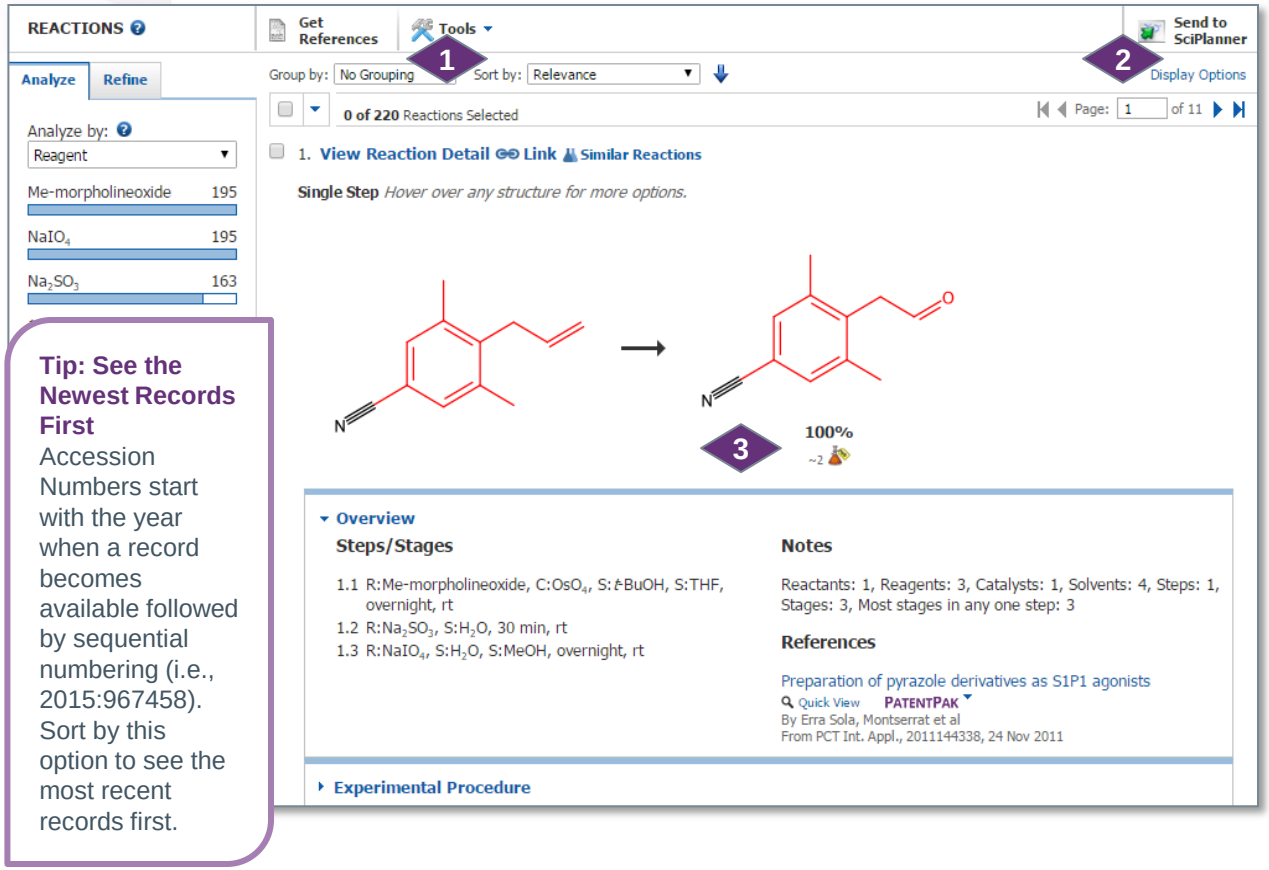
How to… Work with a Reaction Answer Set

Find all relevant reactions based on criteria you specify

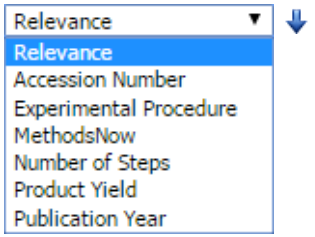
Quickly retrieve relevant information from the world's largest, publicly available reaction collection. This guide provides an overview of the tools in SciFinder® that you can use to evaluate and narrow even a large answer set. From there, a single click retrieves references associated with your reaction(s) 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 when a record becomes available followed by sequential numbering (i.e., 2015:967458). Sort by this option to see the most recent records first.

1. By default, answers are sorted from most to least relevant.
   - Click the blue 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.

