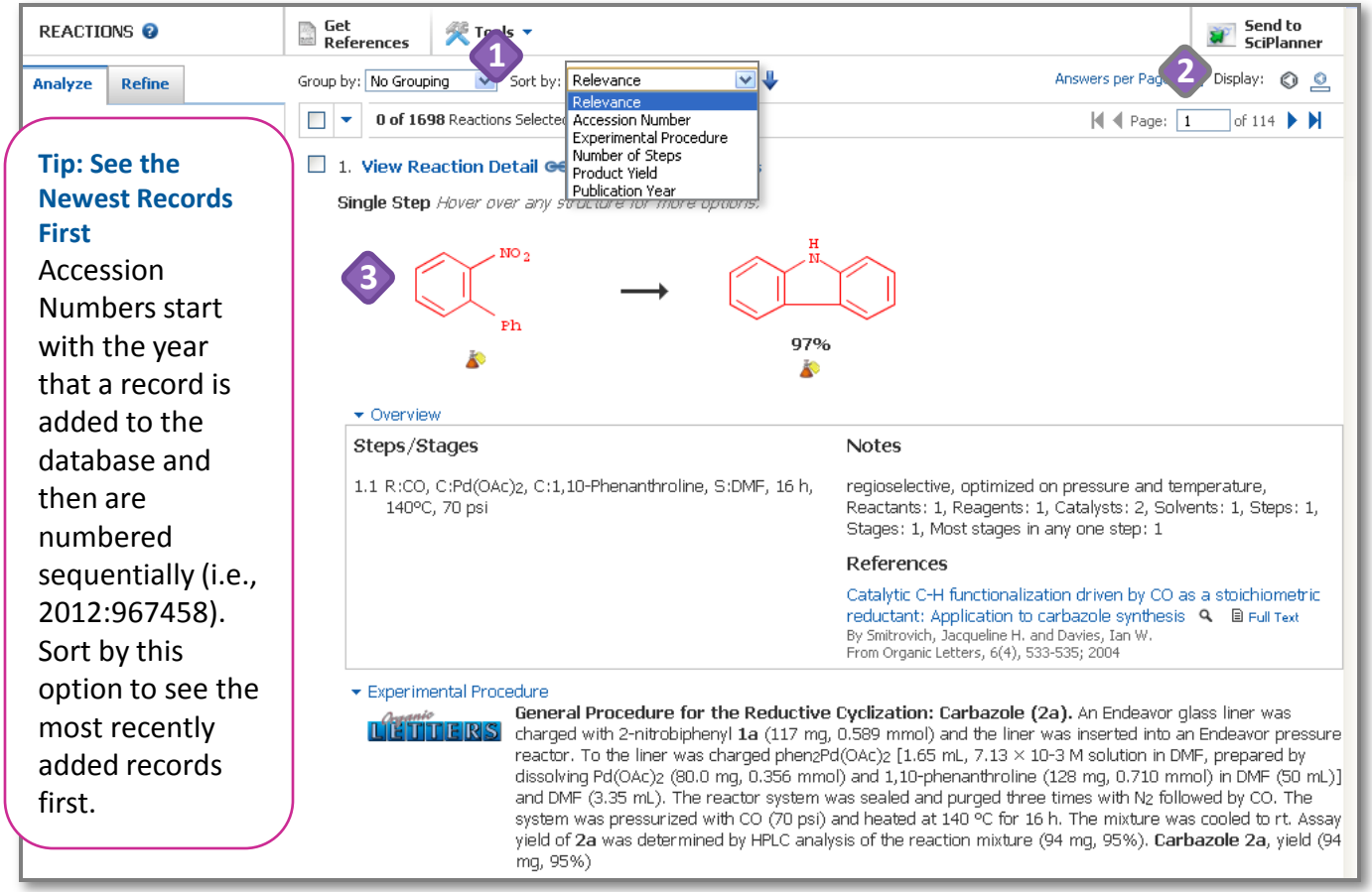
How to… Work with a Reaction Answer Set

SciFinder®

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



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.

