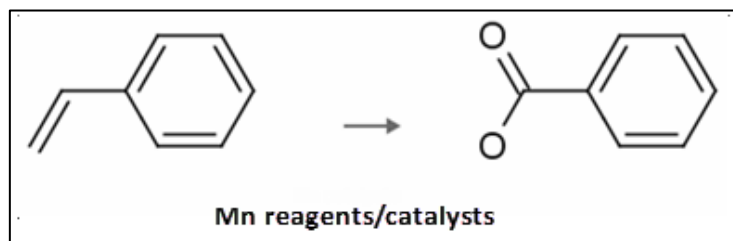# Reaction Searching

I would like to find information on the oxidative cleavage of c-c bonds (like those found in styrene) into carboxylic acids using manganese-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 attach a generic group at various points in the structure
- How to search for reactions "As drawn"
- How to narrow initial answers so that they contain only those with specific reagents/catalysts
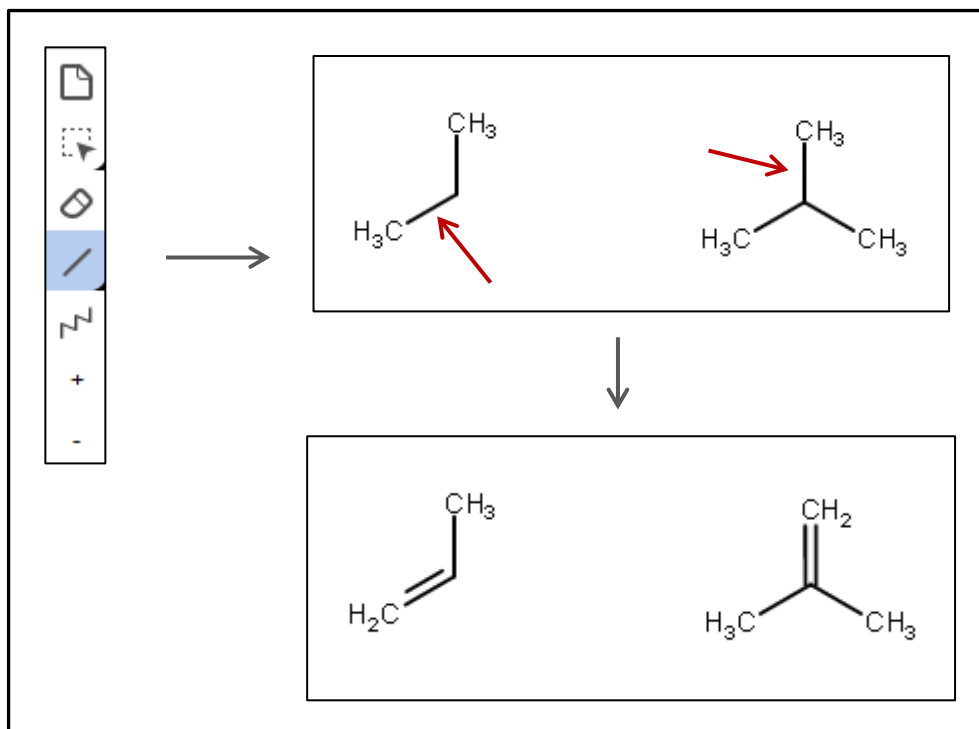
❖ Create a Structure Query

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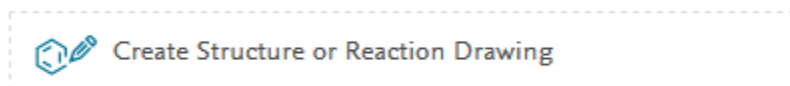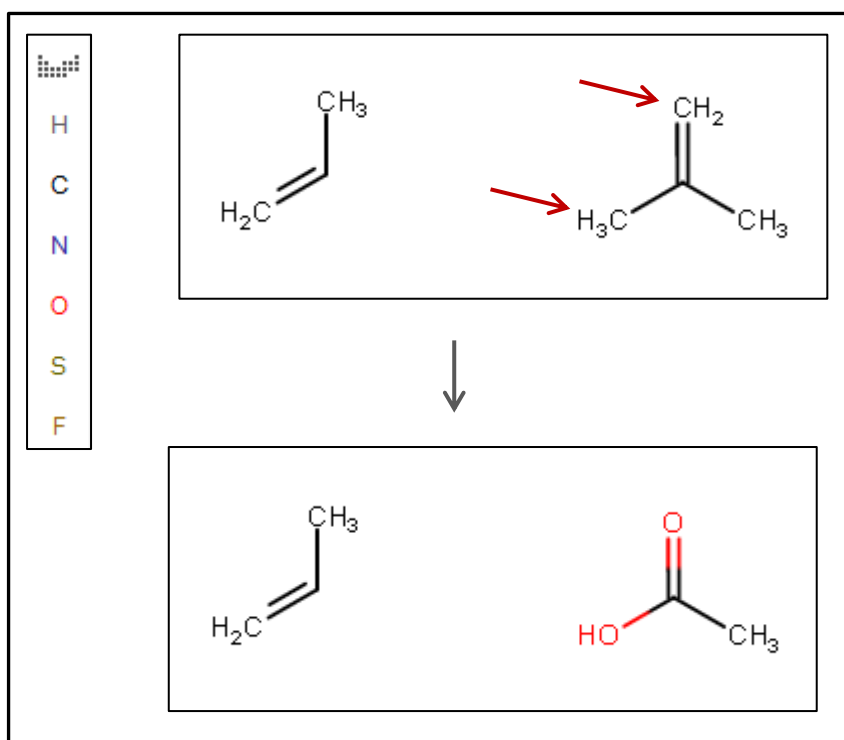

