

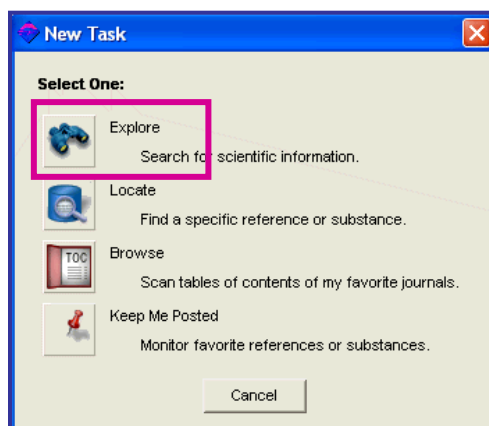
HOW TO

Exploring Reactions: Functional Groups

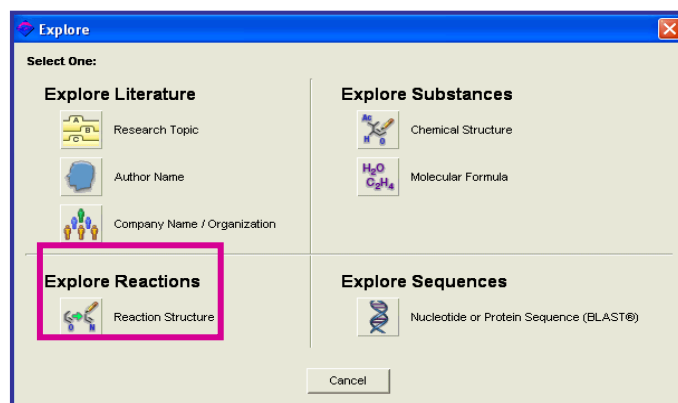


SciFinder[®] provides access to the largest reaction database in the world (CASREACT[®]) with coverage from 1840 to the present. Containing more than 14 million single- and multi-step reactions, with an average of 950 reactions added each week from both patents and journals, CASREACT is a powerhouse of information. You can make your reaction searches more effective by using several unique tools offered by SciFinder. Two tools, **Filters** and **Functional Groups**, can increase the precision of your queries.

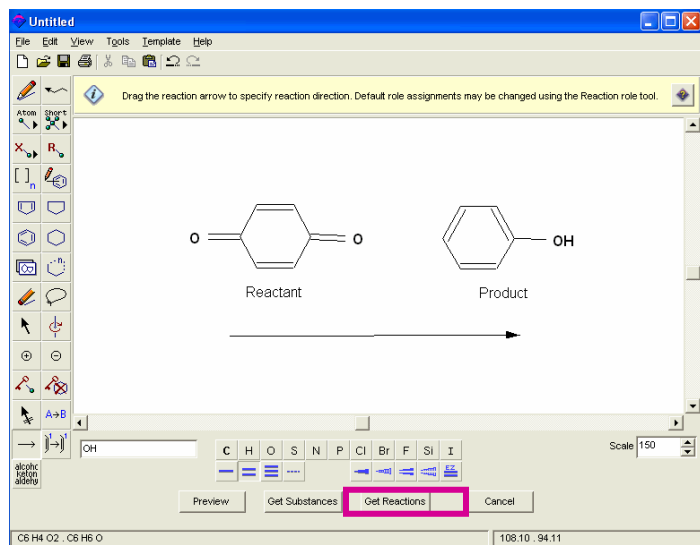
1. Suppose you are interested in transformations of substances containing the moiety p-quinone into substances that contain phenol. To get started, click Explore under New Task.