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. Here, the reaction schema and the **Overview** are displayed, as indicated by the benzene ring with the rectangle under it.
   - Click the benzene ring to see only the reaction schema.
3. Hit structures are red.
   - Click the red flask below a structure to see supplier catalog information for that substance.

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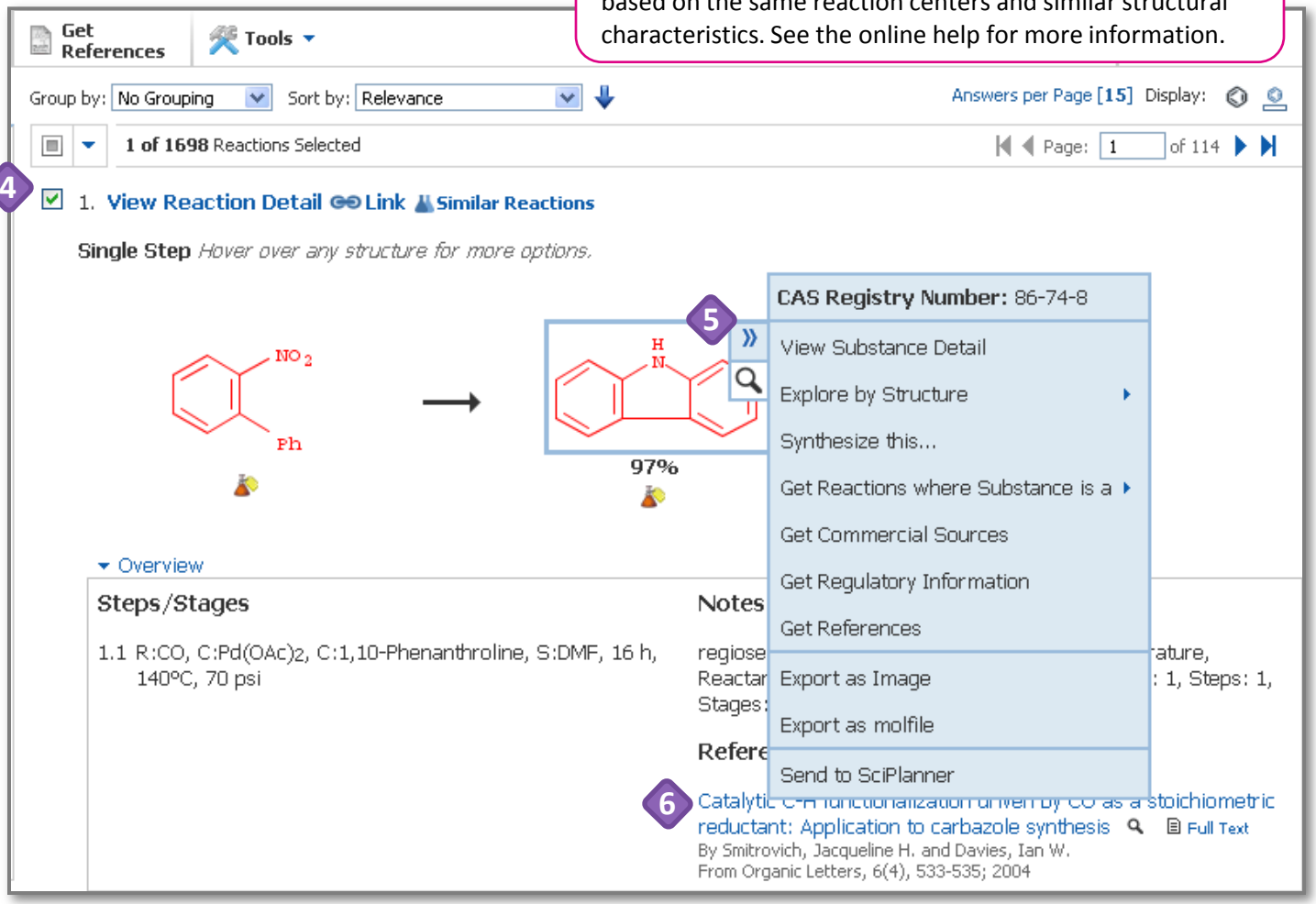
Tip
Click the **Similar Reactions** link to search for reactions based on the same reaction centers and similar structural characteristics. See the online help for more information.