2. Draw the propylene and acid fragments:
   a. Select the ***Single bond*** tool
    b. Add bonds as shown
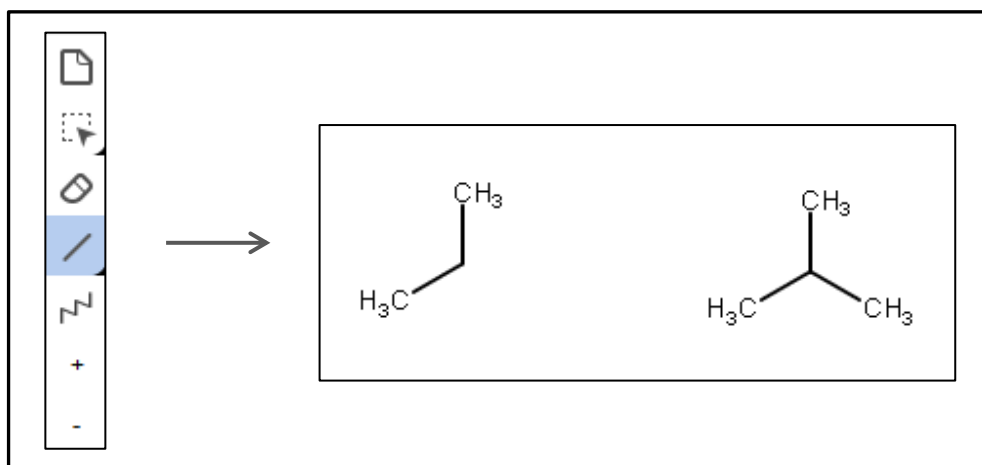
3. Define two double bonds:
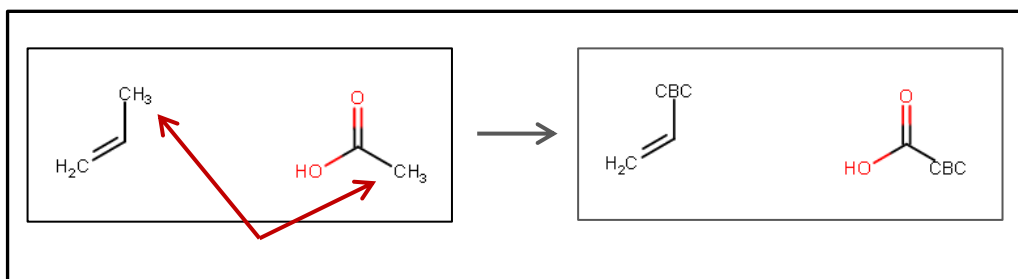   a. With the **Single bond** tool still selected, click the two bonds as shown

4. Change atoms as necessary:
   a. Click '**O**' in the atom toolbar, click the '**CH₂**' atom
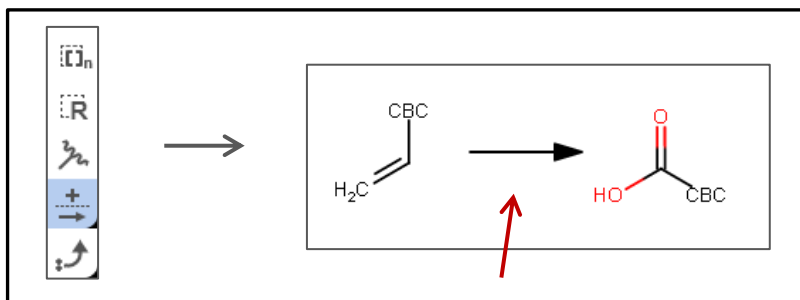   b. Click the '**H₃C**' atom

