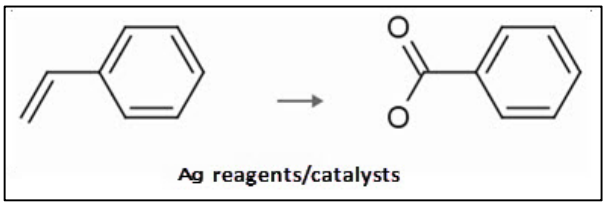
Reaction Searching

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.



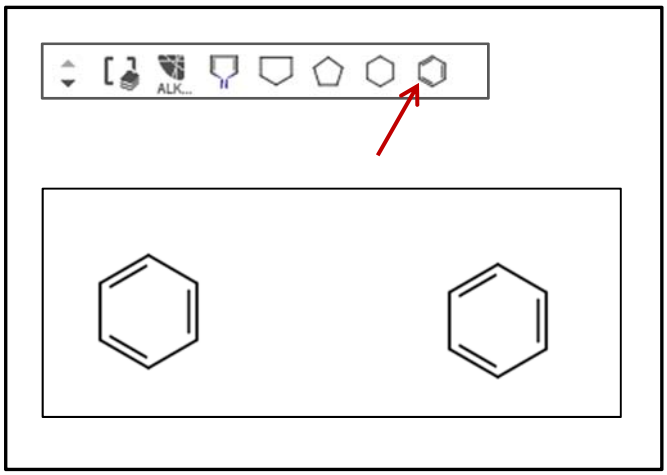
In this workflow we show examples that include:

- 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

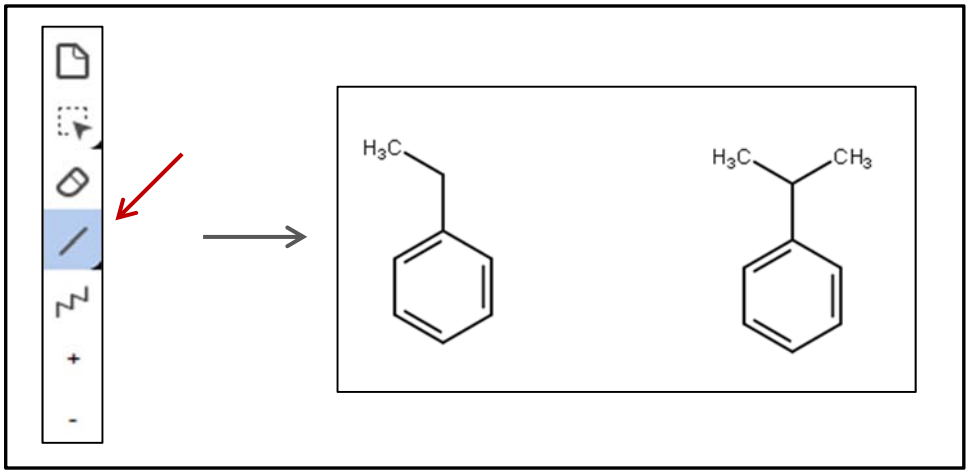
❖ Create a Structure Query

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

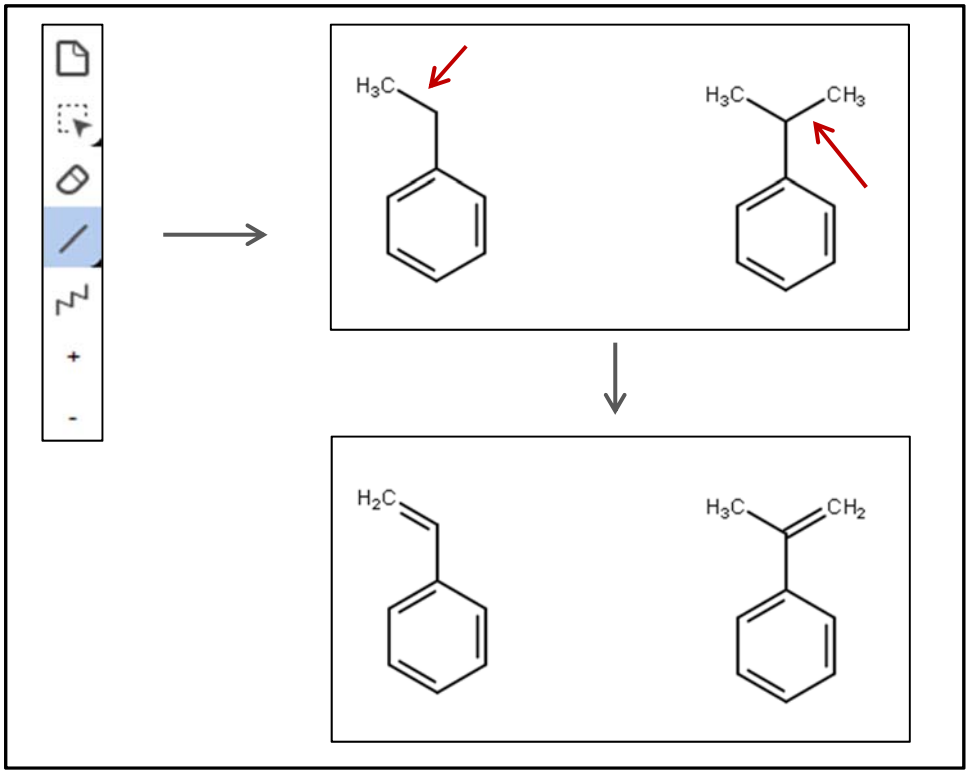
2. Draw an aromatic system.
   a. Select the ***Benzene*** tool
   b. Create two benzene rings as shown



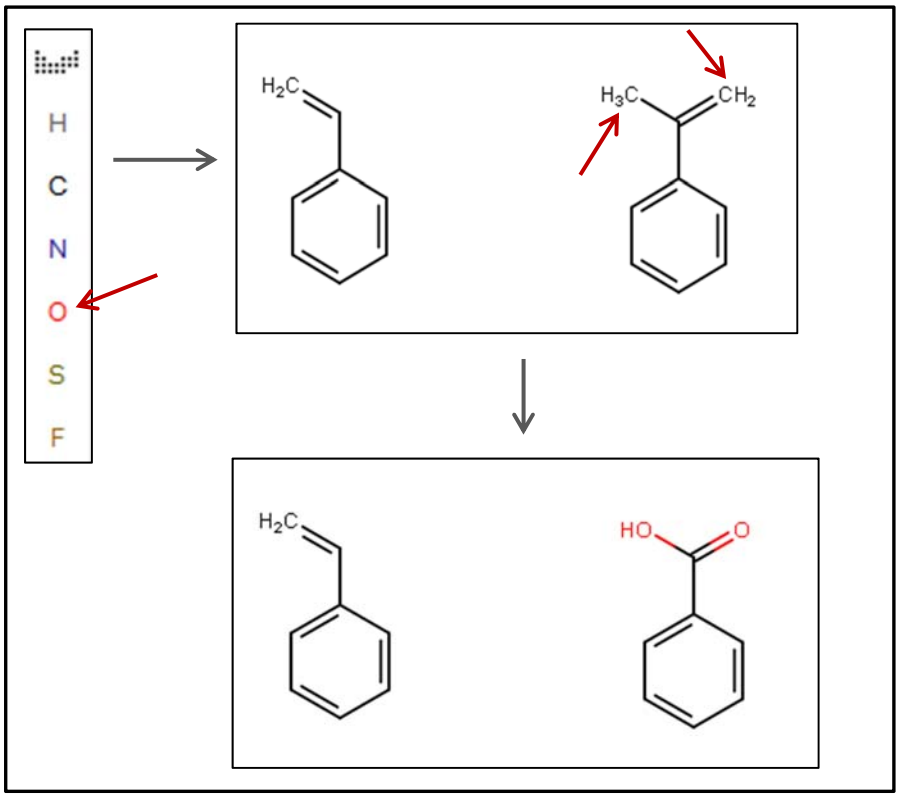
3. Select the ***Single bond*** tool
    a. Add bonds as shown



