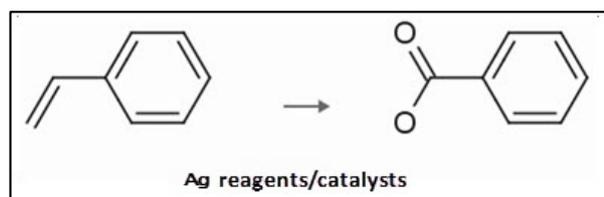


Reaction Searching

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:

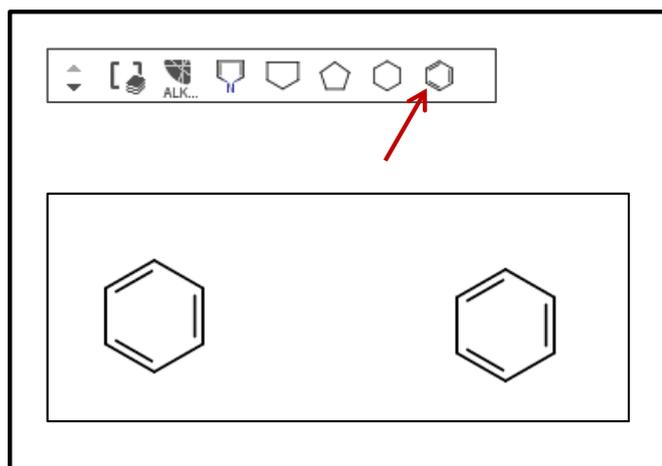
- How to create a reaction query
- How to map atoms between starting materials and products
- How to change the bond defaults
- How to search for reactions "As substructure"
- How to narrow initial answers so that they contain only those with specific reagents/catalysts

❖ Create a Structure Query

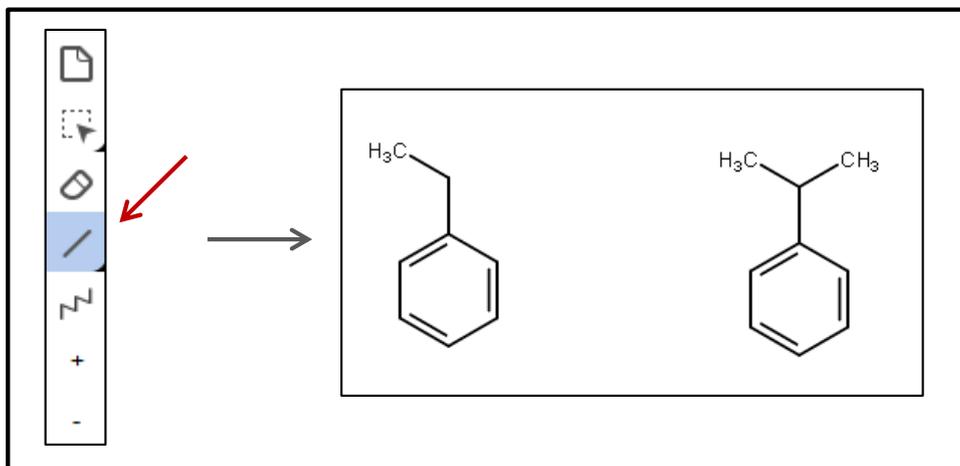
1. On the Reaxys home page click the **Create Structure or Reaction Drawing** box to open the structure editor (Marvin JS from ChemAxon).



