SciFinder® SciFinder Training Materials

On-demand SciFinder training resources are available at CAS web site:
http://www.cas.org/training/scifinder

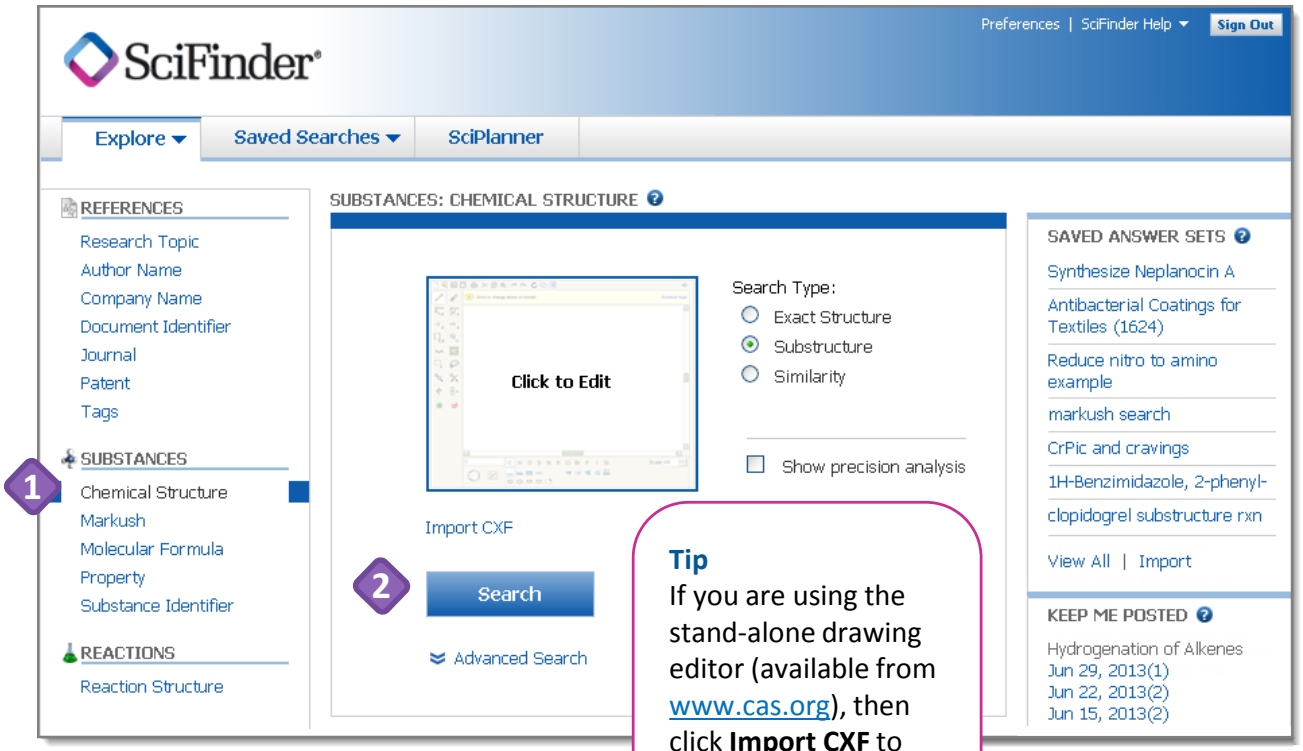
How to Create a Substance Answer Set

SciFinder®

Select among five search techniques to find substances

Since substances can be described by multiple names or other characteristics, SciFinder gives you the flexibility to approach a substance search from different starting points, depending on your research needs. No matter how you begin, your results are from the CAS REGISTRY℠ database, the most trusted and comprehensive collection of publicly available chemical substances in the world. Refer to "How to … Work with Substance Answer Sets" for ways to evaluate the results and hone in on the most relevant answers. To learn more about using SciFinder, consult the online Help or visit www.cas.org/training/scifinder.

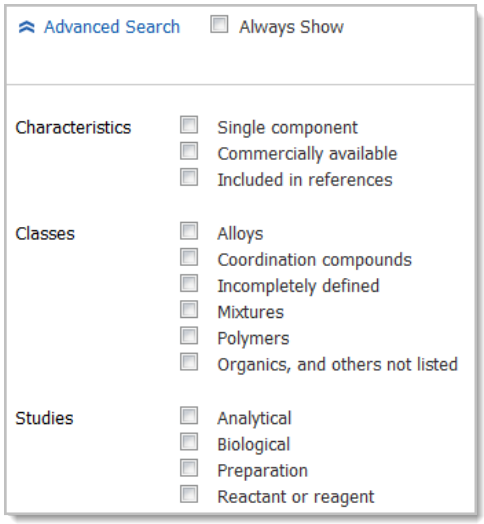
Types of Substance Searches



Tip
If you are using the stand-alone drawing editor (available from www.cas.org), then click **Import CXF** to upload the structure.