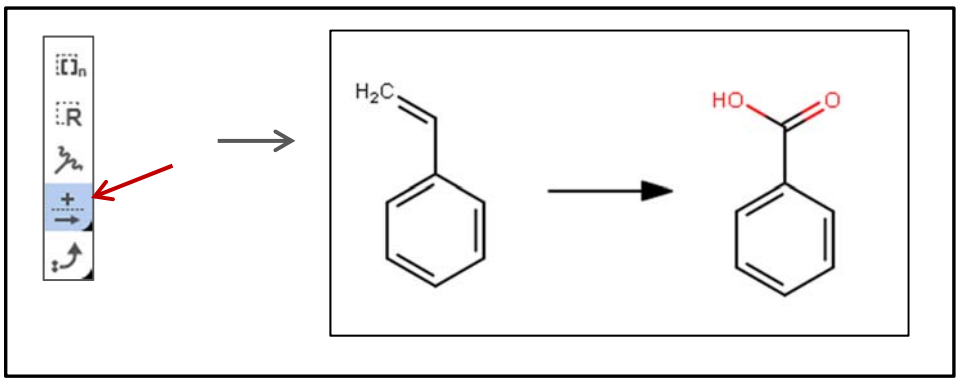
4. Define two double bonds:
    a. With the ***Single bond*** tool still selected, click the two bonds as shown