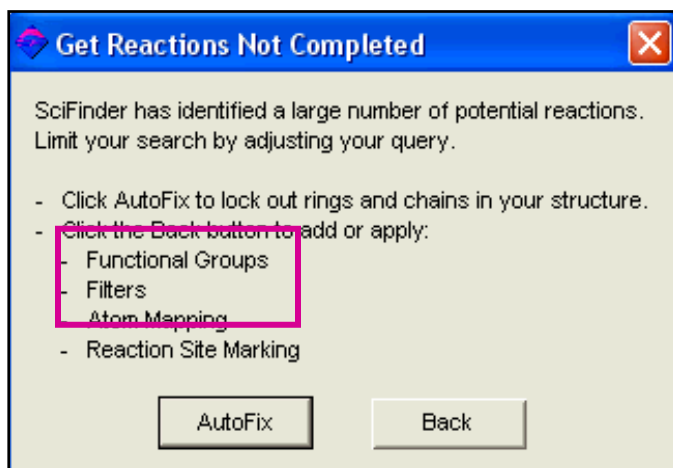
2. You can locate reaction information with any type of SciFinder exploration, but most searchers begin with the structure-drawing window. Click Explore Reactions.



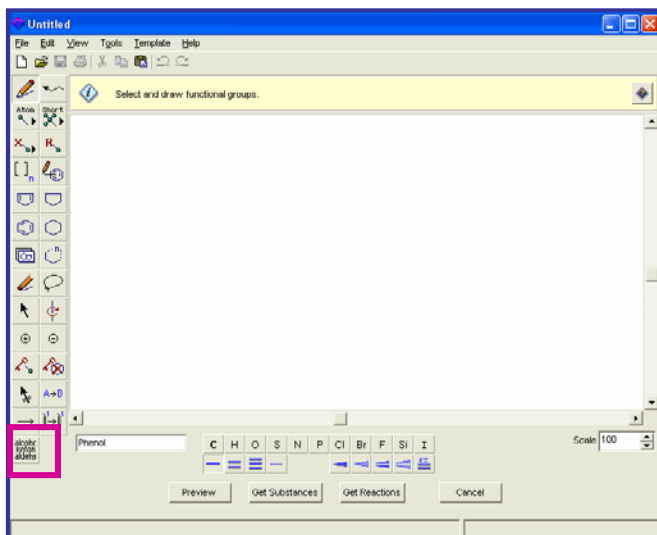
3. You do not need to draw entire substances to explore transformations of interest. Just draw the moieties and use either the A-to-B reaction labeling tool or the reaction arrow to designate roles. Click Get Reactions.



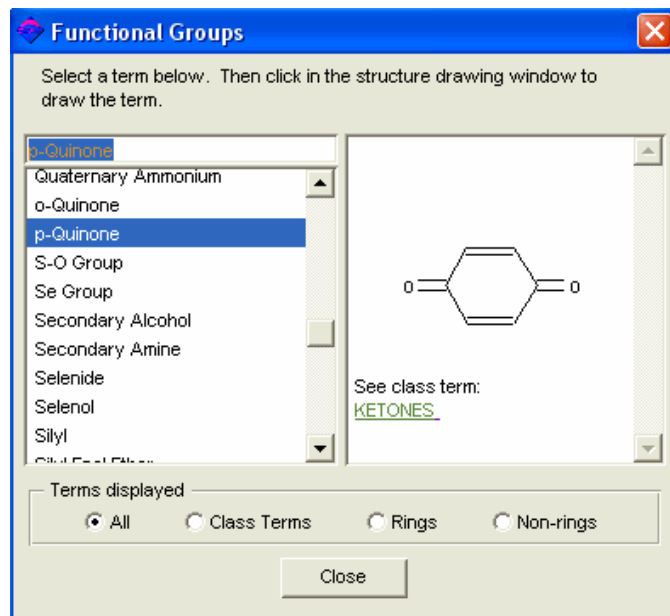
4. SciFinder will inform you if it cannot complete the reaction search as drawn. As in this case, the transformation we have specified is too broad and retrieves too many candidates. SciFinder offers some tips to work around this situation, e.g., Functional Groups and Filters.