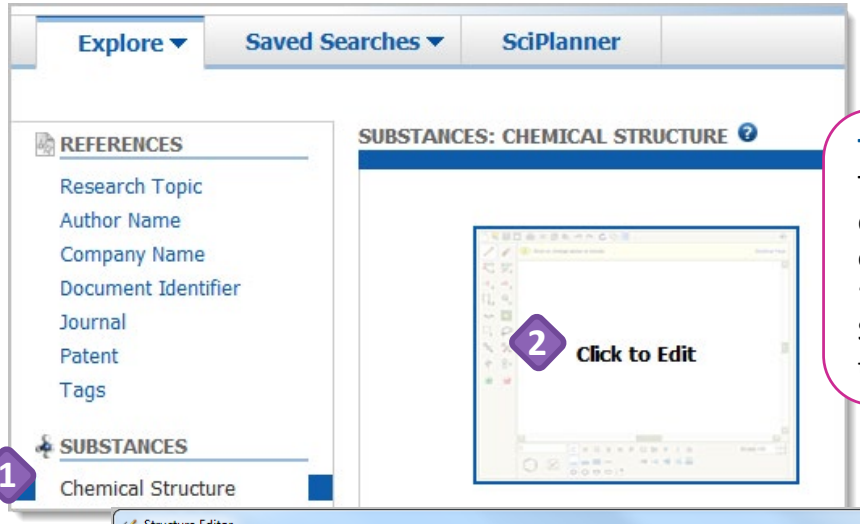
1. On the **Explore** tab, under **SUBSTANCES**, you can search by any of the five options.

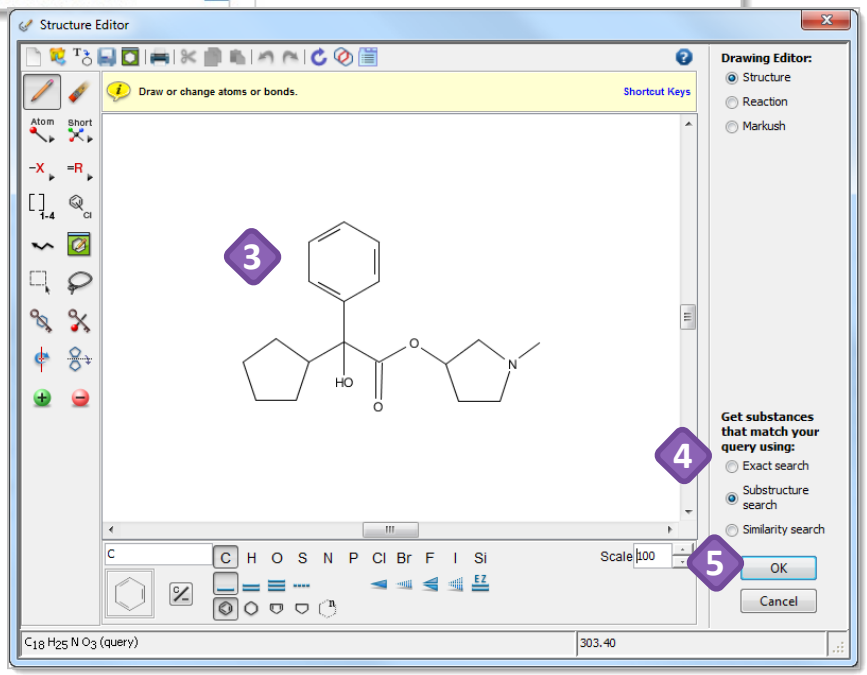
2. Click **Advanced Search** to see criteria that you can add to a search to make it more specific:



- These search limiters are available as part of the **Refine** and **Analyze** functions, so you can also apply them later in your search process.