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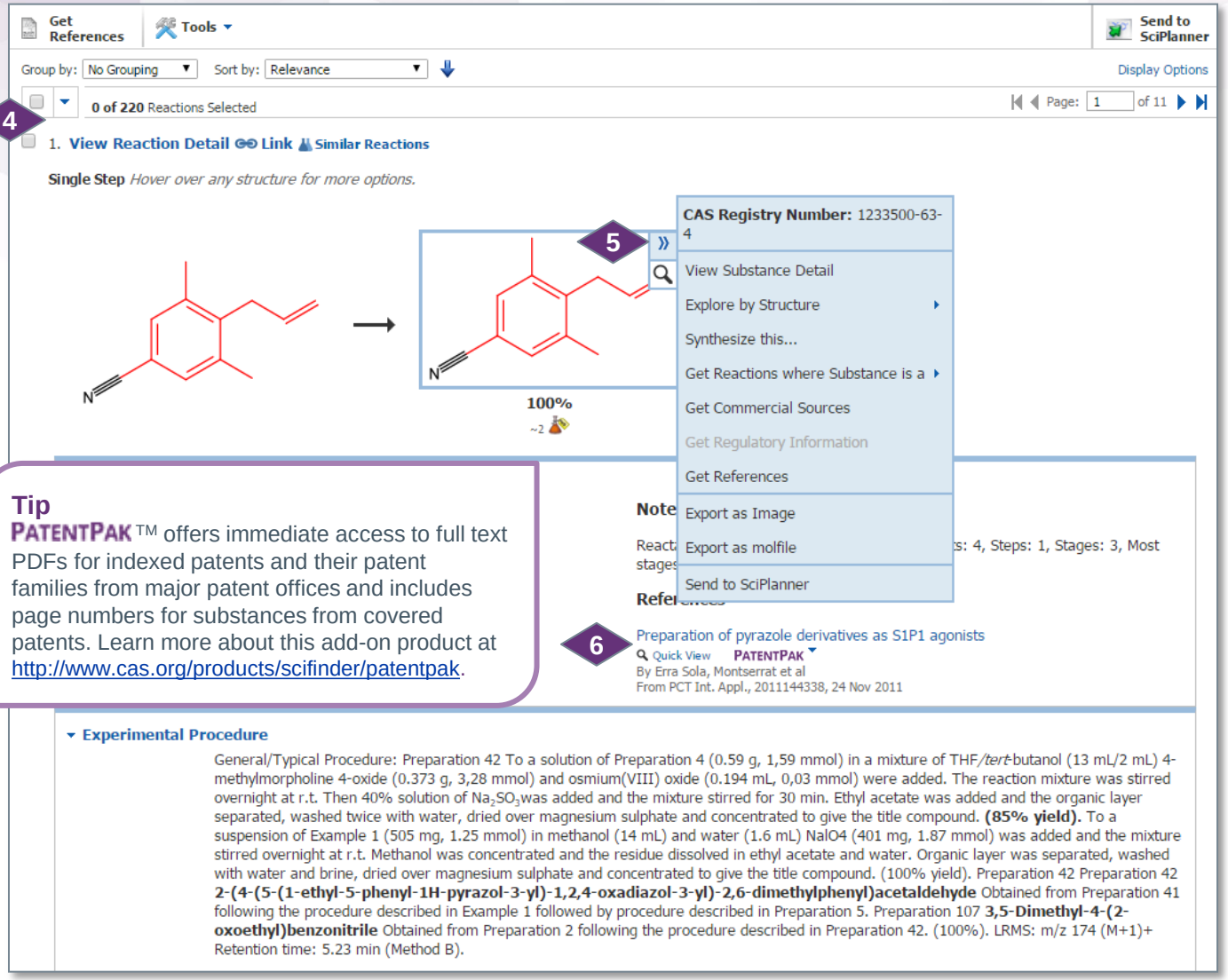

4 Click the box beside an answer number to select it. You can work with selected items several ways, such as saving them or getting references for them.

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 Detail** 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.

