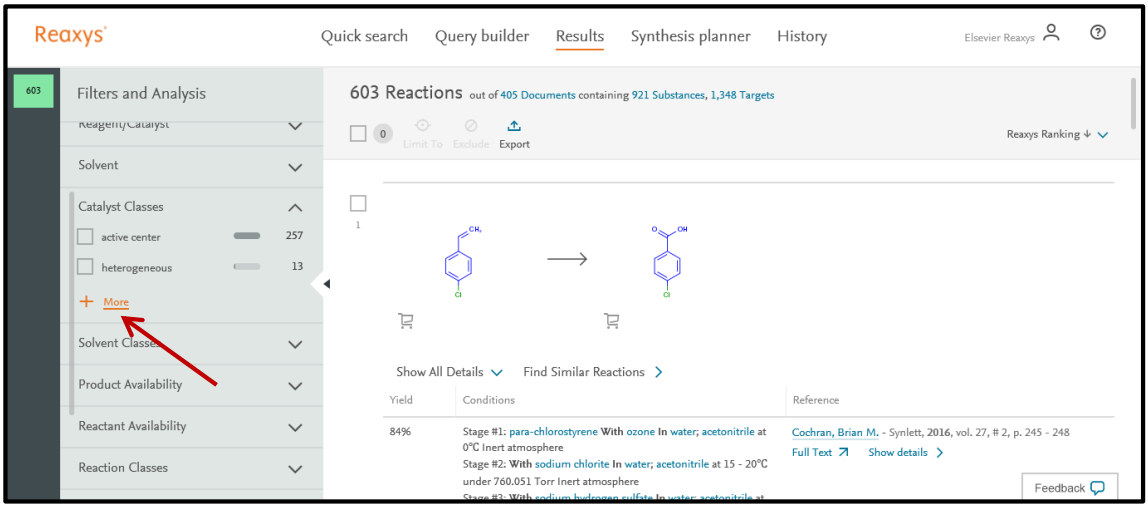
❖ Analyze the Results

Use the Filter & Analysis panel to visualize information about substances involved in the reactions. For example: I want to determine which reactions use silver containing reagents/catalysts.

1. Substances are classified into the roles they play in chemical reactions, and in Reaxys reagents/catalysts are generally grouped under the heading *Catalysts Classes*. The list presented in the filter panel is the first level of a hierarchically organized taxonomy.
   a. Expand the ***Catalyst Classes*** taxonomy



   b. Click ***+ More*** to browse through the branches of the ***Catalyst Classes*** taxonomy.

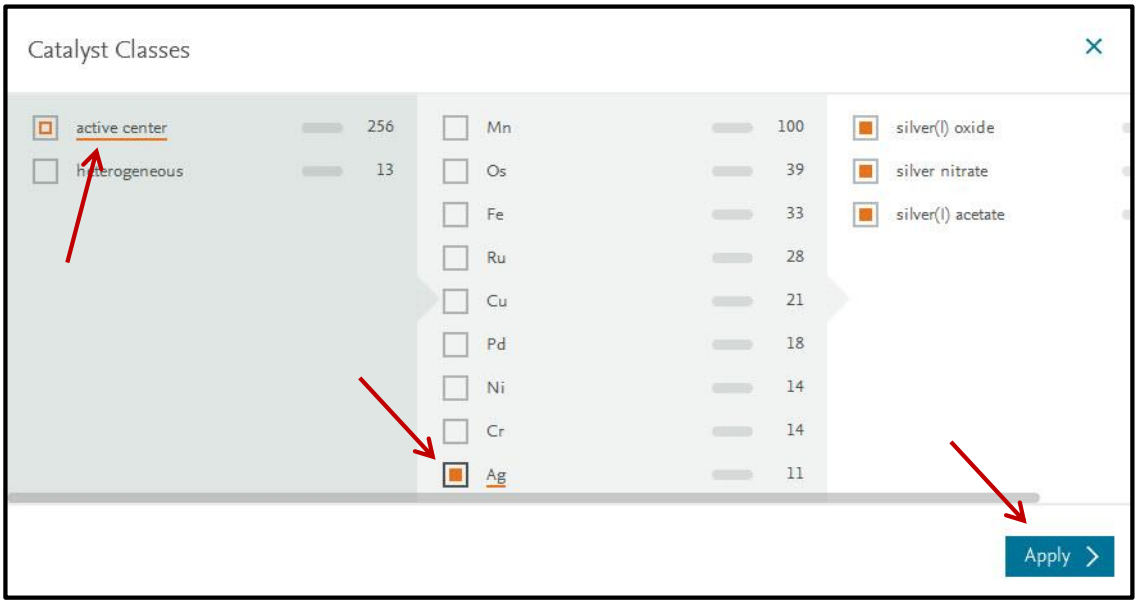


c. Click the text ***active center***

d. Check the box for ***Ag*** – this will limit the result set to 11 reactions.

   i. Silver oxide, silver nitrate and silver acetate

e. Click ***Apply***



The results are now filtered to show only reactions for substances using silver containing reagents/catalysts.