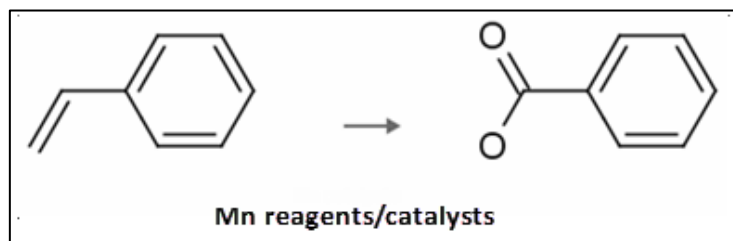


Reaction Searching

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.

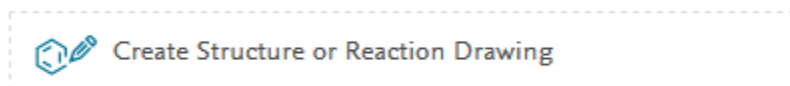


In this workflow we show examples that include:

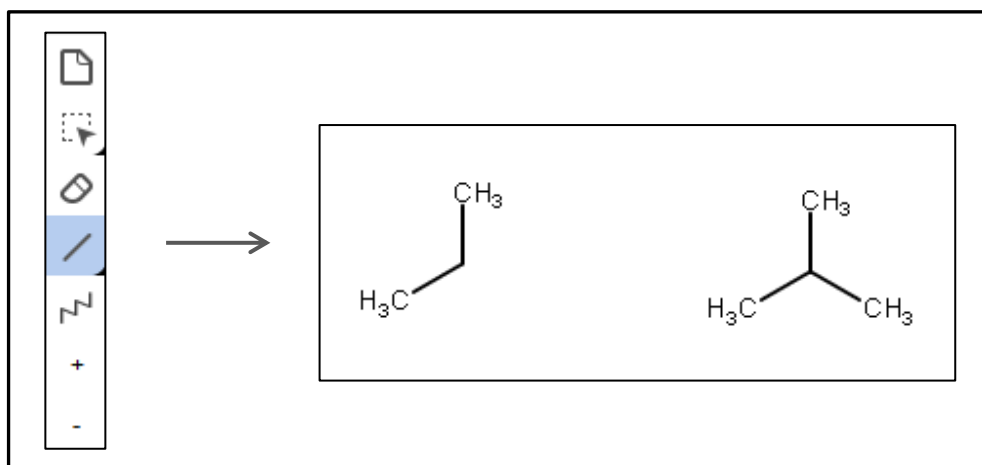
- How to create a reaction query
- How to map atoms between starting materials and products
- How to change the bond defaults
- How to attach a generic group at various points in the structure
- How to search for reactions “As drawn”
- How to narrow initial answers so that they contain only those with specific reagents/catalysts