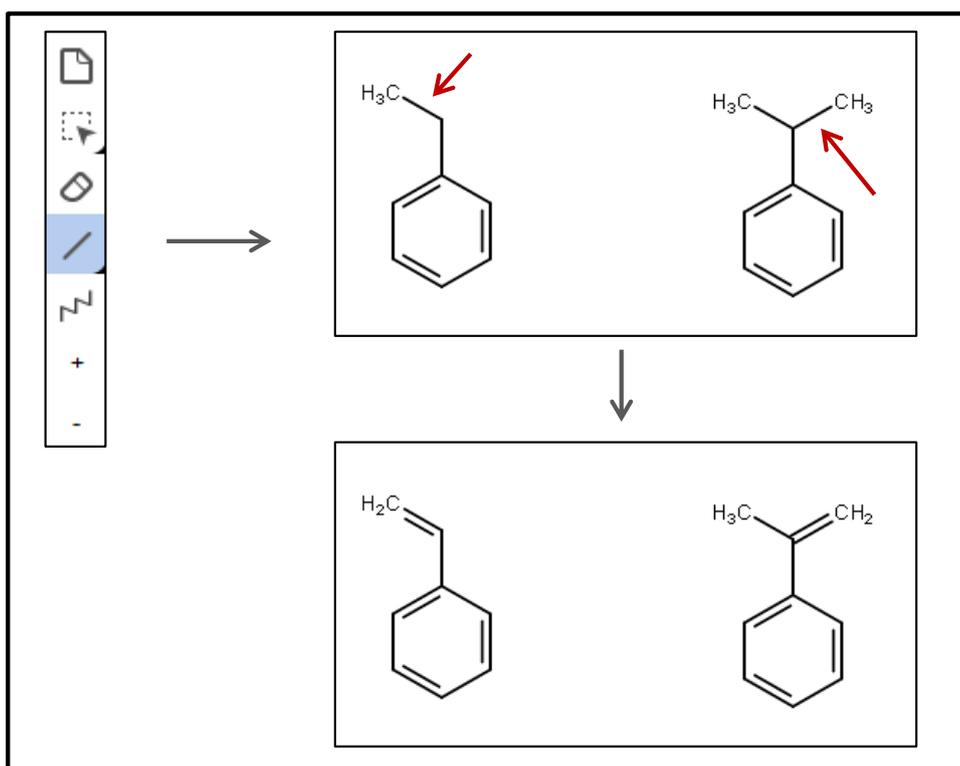
2. Draw an aromatic system.
 - a. Select the **Benzene** tool
 - b. Create two benzene rings as shown



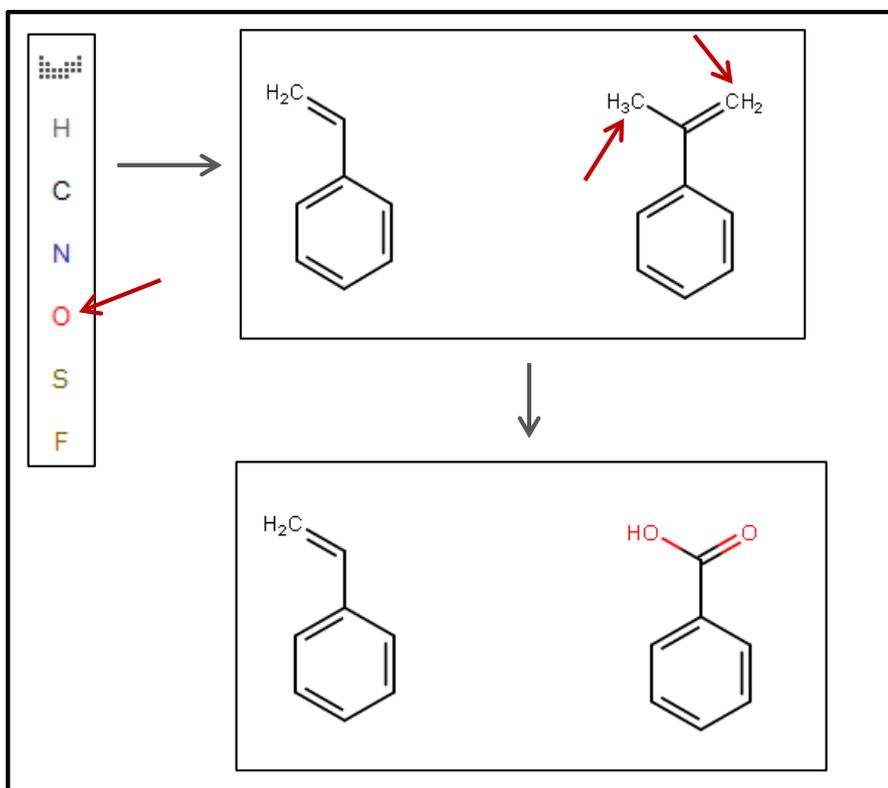
3. Select the **Single bond** tool
 - a. Add bonds as shown