5. Add the appropriate **Reaxys Generic Group (CBC)**:
   a. Click the **ALK...** tool
   b. Click the **Cyclic** tab
   c. Click the abbreviation, in this instance **CBC**
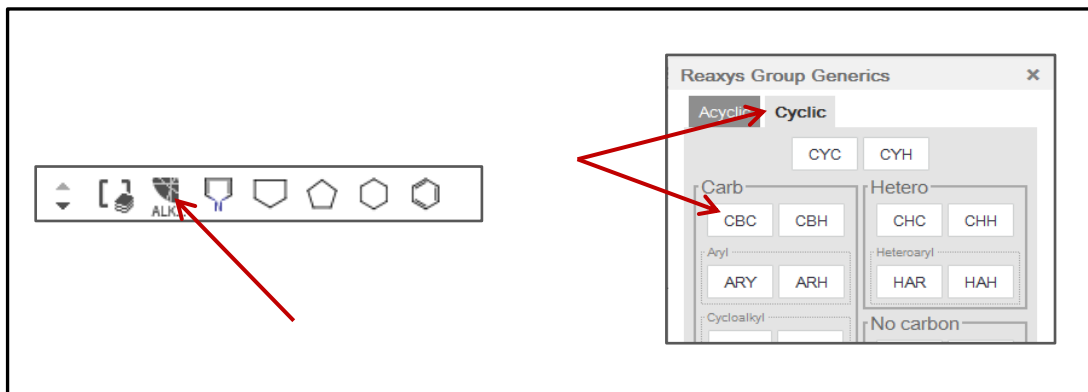

   d. Click the appropriate carbons in the reaction.

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).
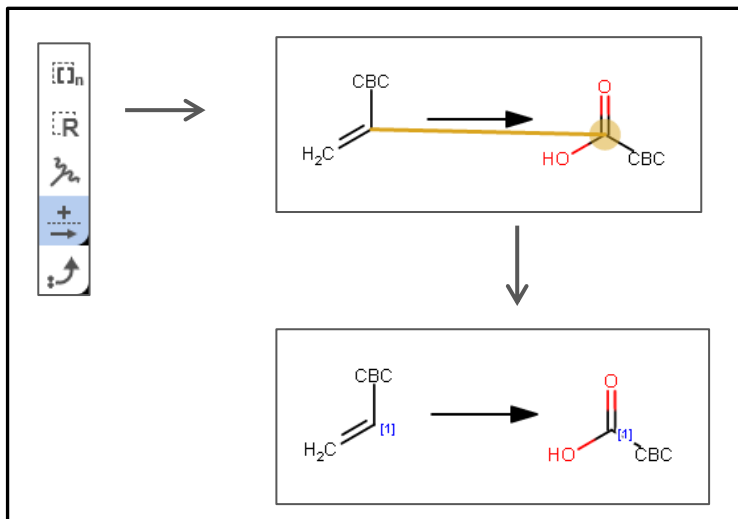
The final query looks like this:

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:

   ⊙ As substructure
      ⊙ On all atoms
      ○ On heteroatoms
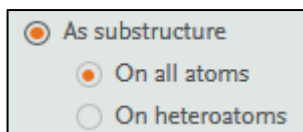
     - **On all atoms** will substitute any explicit or implicit hydrogen with any other atom or group
     - **On heteroatoms** will do the same but only on heteroatoms
   - **Similar**: Reaxys will find results for a similarity search based on the drawn query
   a. Click **as drawn** (the query already contains substructure search features: CBC)

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:

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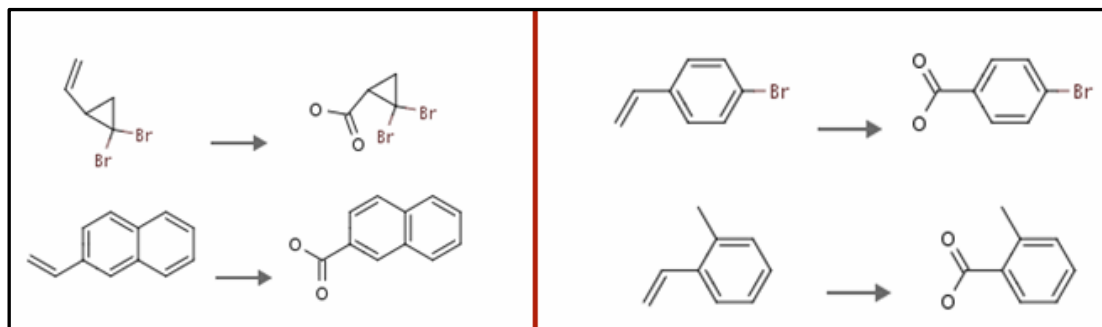
❖ Analyze the Results

Use the Filter & Analysis panel to visualize information about substances involved in the reactions. For example: I want to determine which reactions use manganese 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. Collapse the *Yield, Reagent/Catalyst* and *Solvent* filters
   b. Expand the *Catalyst Classes* taxonomy
   c. Click *+ More* to browse through the branches of the *Catalyst Classes* taxonomy.

   d. Click the text *active center*
   e. Check the box for *Mn* – this will limit the result set to 81 reactions.
   f. Click *Apply*

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