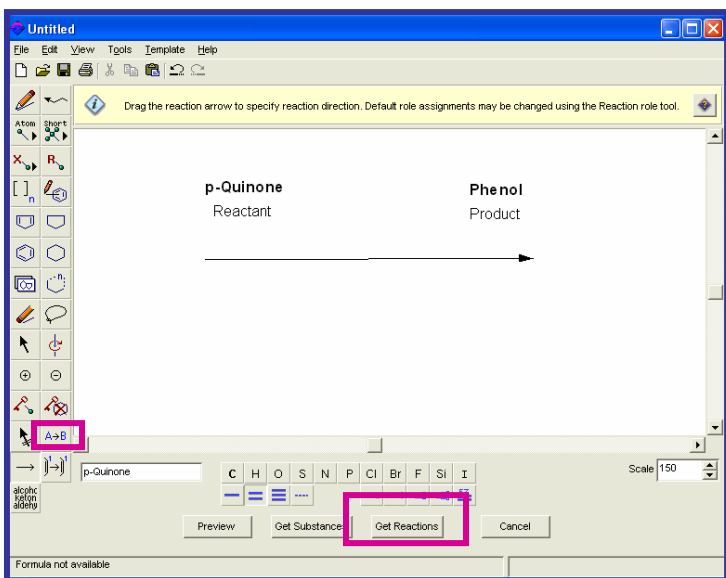
5. **Why does the Functional Groups tool improve the chances for your reaction search to run to completion?** When Functional Groups are specified, SciFinder switches from chemical structures to exploring by CA index terms. Term searching requires far fewer computing resources than does an atom-by-atom, bond-by-bond iterative structure search of the 33-plus million substances in the CAS RegistrySM. To specify Functional Groups, start with a fresh search and click the Functional Groups button.



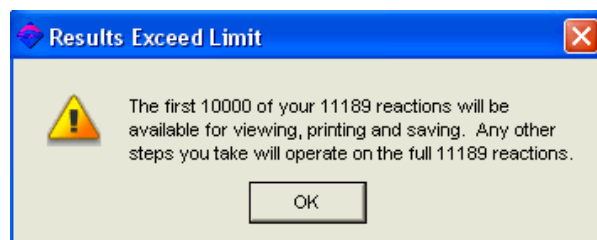
6. The Functional Groups menu provides you with many choices. Scroll down to select p-quinone, click in the structure drawing window to add this functional group. Do the same for phenol.



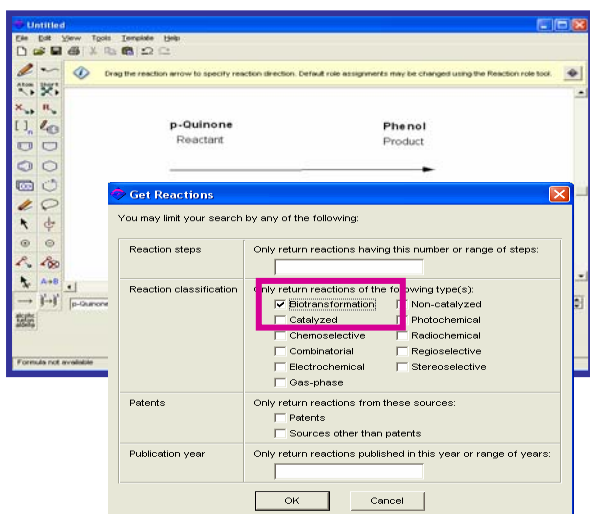
7. Specify reaction roles for the functional groups in your reaction query, click Get Reactions.



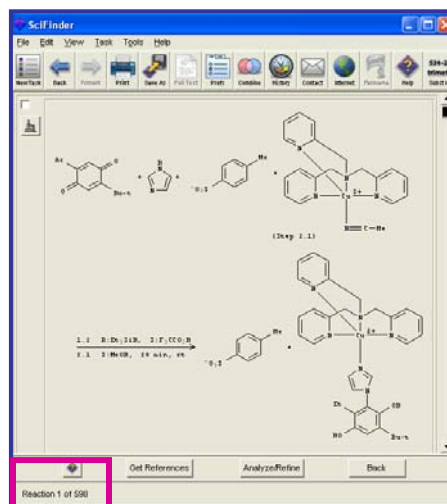
8. The reaction search using the Functional Groups tool runs to completion. SciFinder will warn you if your search results exceeds system limits. To pare down your answer set, employ the Filter tool.