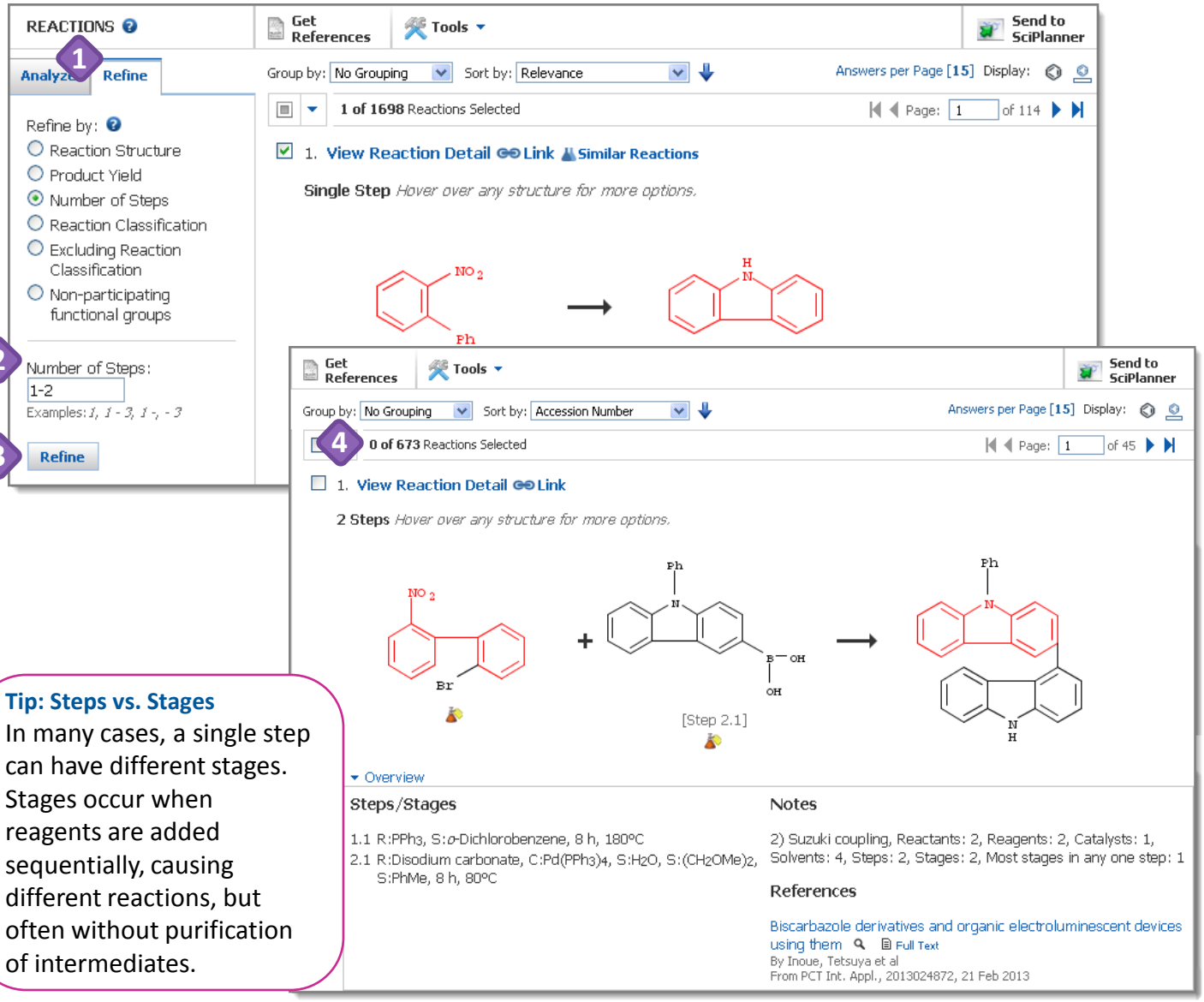
4 Click the box beside an answer number to select it. You can work with selected items several ways, such as saving them or getting references for them.

