How to… Work with a Reaction Answer Set

Find all relevant reactions based on criteria you specify
Quickly retrieve relevant information from the world’s largest, publicly available reaction database. This guide provides an overview of the tools in SciFinder that you can use to evaluate and narrow even a large answer set. From there, a single click retrieves references associated with your reaction(s) of interest. For more detailed information and additional training resources, consult the online Help or visit www.cas.org/training/scifinder.

Reaction Search Results

These answers are grouped by Document and sorted by Number of Steps.

1. By default, answers are sorted from most to least relevant.
   - Click the drop-down arrow to select other sorting criteria.
   - Click the blue arrow to reverse the sort order.

2. Click Display Options to specify the number of answers displayed per page (15, 20, 25 or 50) and to select whether the Overview is opened or closed by default.

3. Hit structures are red.
   - Click the flask below a structure to see commercial source information for the substance.

Tip: See the Newest Records First
Accession Numbers start with the year that a record is added to the database and then are numbered sequentially (i.e., 2012:967458). Sort by this option to see the most recently added records first.

Continued
Click the box beside an answer number to select it. You can work with selected items several ways, such as saving them or getting references for them.

Mouse over a structure to access additional substance information and search options.

- Click the blue arrows to see related search options.
- Click the magnifying glass to see the Substance Detail in a separate window (called a Quick View).

Click the reference title to go to the Reference Detail page, or click the magnifying glass to open the reference information in a Quick View window.

Tip

PatentPak® offers immediate access to full text PDFs for indexed patents and their patent families from 11 major patent offices and includes page numbers for substances from covered patents. Learn more about this add-on product at http://www.cas.org/products/scifinder/patentpak.
Refine to Narrow the Answer Set

On the Refine tab, click a radio button to select a Refine by: option.

Below the radio buttons, further define the refine criteria.

Click Refine.

The answer set is narrowed based on the criteria you specified.

Tip: Steps vs. Stages
In many cases, a single step can have different stages. For example, stages occur when reagents are added sequentially, causing different reactions, but often without isolation of intermediates.
Group by Document or Transformation

1. **Group by: Transformation** groups single-step reactions based on transformation types so you can quickly evaluate synthesis options and preferred pathways.
   - Reactions can fall into more than one category
   - Unclassified single- and multi-step reactions (if any) appear at the end of the answer set

2. **Group by: Document** shows all the reference titles for the answer set, the total number of reactions associated with each title and a representative reaction for each title.

**Tip:** By default, answers are sorted by frequency. Click the drop-down arrow for other sort options.

**Tip:** You can run a Similar Reactions search when the link is available. This search uses the same reaction center and similar structural characteristics as your initial search. You select how narrow or broad you want the new search to be.

**Tip:** Click the number of reactions to see just those reactions.
Analyze to See Subsets of Information

1. Click the Analyze tab.
2. Click the drop-down arrow to select an Analyze by: option.

- Narrow results with bibliographic data using:
  - Author Name
  - Company-Organization
  - Document Type
  - Journal Name
  - Language
  - Publication Year

- Narrow results with reaction data using:
  - Catalyst
  - Number of Steps
  - Product Yield
  - Reagent
  - Solvent

- Narrow results based on the availability of actual experimental details using:
  - Experimental Procedure

Tip
The top ten subsets appear on the Analysis tab. When additional subsets are available, click the Show More button at the bottom of the tab to see a complete list or to select more than one subset.

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### General Procedure for the Reductive Cyclization: Carbazole (2a)

An Endeavor glass liner was charged with 2-nitrobenzyl alcohol and the liner was inserted into an Endeavor pressure reactor. To the liner was added Pd(OAc)\(_2\) (0.058 mmol) and 1,10-phenanthroline (0.058 mmol) in DMF (50 mL). The reactor system was sealed and purged three times with N\(_2\) followed by CO. The system was pressurized with CO (70 psi) and heated at 140 °C for 16 h. The mixture was cooled to rt. Assay yield of 2a was determined by HPLC analysis of the reaction mixture (94 mg, 95%). Carbazole 2a, yield (94 mg, 95%).

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Tip

Click 6 to see context-specific, online help.
Manage Your Searching


2. Click the Explore drop-down arrow to start a new references, substances or reactions search.

3. Click the Saved Searches drop-down arrow to access Saved Answer Sets, Keep Me Posted answer sets, and your search History.

4. Click SciPlanner to open the SciPlanner workspace.
   - SciPlanner is an interactive window where you can store and organize reference, substance, and reaction search results. Use it to gather information for a project, create a report, or export research to share with colleagues.
   - Three short videos about using SciPlanner are available the first time you open it and also in the online Help.

5. Click Save, Print or Export to open a dialog window and initiate each of these processes. See “How to... Print, Save and Export” for more information.

6. The breadcrumb trail shows each step in your current search history. Mouse over a step to see more information about it. Click a step to return to that part of the search.

7. Click Get References to retrieve references for part or all of your answer set.

8. Click the Tools drop down arrow to access Combine Answer Sets.

9. Click Send to SciPlanner to send selected answers to the SciPlanner workspace.