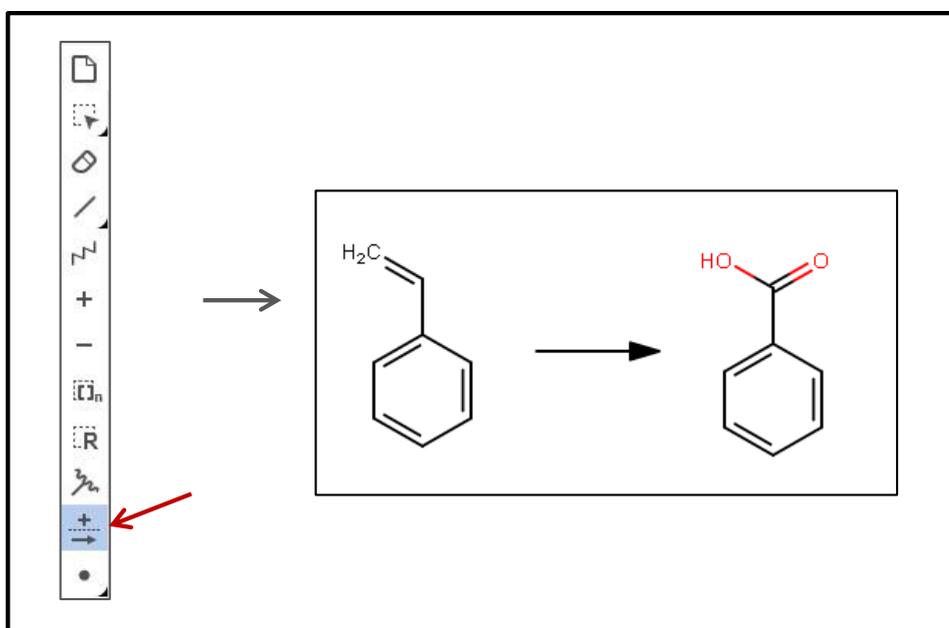
4. Define two double bonds:
 - a. With the **Single bond** tool still selected, click the two bonds as shown



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



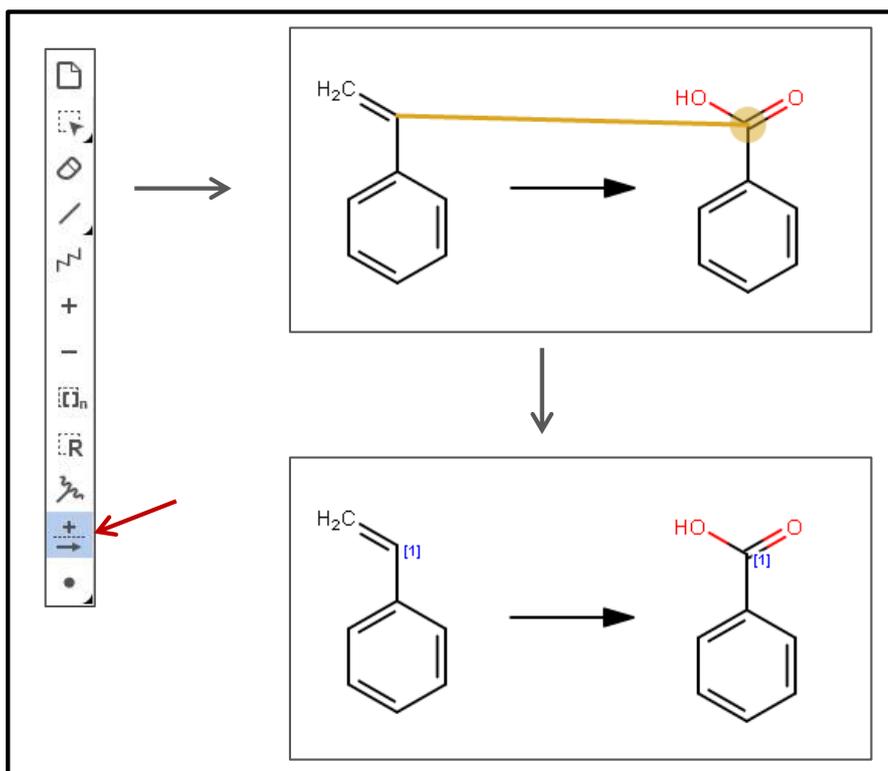
6. Create a reaction:
 - a. Click and drag to draw the arrow using the *Straight arrow / Reaction* tool.