5 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 Details** in a separate window (called a **Quick View**).

6 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.

Refine to Narrow the Answer Set

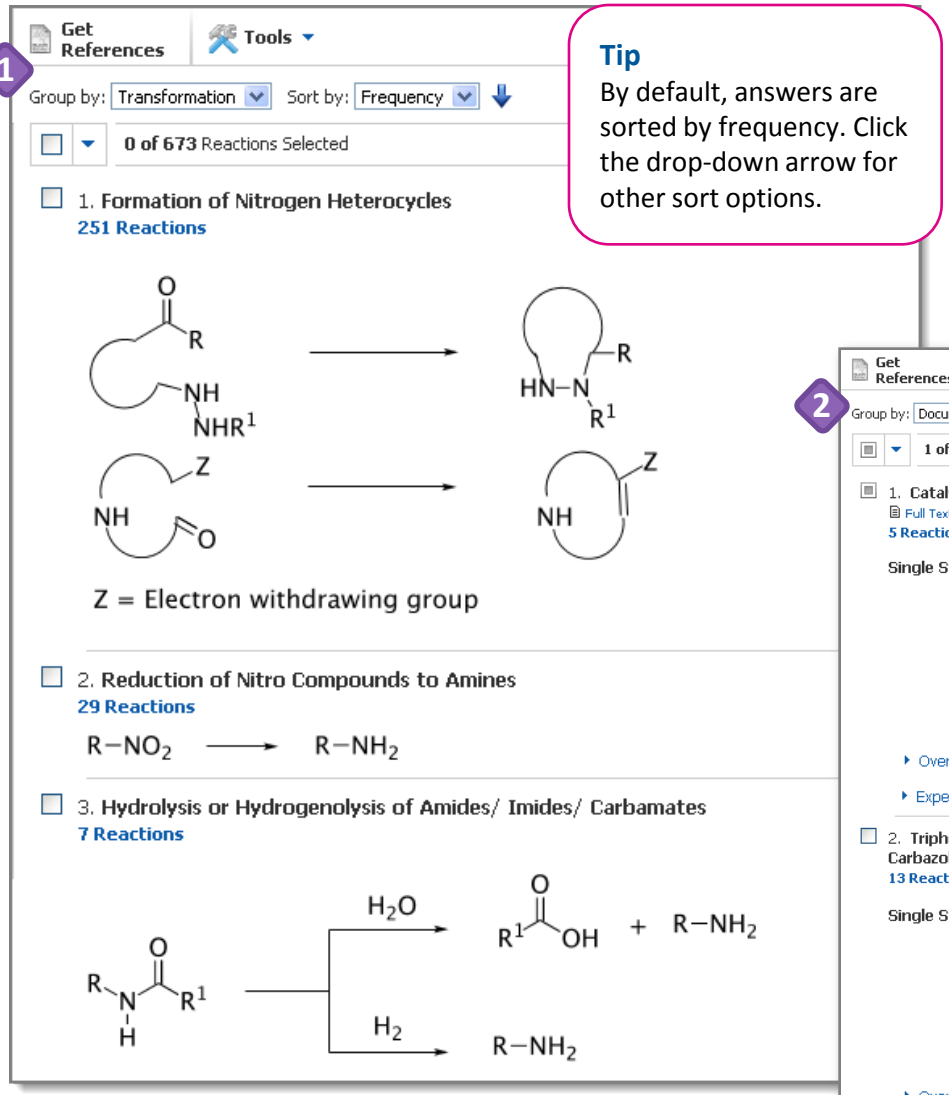


1. On the **Refine** tab, click a radio button to select a **Refine by:** option.
2. Below the radio buttons, further define the criteria by which you want to refine.
3. Click **Refine**.
4. The answer set is narrowed according to the criteria you specified.

Tip: Steps vs. Stages

In many cases, a single step can have different stages. Stages occur when reagents are added sequentially, causing different reactions, but often without purification of intermediates.