Search by Chemical Structure



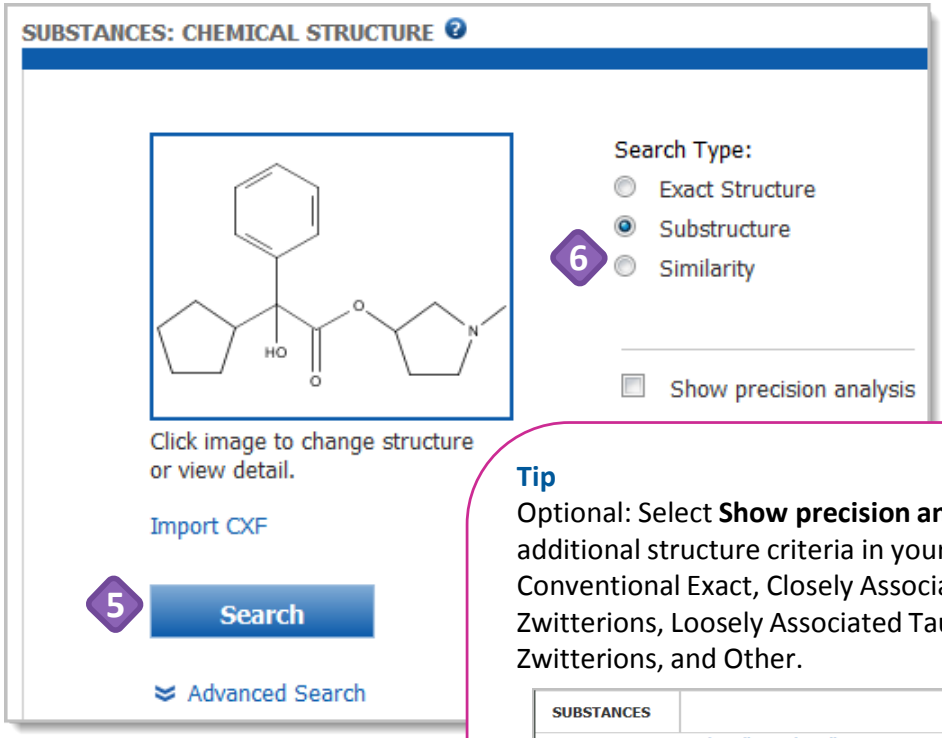


Tip
To learn about structure drawing, refer to the online help or the "Introduction to the SciFinder Drawing Editor" tutorial on cas.org.

1. Select **Chemical Structure** (the default).
2. Click the picture of the structure drawing window to launch the **Structure Editor**.
3. Draw your structure.
4. Specify the type of structure search.
5. Click **OK** to transfer the structure and type of search to the search page.

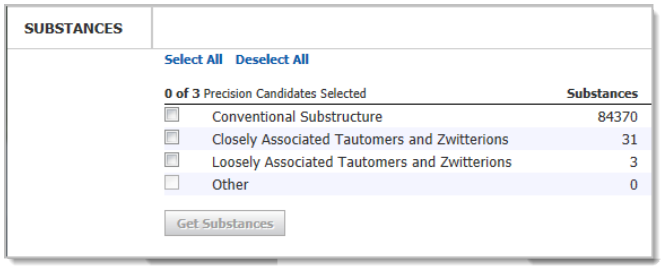
Continued

SELECT…	IF YOU WANT TO RETRIEVE…
Exact Search	The specific structure as drawn in the query, including: • Stereoisomers • Salts and mixtures • Polymers with one exactly matching monomer • Isotopes • Tautomers
Substructure Search	The structure as drawn or as part of a larger molecule in which there is: • Substitution at open positions • Additional ring fusion
Similarity Search (Queries cannot include variable groups, repeating groups, or variable attachment positions)	Similar chemical structures containing: • Positional isomers • Different or fewer substituents • Different ring systems



Tip

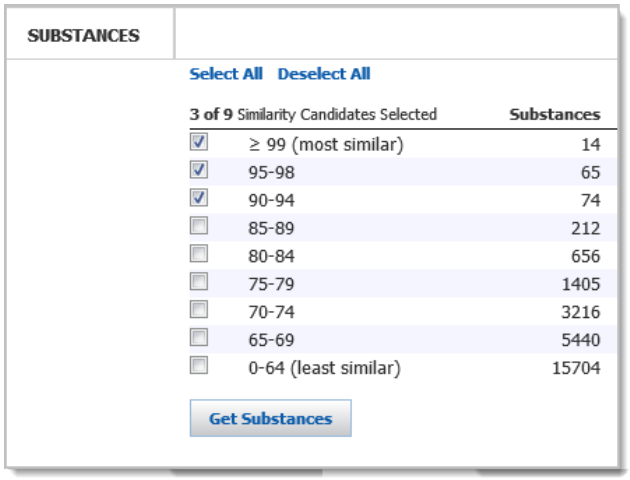
Optional: Select **Show precision analysis** to include additional structure criteria in your search: Conventional Exact, Closely Associated Tautomers and Zwitterions, Loosely Associated Tautomers and Zwitterions, and Other.