7. Atom Mapping

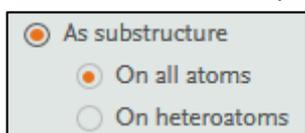
- a. Using the same ***Straight arrow / Reaction*** tool, click and drag to define the atom mapping between the carbon atom on the reactant and the analogous carbon atom on the product.

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:

- Click **As substructure + On all atoms**
- Turn off all **Include** features

The screenshot shows the Reaxys interface with a chemical reaction in the center: styrene (left) reacting to form styrene-1-carboxylic acid (right). On the right side, the 'Search this structure as:' panel is open. The 'As substructure' option is selected, and under it, 'On all atoms' is also selected. Below these, the 'Include' section is expanded, showing a list of features with all checkboxes turned off: Tautomers, Stereo, Additional ring closures, Related Markush, Salts, Mixtures, Isotopes, Charges, and Radicals. A red arrow points from the 'On all atoms' option to the 'Include' section.

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

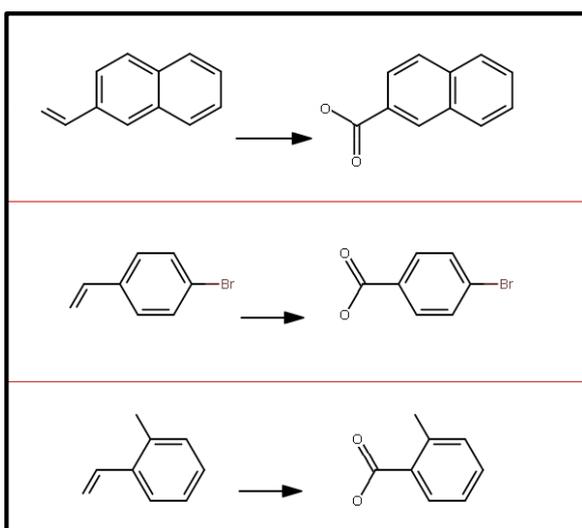
The **Results Preview** is displayed. Each result option has a **Preview Results** feature that presents the top 3 results for the given query. You can check the results of your query before continuing to the full result set.

The screenshot shows the Reaxys search results page. At the top, there are navigation tabs: Quick search, Query builder, Results, Synthesis planner, and History. Below the navigation, there are icons for 'New' and 'Edit'. The main content area displays '603 Reactions' for the query 'substructure'. A red box highlights the 'Preview Results' button, and a 'View Results >' button is also visible. A 'Feedback' button is located at the bottom right.

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

This screenshot is similar to the previous one, but a red arrow points to the 'View Results >' button, indicating the next step in the process. The 'Preview Results' button is now blue and has a dropdown arrow.