❖ Create a Structure Query

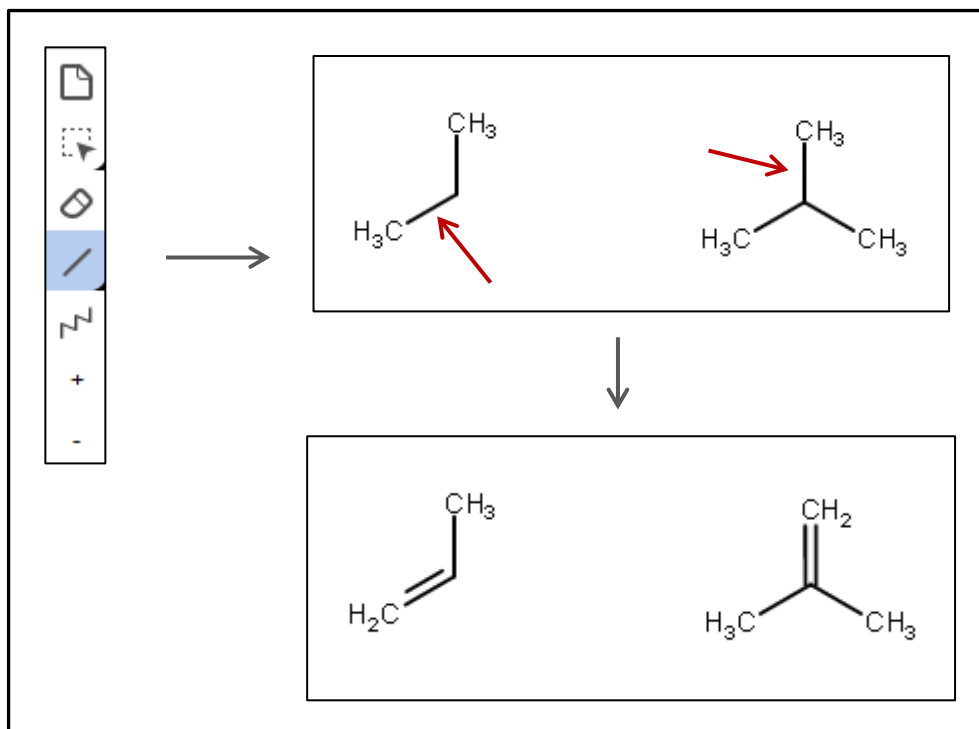
1. On the Reaxys home page click the **Create Structure or Reaction Drawing** box to open the structure editor (Marvin JS from ChemAxon).



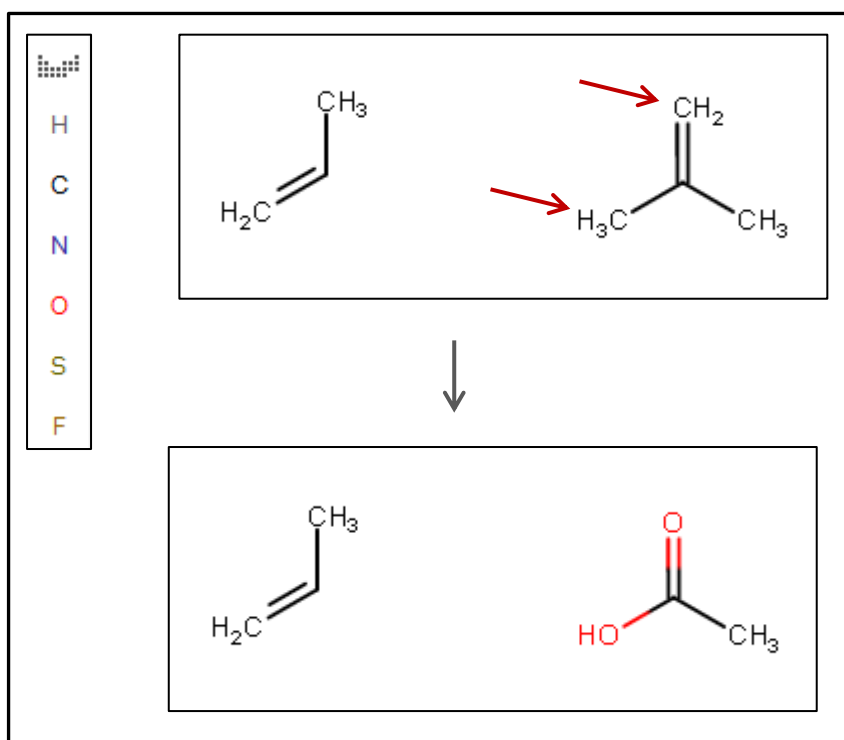
2. Draw the propylene and acid fragments:
 - a. Select the **Single bond** tool
 - b. Add bonds as shown