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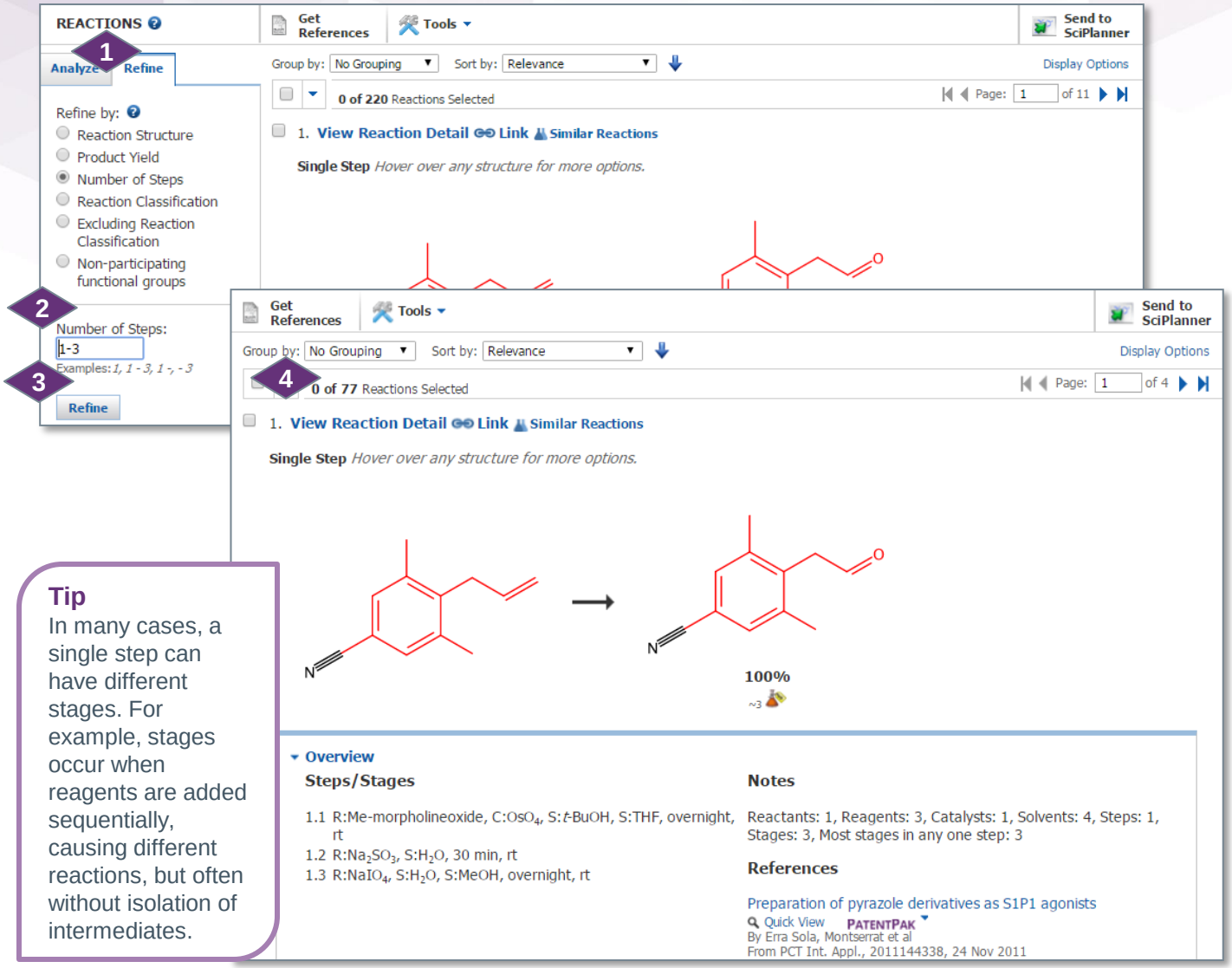
Refine to Narrow the Answer Set



Tip
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.