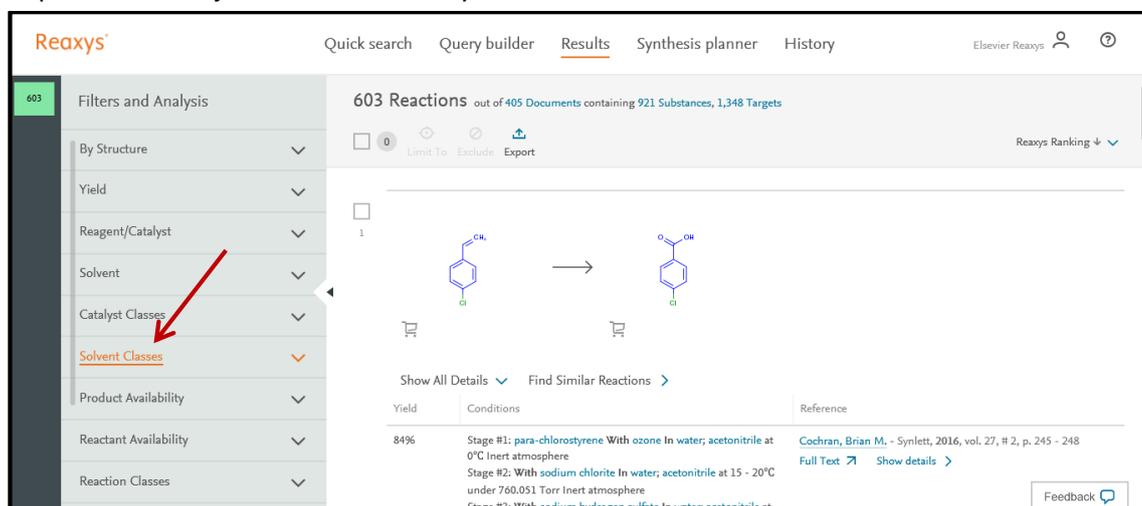
Several hundred reactions, like these, are retrieved:



❖ Analyze the Results

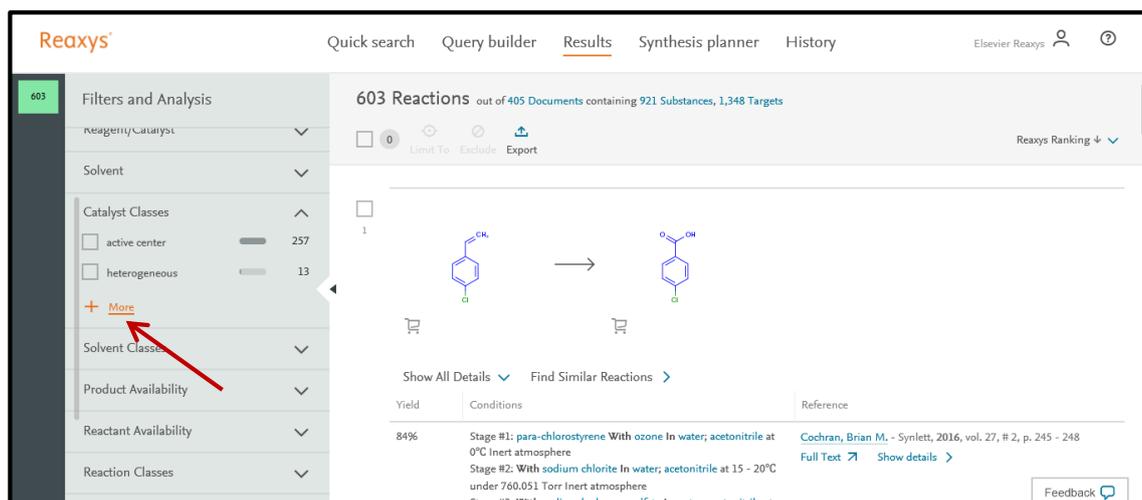
Use the Filter & Analysis panel to visualize information about substances involved in the reactions. For example: I want to determine which reactions use silver containing reagents/catalysts.