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

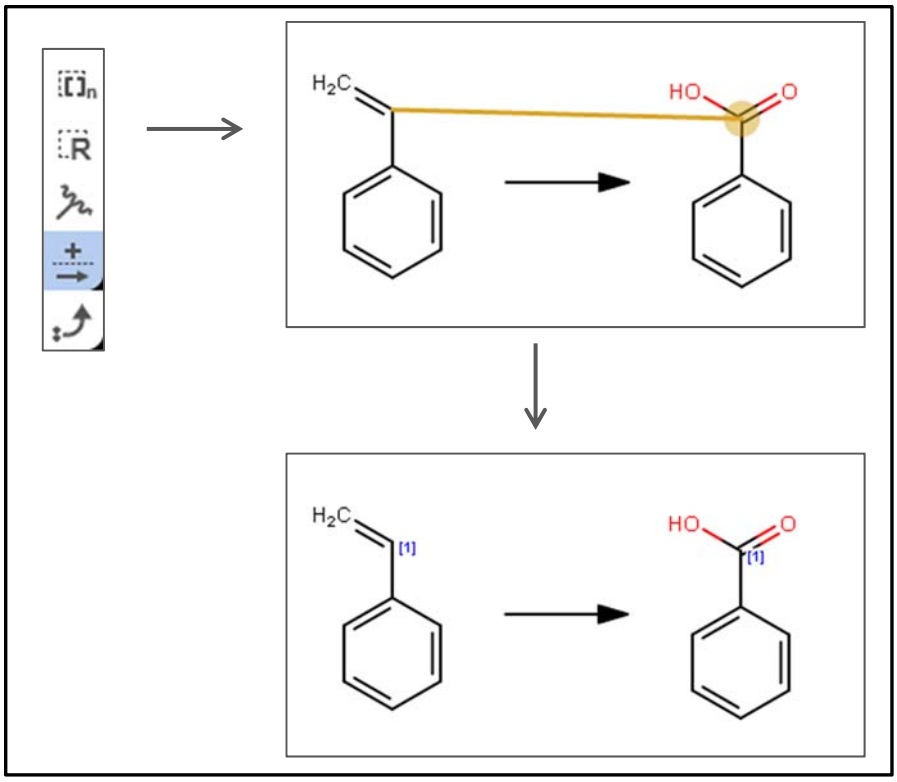


6. Create a **reaction**:
   a. Draw the arrow using the ***Straight arrow / Reaction*** tool.

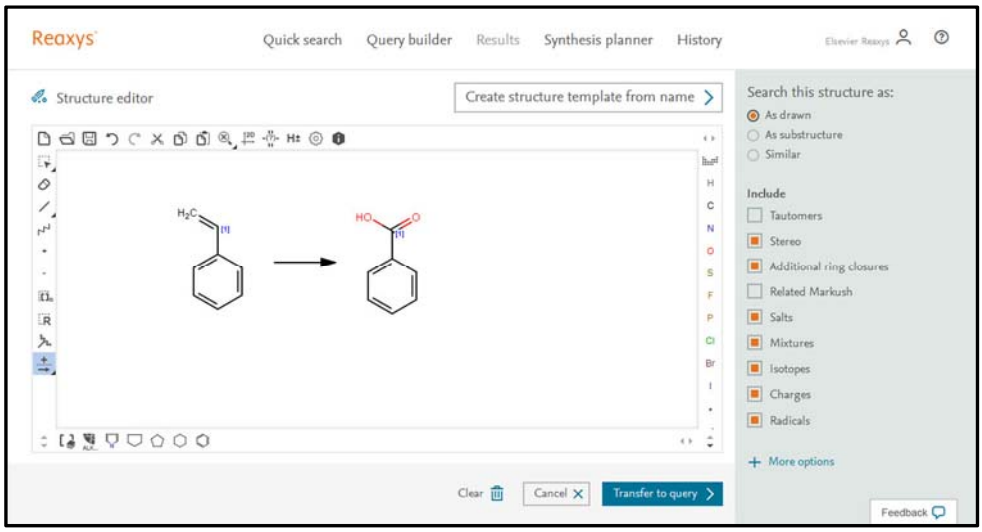


7. **Atom Mapping**
   a. Using the same ***Straight arrow / Reaction*** tool, draw an arrow between the carbon atom on the reactant and the analogous carbon atom on the product.

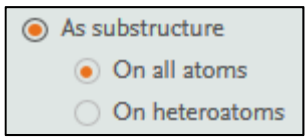
      This will map the two atoms (alternatively right-click the carbon atom on the reactant and add a 1 in the Map field of the Atom properties dialog. Do the same for the analogous carbon atom on the product).



The final query looks like this:



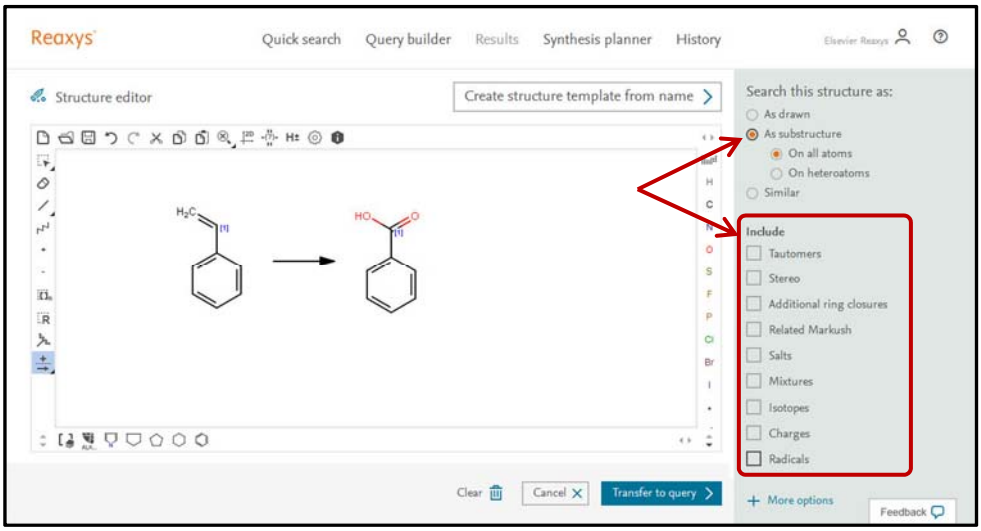
8. In the ***Search this structure as:*** panel, there are three options.
   - **As drawn***:* Reaxys will find results for the query as drawn
   - **As substructure***:* Reaxys offers two sub-options:



     - **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

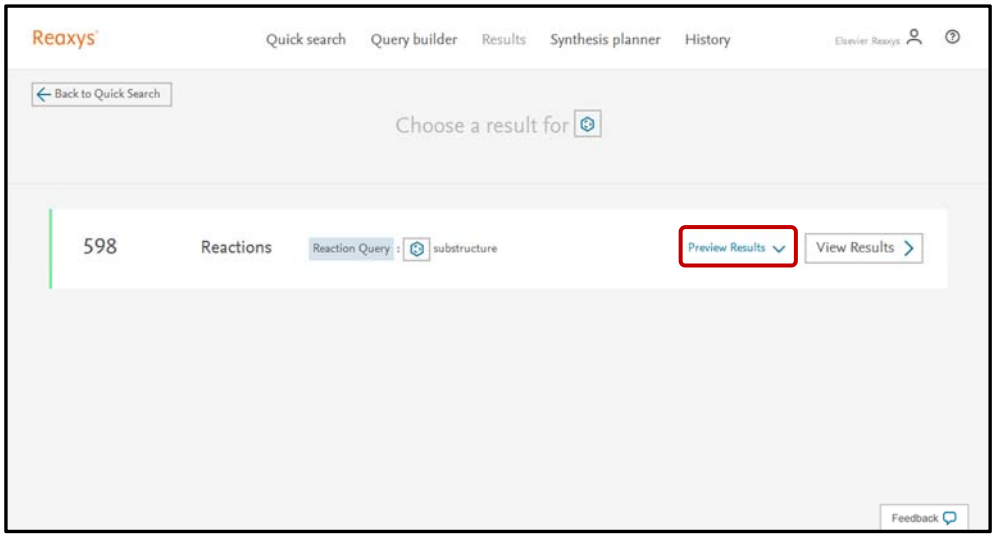
   Since this is a substructure search and we want substitutions on all the atoms:

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

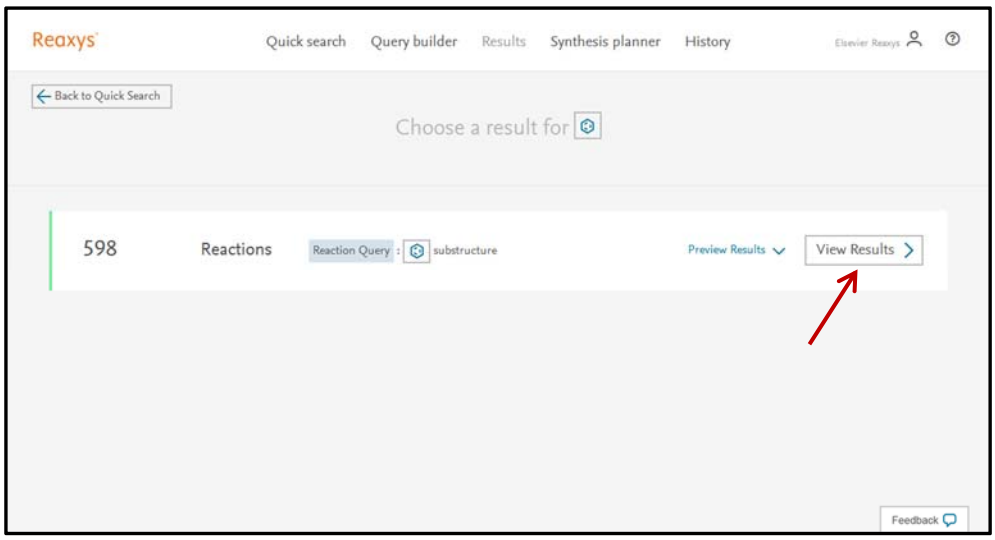


9. Click ***Transfer to query*** and click ***Search***.

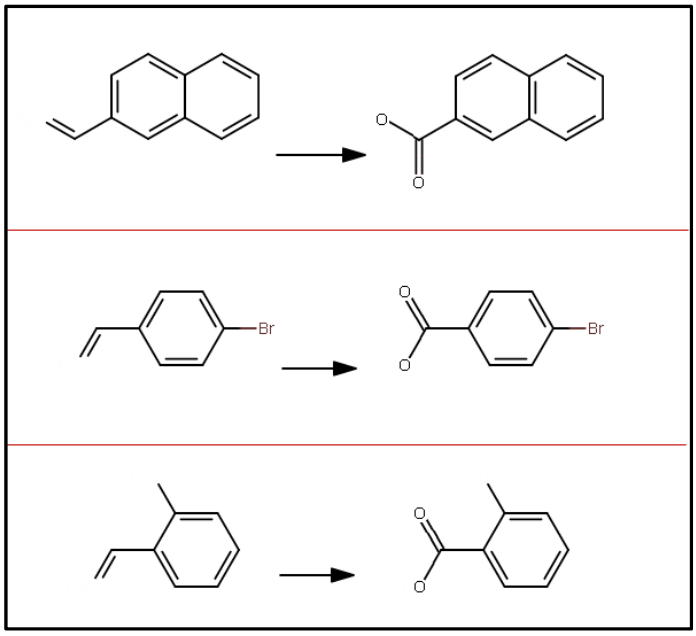
   The **Results Preview** is displayed. Each result option has a ***Preview Results*** feature that presents the top 3 results for the given query. You can check the results of your query before continuing to the full result set.