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

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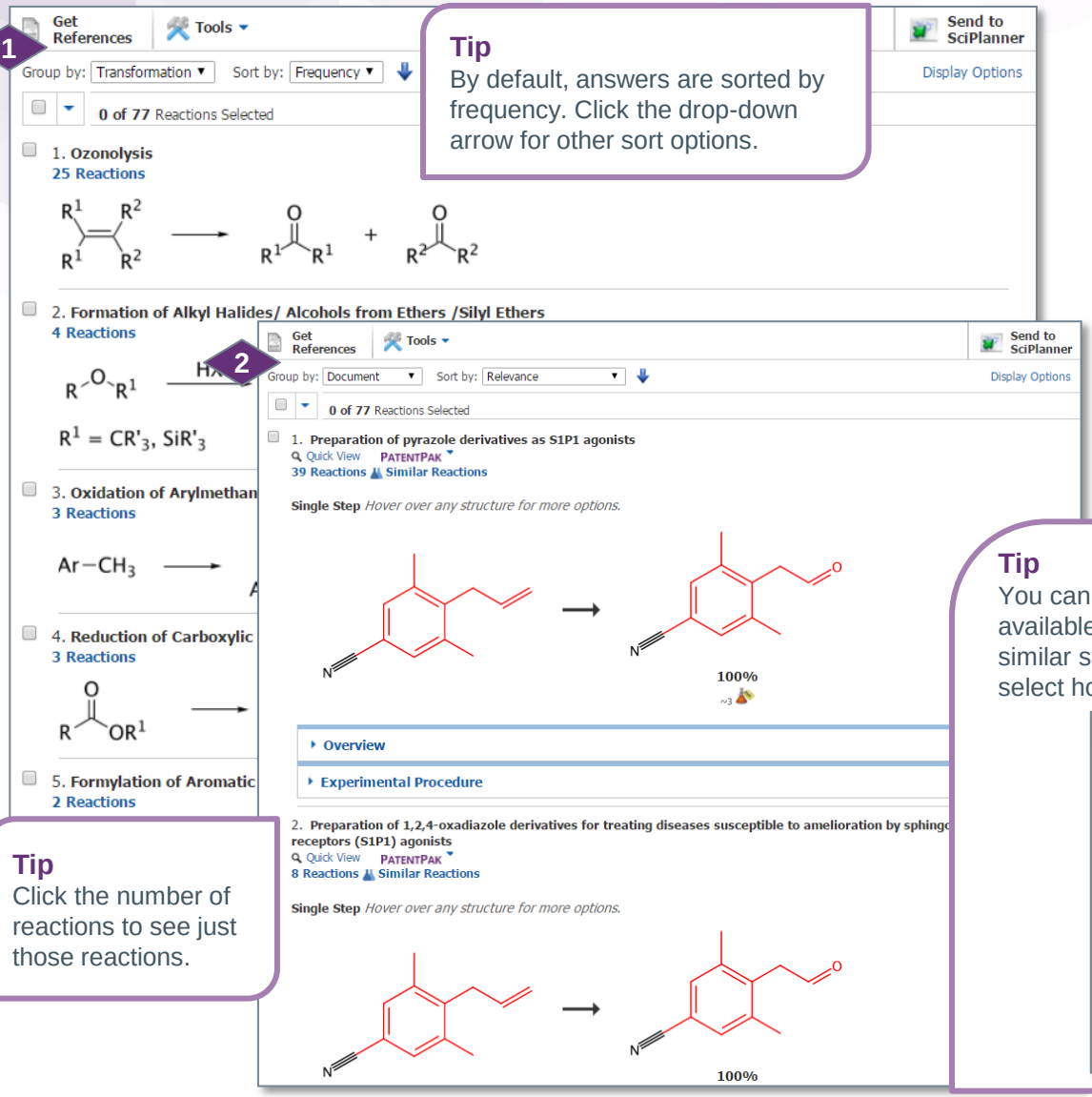
Group by Document or Transformation



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

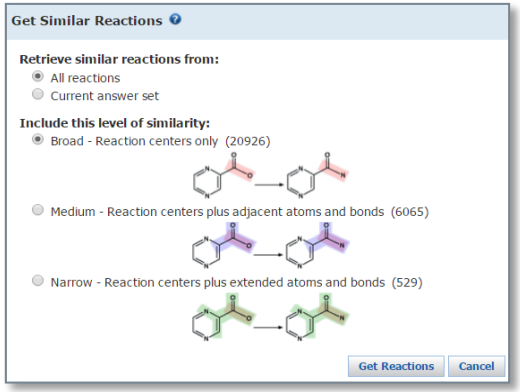
Tip
Click the number of reactions to see just those reactions.

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
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.