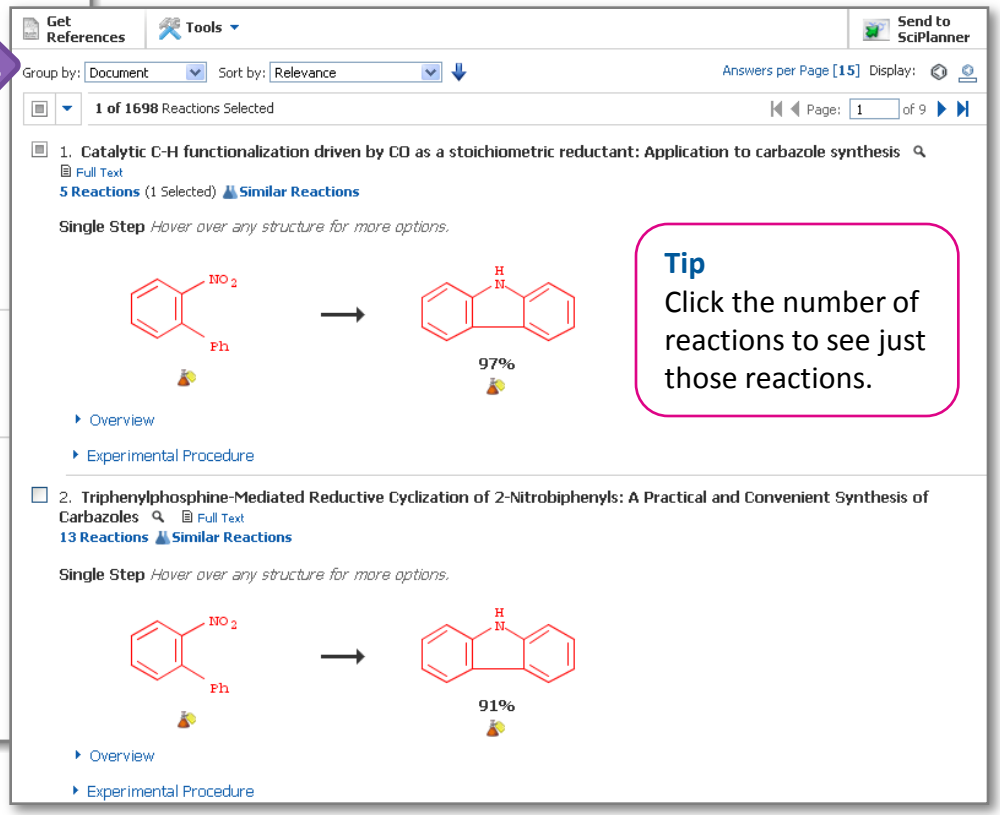
Group by Document or Transformation



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

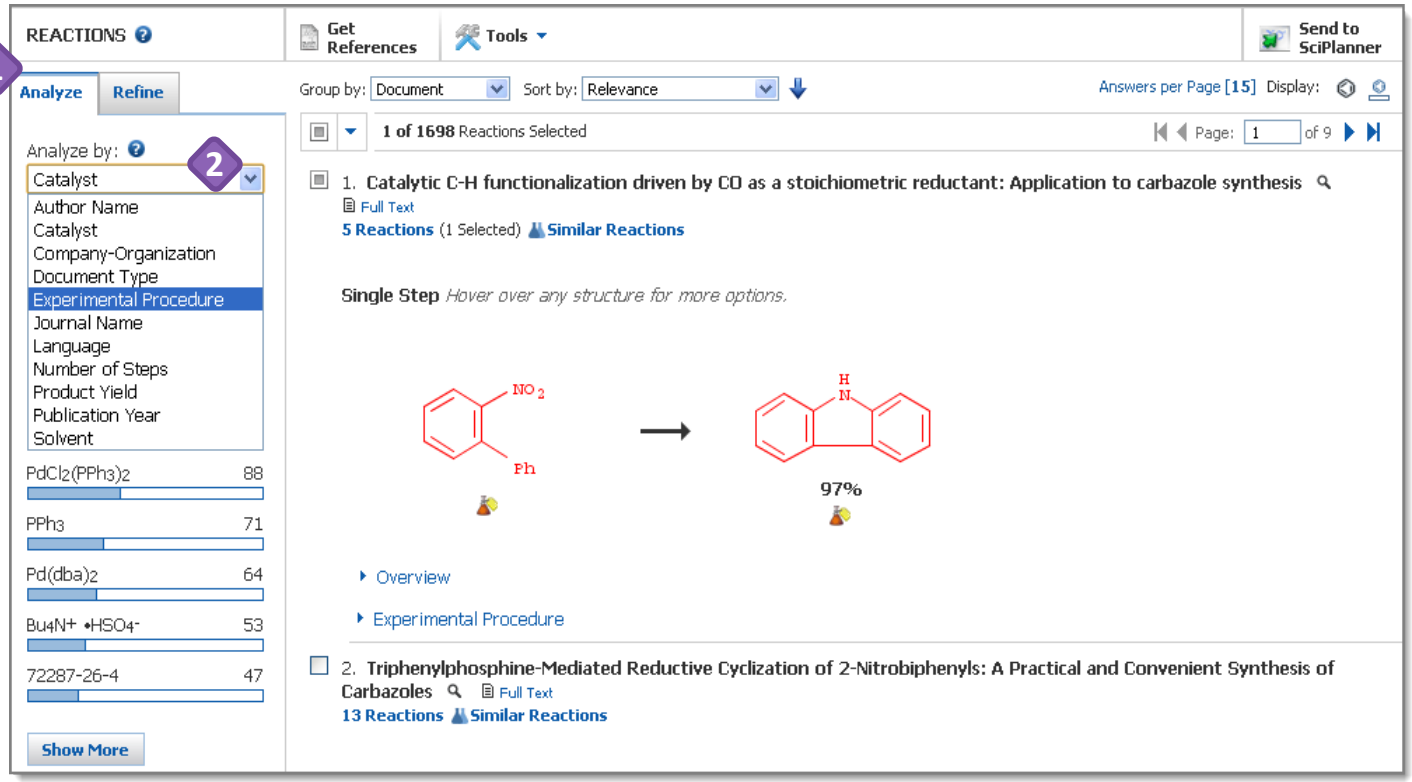
1. **Group by: Transformation** groups single-step reactions based on transformation types so you can quickly evaluate synthesis options and preferred pathways.
   - Reactions can fall into more than one category.
   - Unclassified single- and multi-step reactions (if any) appear at the end of the answer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

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



Tip
Click the number of reactions to see just those reactions.