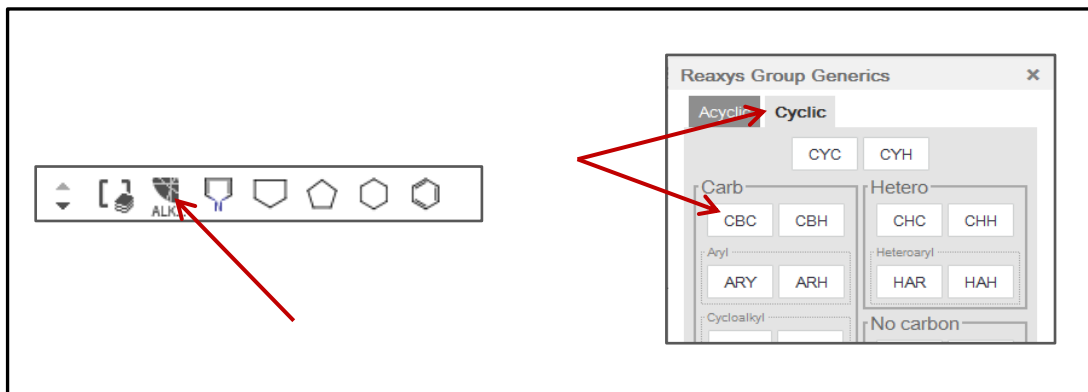
3. Define two double bonds:
 - a. With the **Single bond** tool still selected, click the two bonds as shown



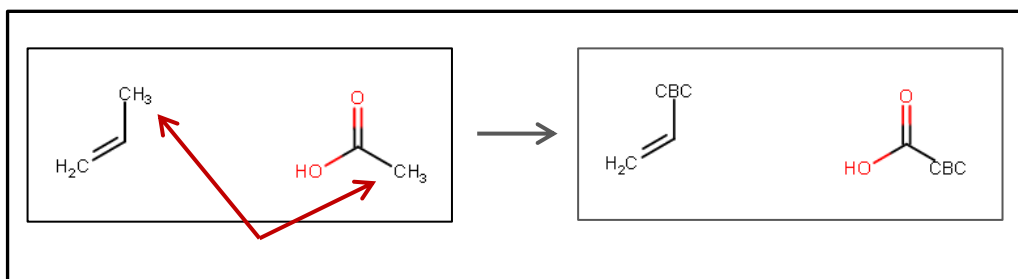
4. Change atoms as necessary:
 - a. Click 'O' in the atom toolbar, click the 'CH₂' atom
 - b. Click the 'H₃C' atom



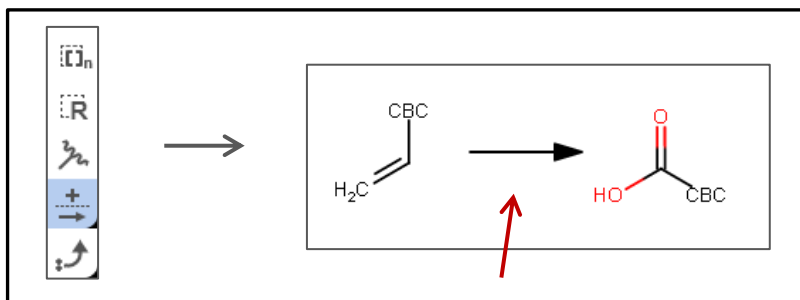
5. Add the appropriate **Reaxys Generic Group (CBC)**:
 - a. Click the **ALK...** tool
 - b. Click the **Cyclic** tab
 - c. Click the abbreviation, in this instance **CBC**



- d. Click the appropriate carbons in the reaction.



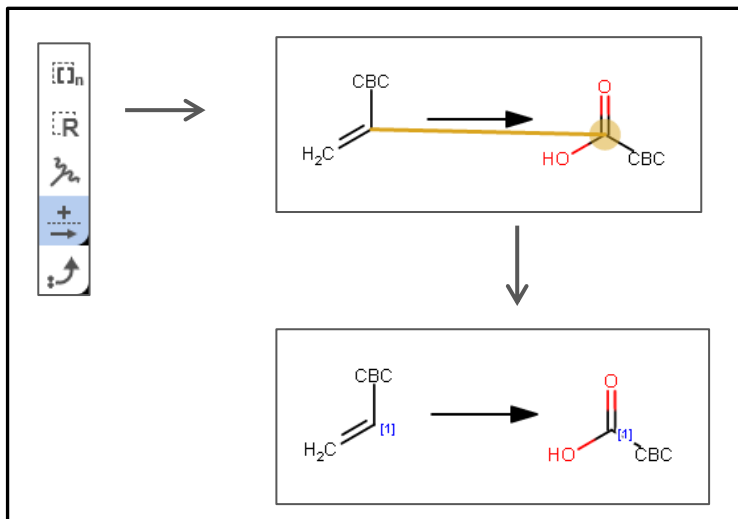
6. Create a **reaction**:
 - a. Draw the arrow using the **Straight arrow / Reaction** tool.