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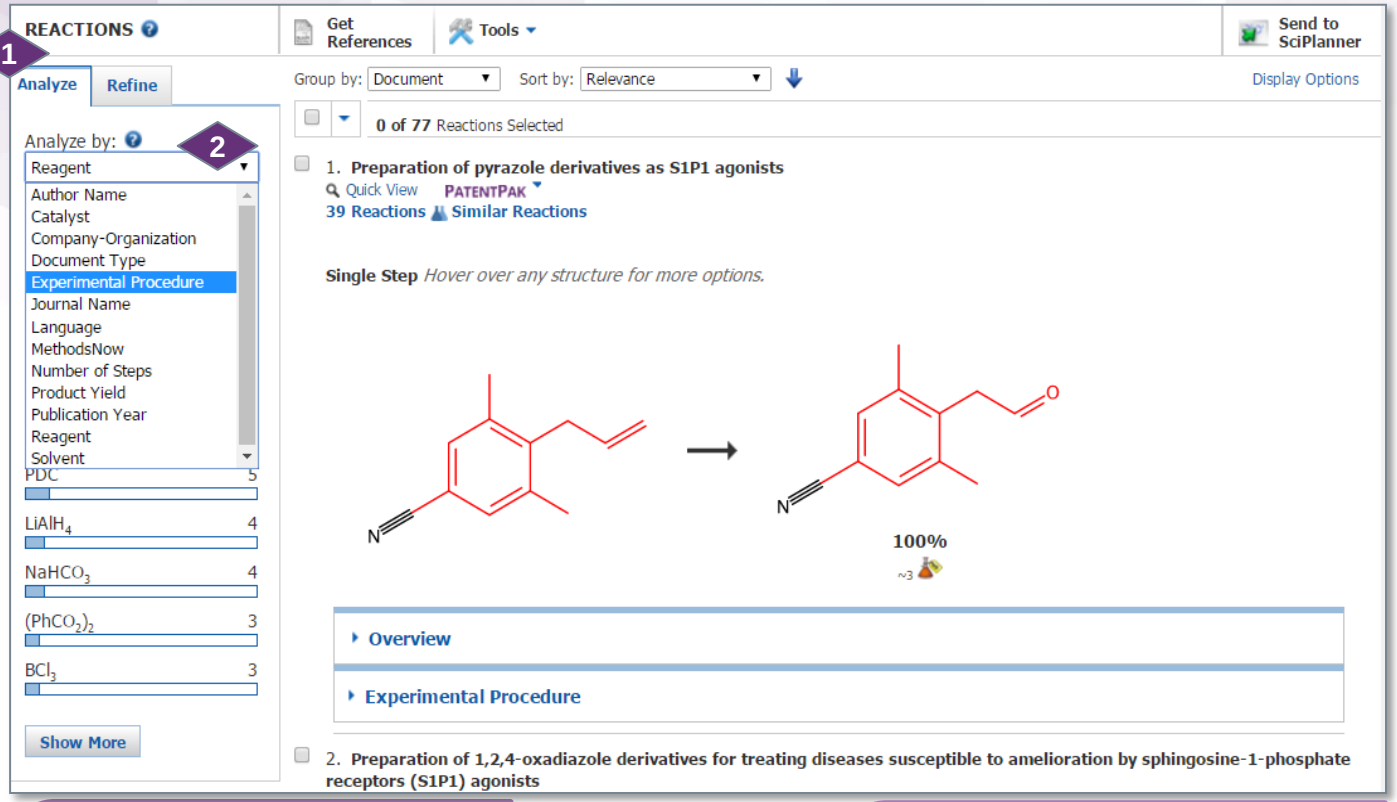
Analyze to See Subsets of Information



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**
- **MethodsNow**

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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.

Tip
MethodsNow™ features step-by-step instructions for analytical and synthetic methods. This add-on product displays experimental details in easy-to-read table format and includes materials, instrumentation, conditions and more.