Analyze to See Subsets of Information



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

- Narrow results with bibliographic data using:
  - **Accession Number**
  - **Company-Organization**
  - **Document Type**
  - **Journal Name**
  - **Language**
  - **Publication Year**
- Narrow results with reaction data using:
  - **Catalyst**
  - **Number of Steps**
  - **Product Yield**
  - **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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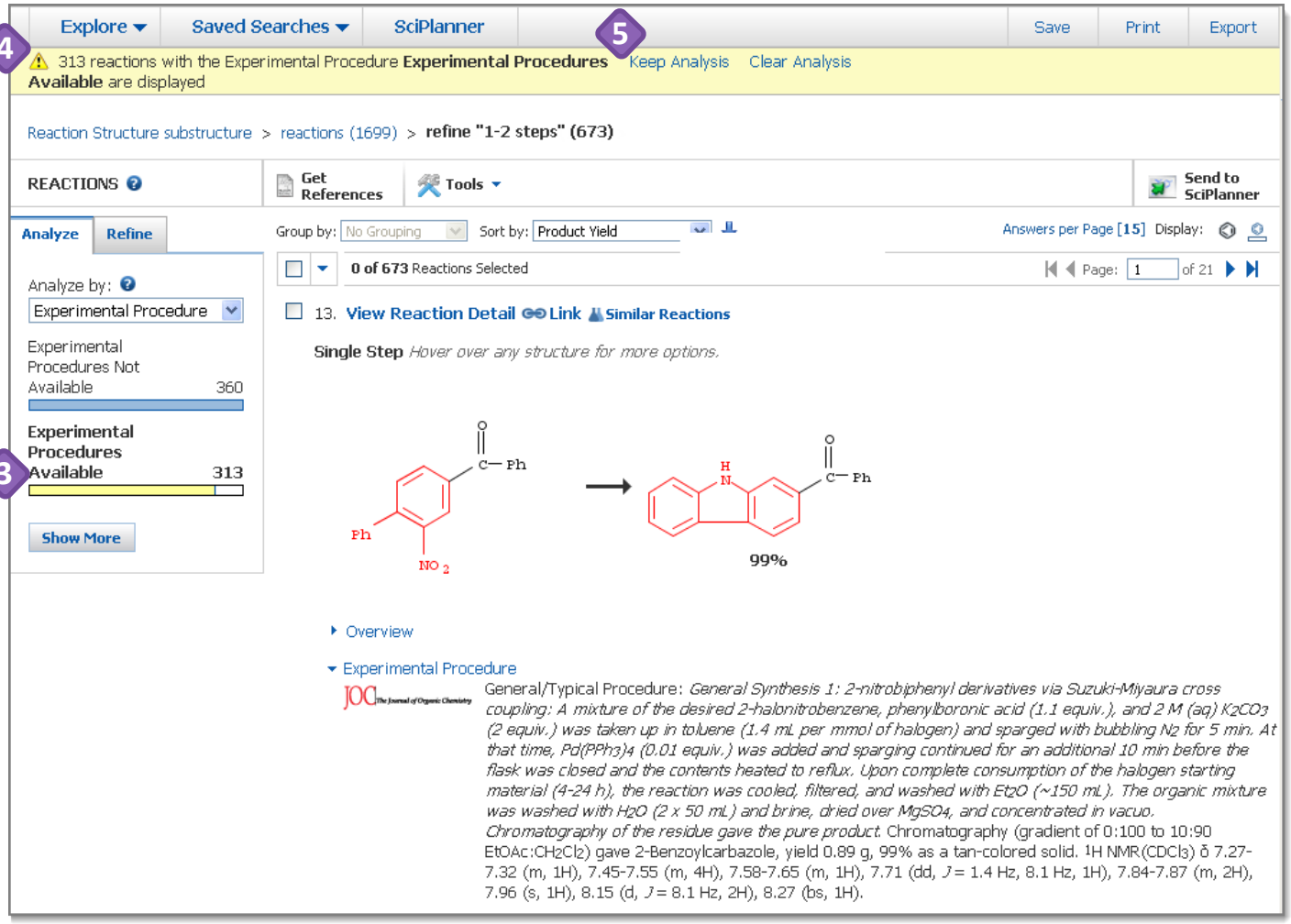


Your answer set is divided into subsets based on the analysis criteria.