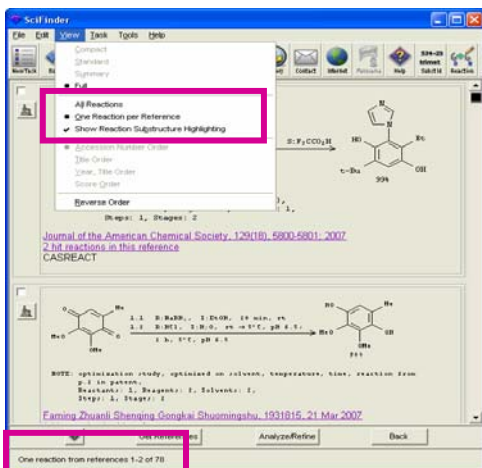
9. Return to the Functional Groups query. This time when we click Get Reactions, we will select the reaction classification Biotransformation.



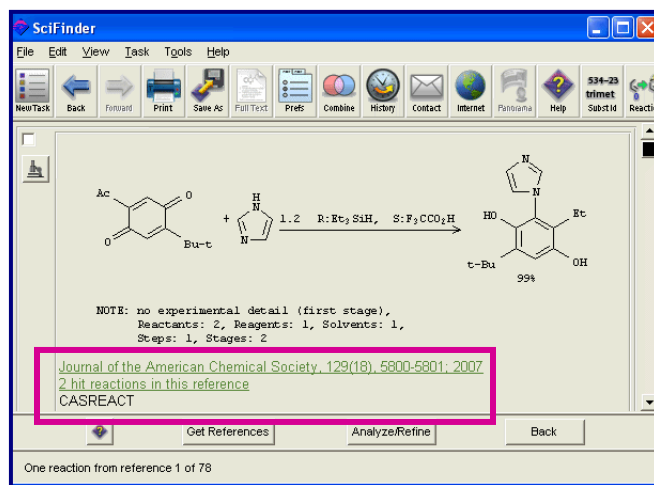
10. SciFinder retrieves 598 reactions that involve a biotransformation of p-quinone into substances that contain phenol. Yet, 598 reactions are too many to view one-by-one.



11. To evaluate your answer set quickly and easily, choose the viewing option that shows just one reaction for each reference. This option condenses the answer set to 78 references, each showing one representative reaction.

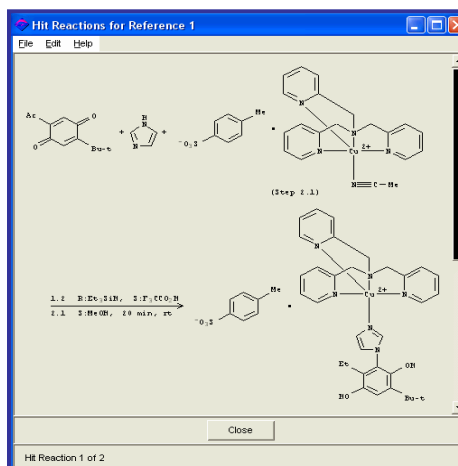




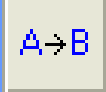

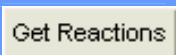

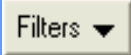
12. Now you can scan the list of 78 references to find one of interest, such as the one below, which contains two reactions. Note the links below the reference.



13. The first link allows you to view the abstract.

14. The second link enables you to view any of the associated reactions.



When you want to . . .	Click
Explore reaction information	
Explore reactions by structure diagram queries	
Assign reaction roles to structure drawing queries	
Explore reaction information	
Explore reactions by structure diagram queries	
Assign reaction roles to structure drawing queries	
Apply a Filter	

Contact CAS Customer Care at help@cas.org or call 800-753-4227 (North America) or 614-447-3700 (worldwide).