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.

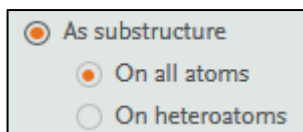
This will map the two atoms (alternatively right-click the carbon atom on the reactant and add a 1 in the Map field of the Atom properties dialog. Do the same for the analogous carbon atom on the product).



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:



- **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)

The screenshot shows the Reaxys interface with the 'Structure editor' on the left and the 'Search this structure as:' panel on the right. The structure editor displays a chemical reaction: C=C(CBC) >> OC(=O)N(CBC). The search panel has 'As drawn' selected. A red arrow points to the 'As drawn' option.

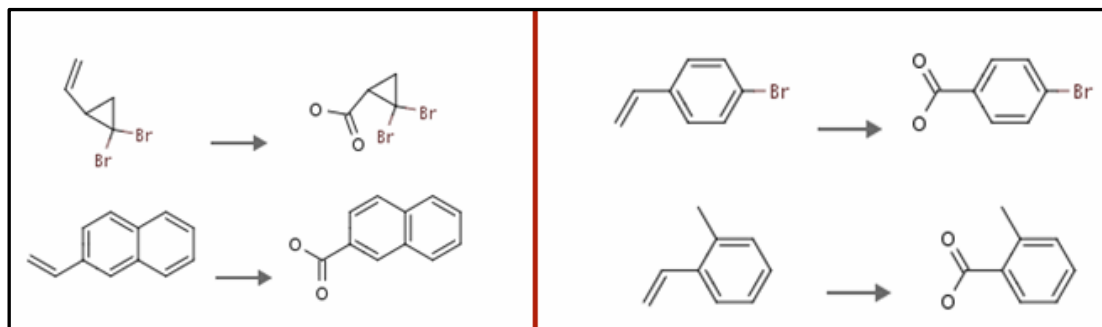
9. Click **Transfer to query** and click **Search**.

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.

The screenshot shows the 'Results Preview' page in Reaxys. It displays '300 Reactions' and a 'Reaction Query' of 'as drawn'. A 'Preview Results' button is highlighted with a red box, and a 'View Results' button is also visible.

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 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**

Filter	Count	Filter	Count
<input checked="" type="checkbox"/> active center	203	<input checked="" type="checkbox"/> Mn	81
<input type="checkbox"/> heterogeneous	8	<input type="checkbox"/> Ru	49
		<input type="checkbox"/> Os	42
		<input type="checkbox"/> Cr	27
		<input type="checkbox"/> B	11
		<input type="checkbox"/> Ni	11
		<input type="checkbox"/> Fe	10
		<input type="checkbox"/> Pd	6
		<input type="checkbox"/> Si	5

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

The screenshot shows the Reaxys search results page. On the left, the 'Filters and Analysis' sidebar is active, showing a 'Yield' filter with a range of >65 - 70 selected (6 results) and a 'Reagent/Catalyst' filter with 'potassium permanganate' selected (78 results) and 'acetone' selected (19 results). The main content area displays '81 Reactions out of 114 Documents containing 162 Substances'. Below this, there is a '0 selected' status and an 'Export' button. The central focus is a chemical reaction scheme showing the conversion of cinnamaldehyde (H₂C=CH-Ph) to cinnamic acid (HOOC-CH=Ph). Below the reaction, there are 'Find Similar Reactions' and 'Feedback' buttons.