3 Click an analysis bar to display only the answers in a subset. The selected bar turns yellow.

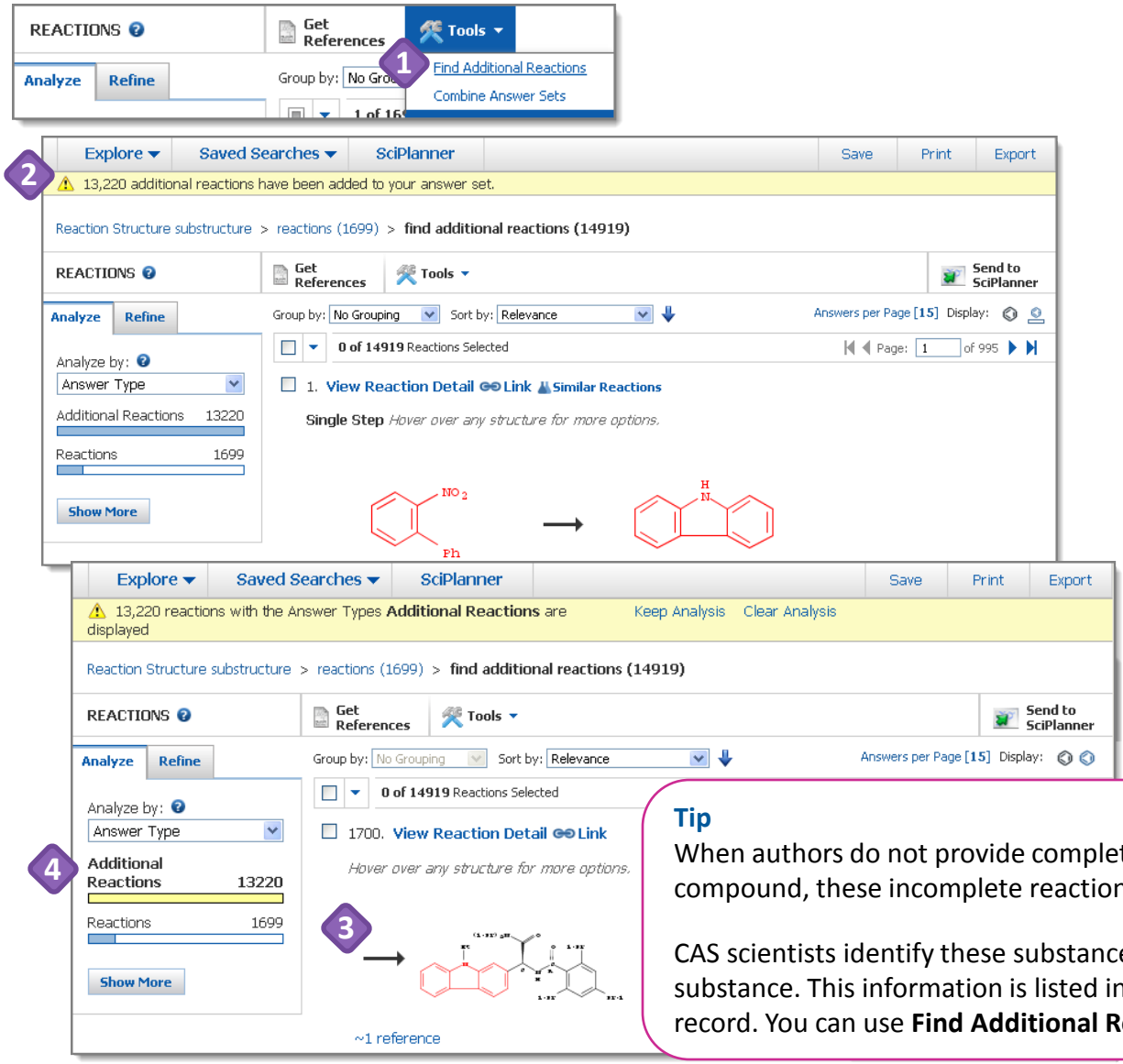
4 The yellow status message indicates the new display.

5 To replace the original answer set with the selected subset, click **Keep Analysis**.

- To return to the original answer set, click **Clear Analysis**.

Tip
Click ? to see context-specific, online help.

Find Additional Reactions



Find Additional Reactions takes advantage of the deep indexing in the CAplus[SM] bibliographic database. This feature identifies synthetically prepared substances in which the complete reaction information is not available but the reference indicates that the compound was synthesized. See the **Tip** for more details.

1. Click the **Tools** drop-down arrow and then click **Find Additional Reactions**.

2. The message in the yellow status bar shows the number of additional reactions that SciFinder found.
   - These reactions appear at the end of the answer set.

3. The synthesized compound is a product and appears to the right of the reaction arrow.

4. The default **Analyze** of the new answer set is **Answer Type**.
   - Select **Additional Reactions** to see only the newly added reactions.

Tip

When authors do not provide complete reaction information for synthesizing a compound, these incomplete reactions cannot be put into the CASREACT® database.

CAS scientists identify these substances and apply the Preparation CAS Role to the substance. This information is listed in the indexing of the CAplus bibliographic record. You can use **Find Additional Reactions** to see these synthesized substances.

Manage Your Searching

1. Access **Preferences** and **SciFinder Help** options: **Help**, **Training**, **What's New** and **Contact Us**.

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 **Find Additional Reactions** and **Combine Answer Sets**.

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