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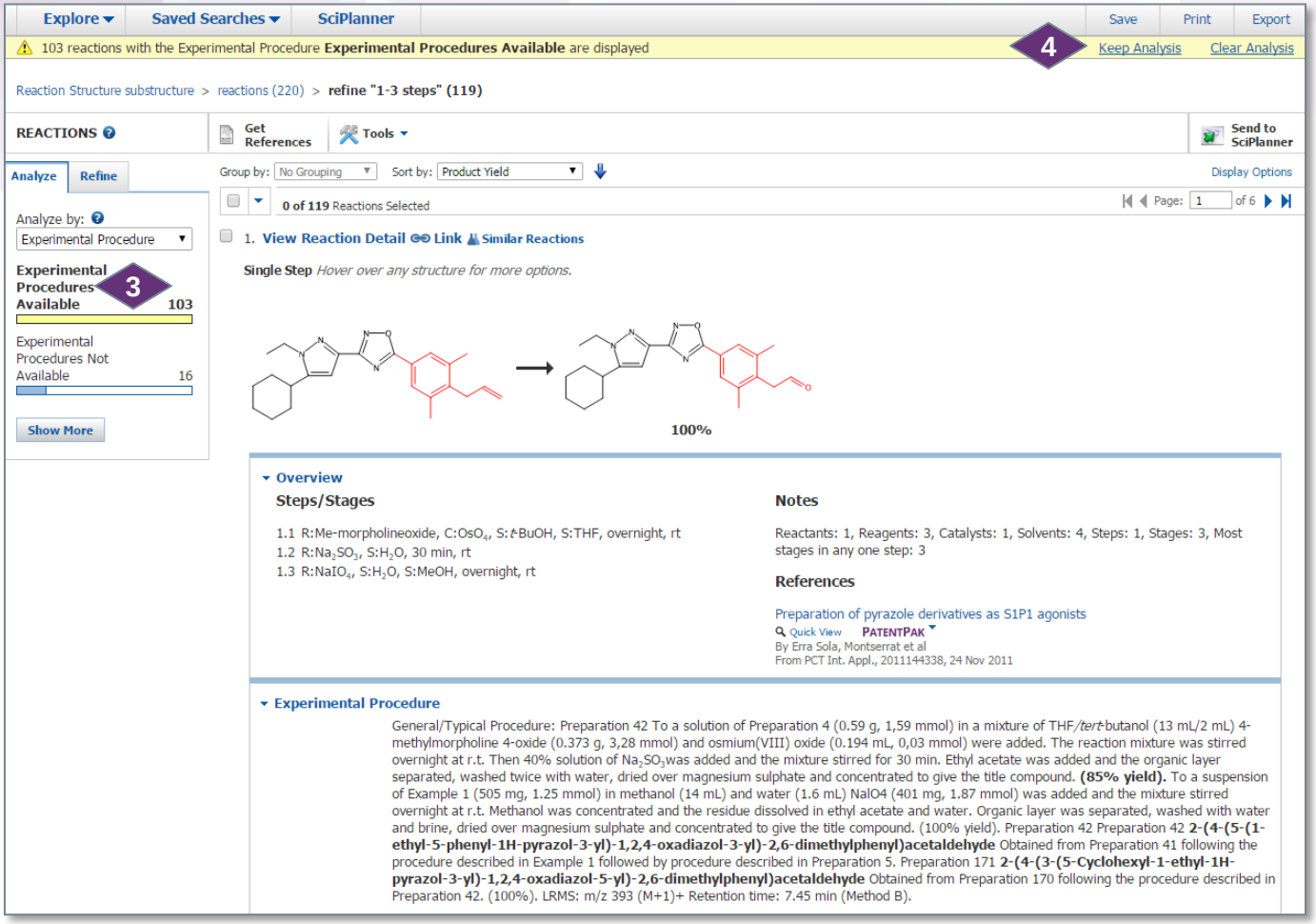


Your answer set is divided into subsets based on the analysis criteria.

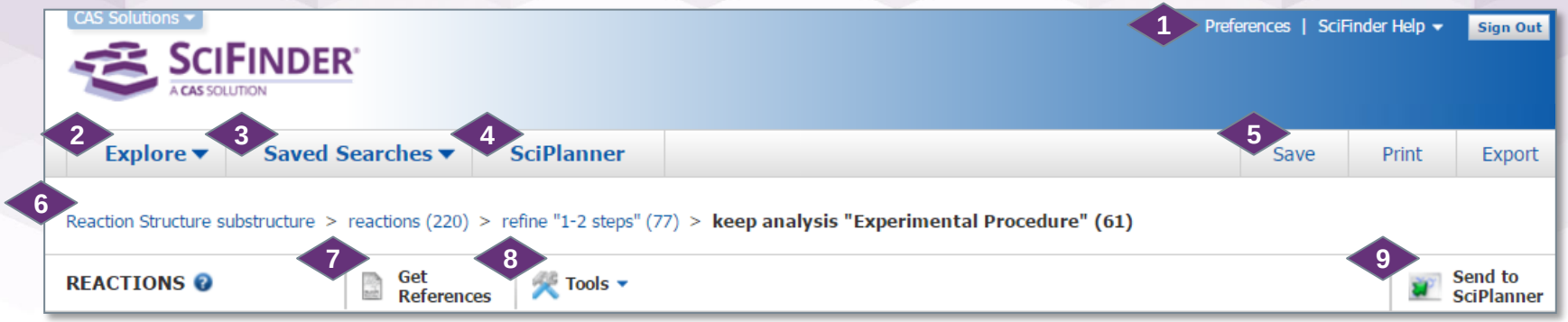
3 Click an analysis bar to display only the answers in a subset. The selected bar turns yellow.

4 The yellow status message indicates the new display.

- 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 access context-specific online help.

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 navigation 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.

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