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



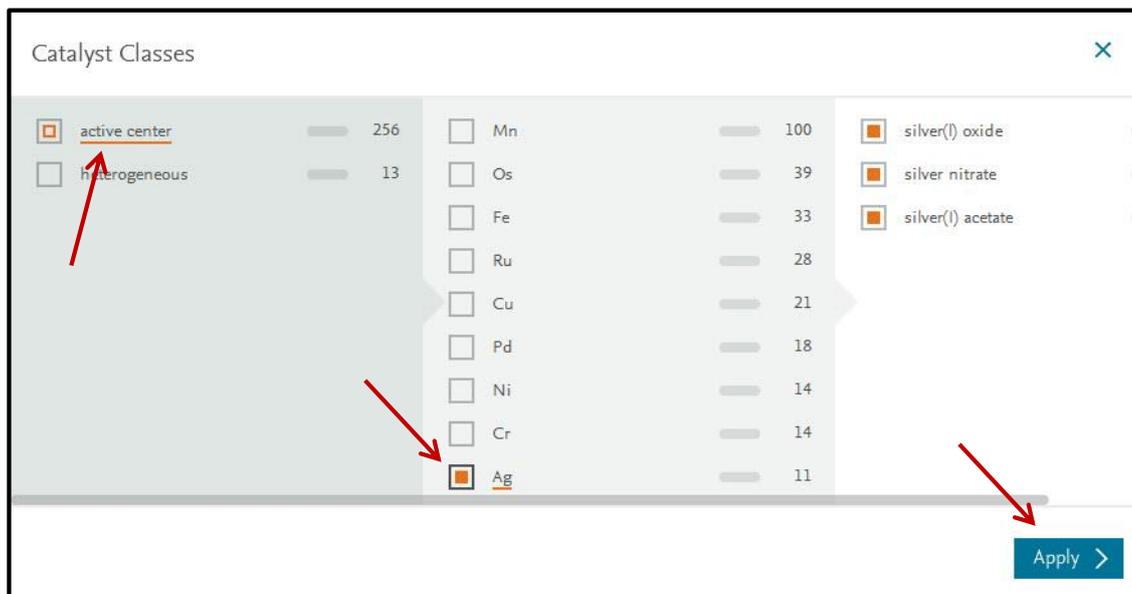
The screenshot shows the Reaxys interface with 603 reactions displayed. The 'Filters and Analysis' panel on the left is expanded to show 'Catalyst Classes'. A red arrow points to the 'Catalyst Classes' dropdown menu. The main reaction area shows a chemical reaction: para-chlorostyrene reacting with ozone in water and acetonitrile at 0°C, followed by sodium chlorite in water and acetonitrile at 15-20°C, and finally sodium hydrogen sulfate in water and acetonitrile. The yield is 84%.

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



The screenshot shows the Reaxys interface with 603 reactions displayed. The 'Filters and Analysis' panel on the left is expanded to show 'Catalyst Classes'. The 'Catalyst Classes' section is further expanded to show 'active center' (257) and 'heterogeneous' (13). A red arrow points to the '+ More' button. The main reaction area shows the same chemical reaction as in the previous screenshot.

- 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.

The screenshot shows the Reaxys search results page. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The left sidebar shows 'Filters and Analysis' with 'Catalyst Classes' expanded to show 'active center' with 11 results. The main content area displays '11 Reactions out of 9 Documents containing 20 Substances, 10 Targets'. The first reaction is shown with a chemical structure of a chlorinated benzene derivative and its corresponding product. The reaction conditions and reference are also visible.

Yield	Conditions	Reference
	Multi-step reaction with 4 steps 1: 85 percent / Zn / dioxane / 16 h / Heating 2: 1.) AgNO ₃ , 2.) Cl ₂ / 1.) H ₂ O, THF, 30 min, 2.) CCl ₄ , 5 min 3: 52 percent / concd. H ₂ SO ₄ / 1 h / 100 °C 4: 85 percent / 20percent aluminum / 1 h / 100 °C	Ballester, Manuel; Castaner, Juan; Riera, Juan; Tabernero, Ignacio - Journal of Organic Chemistry, 1986, vol. 51, # 9, p. 1413 - 1419 Full Text Cited 12 times Show details