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



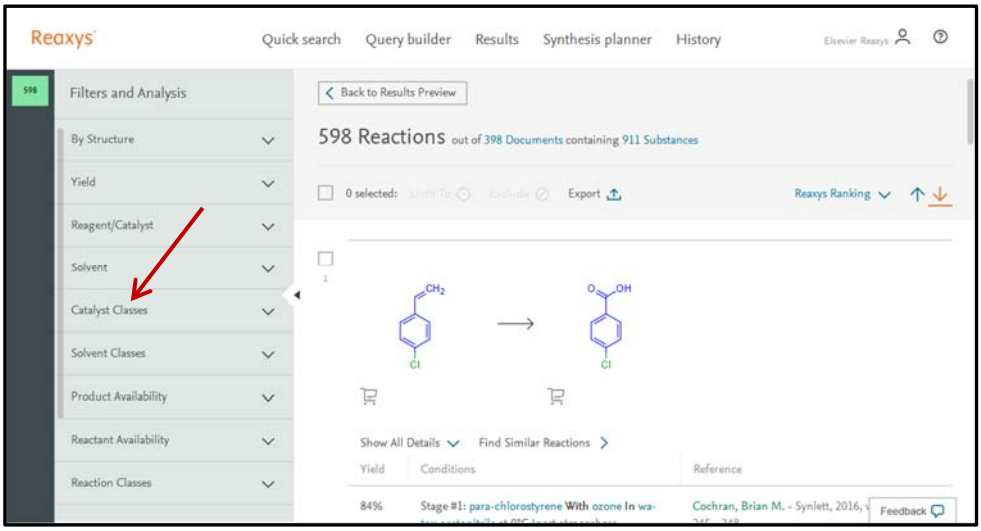
Several hundred reactions, like these, are retrieved:



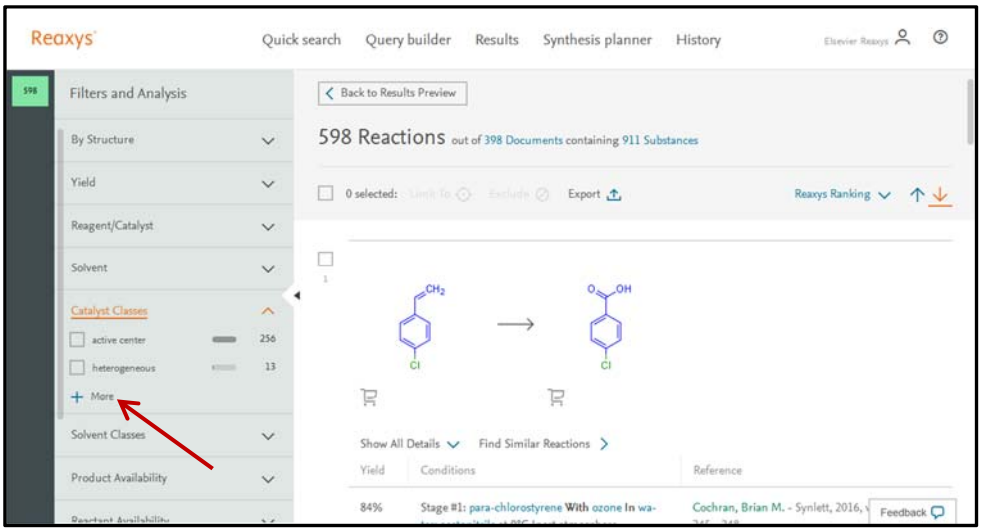
❖ Analyze the Results

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.