Guide to finding experimental procedures for novel reactions

Suppose you wanted to carry out the following epoxidation reaction:

\[
\begin{align*}
\text{substrate} & \quad \rightarrow \quad \text{product} \\
\text{phenylpropene} & \quad \rightarrow \quad \text{epoxide}
\end{align*}
\]

The first step would be to see if this exact reaction has been done before. Unfortunately, a search for this transformation turns up no results with SciFinder. How should you proceed? You could try a topic search for “epoxidation reactions” but this is likely to give thousands of results (and there’s no easy way of sorting through them to find the conditions that would work well for your substrate). A better approach is to do a search for epoxidation reactions on structures that are similar to yours. The following guide provides instructions for how to do this type of search.

- From the main SciFinder window, click on “Explore reactions”

![SciFinder window](https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf)

- Click on the structure editor (up-to-date Java plugin required)
- From here, you have several options for how to proceed:

Option A (search for simple variations of your specific reaction)
- Decide on some simplifications you could make to your substrate that wouldn’t change its overall reactivity. For example, you might simplify or even remove some of the substituents to search for:

\[
\begin{align*}
\text{substrate} & \quad \rightarrow \quad \text{epoxide} \\
\text{phenylpropene} & \quad \rightarrow \quad \text{epoxide}
\end{align*}
\]
• Draw the reactant and product in the SciFinder Structure Editor window.
• Assign a role to each structure by drawing in a reaction arrow (roles will automatically be assigned when you draw in the reaction arrow; structures to the left of the arrow are assigned as reactants; structures to the right are assigned as products):

- Select the radio button “variable only at the specified positions” to search for exactly the reaction that you drew.
- Click ok (structure editor will close) and then click search (top right of screen).

Option B (search for a generic version of your specific reaction)
• Decide on some generic simplifications you could make to your substrate that won’t significantly change its overall reactivity. For example, you might decide that as long as the groups attached to the double bond are alkyl groups, the method could be used for your reaction:

Where R = any alkyl group
• Draw the core structure of your reactant and product in the SciFinder Structure Editor window.
• Use the Variable Menu tool ("– X") to open the “Variables” menu. Select the type of variable you would like to introduce to your search (for example, select “Ak” for “Any alkyl group”).

• Close the “Variables” menu and click on your structure wherever you would like to introduce the variable.
• Assign a role to each structure by drawing in a reaction arrow as described above.
• Select the radio button “variable only at the specified positions”.
• Click ok (structure editor will close) and then click search (top right of screen).

Option C (substructure search)
• WARNING: This type of search has the potential to generate hundreds of reactions with seemingly NO relationship to what you’re interested in! Avoid using this approach unless you’re really desperate!
• In the Structure Editor window of SciFinder, draw either the exact reaction you’re interested in or a simplified version (perhaps just the core of each structure). For example:

```
\[
\begin{array}{c}
\text{苯乙烯} \\
\text{苯甲酸}
\end{array}
\]
```

• Assign a role to each structure by drawing in a reaction arrow as described above.
• Select the radio button “substructures of more complex structures.” This will tell SciFinder to search for reactions where substitution anywhere on your structures is allowed.
• Click ok (structure editor will close) and then click search (top right of screen).

Regardless of which search method you choose, don’t be discouraged if you aren’t successful on your first try. Some searches will retrieve hundreds of results; others might not retrieve any. You will likely have to try several different searches, allowing different types of variation on your structures in order to find what you’re looking for.

In some cases, you may need to refine your search in order to narrow down the results to a useful/manageable number of results. Once you have a list of results, click on the “Refine” tab on the right hand side of the screen to experiment with different criteria for limiting your search results to what you’re interested in. Some good starting places include: yield, number of steps, reaction classification.