Precision Analysis Window (Unrelated Example)

5 Click **Search** to retrieve the answers that meet your query requirements.

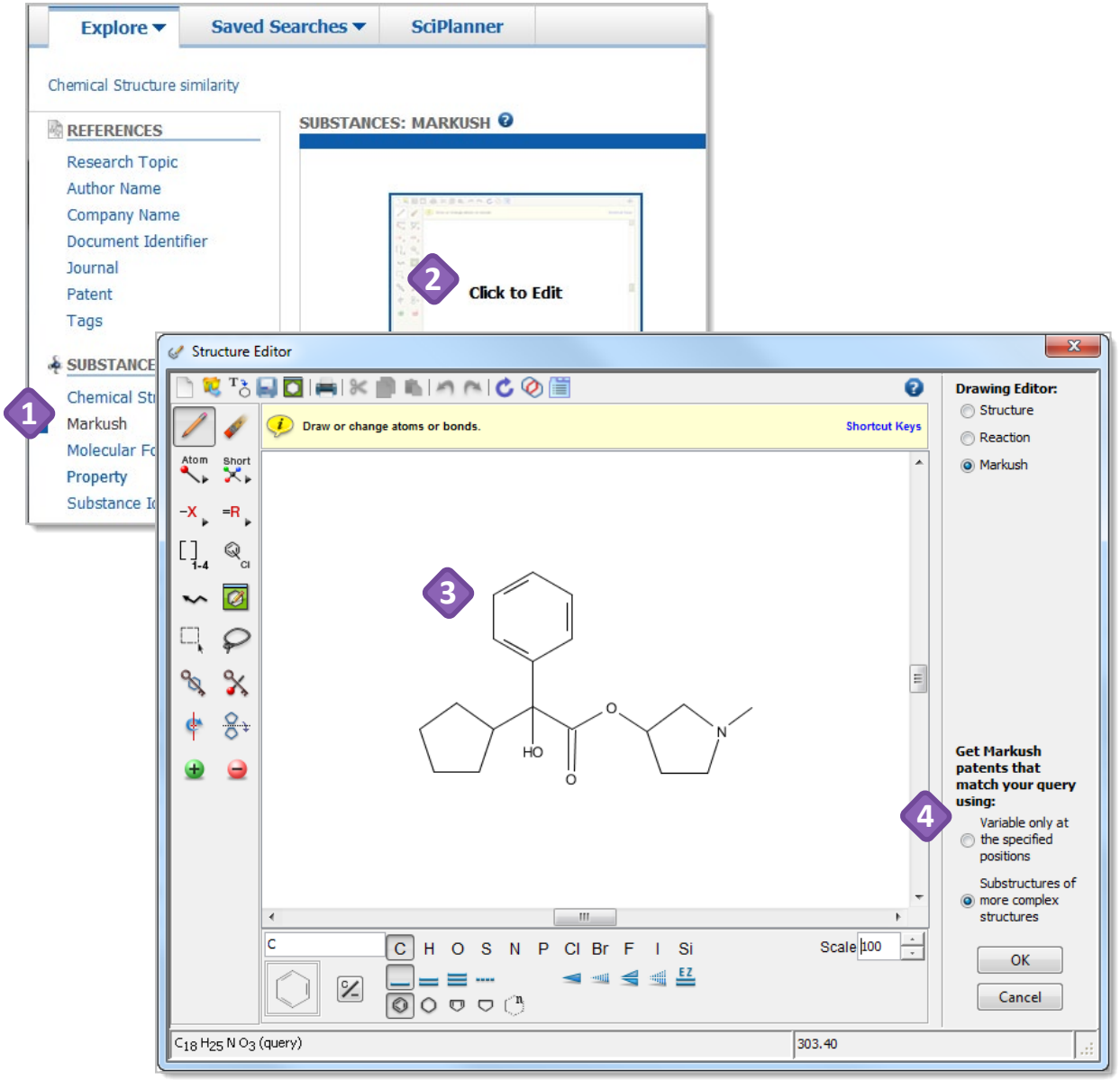
6 For **Similarity** searches, after you click **Search**, you will see a **Similarity Candidates** window. To select the degree(s) of similarity for your answers, check the box(es) of interest. Then, click **Get Substances**.



Now what?

After you click **Search**, SciFinder will retrieve the answers that meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with a Substance Answer Set."

B. Search by Markush Structure

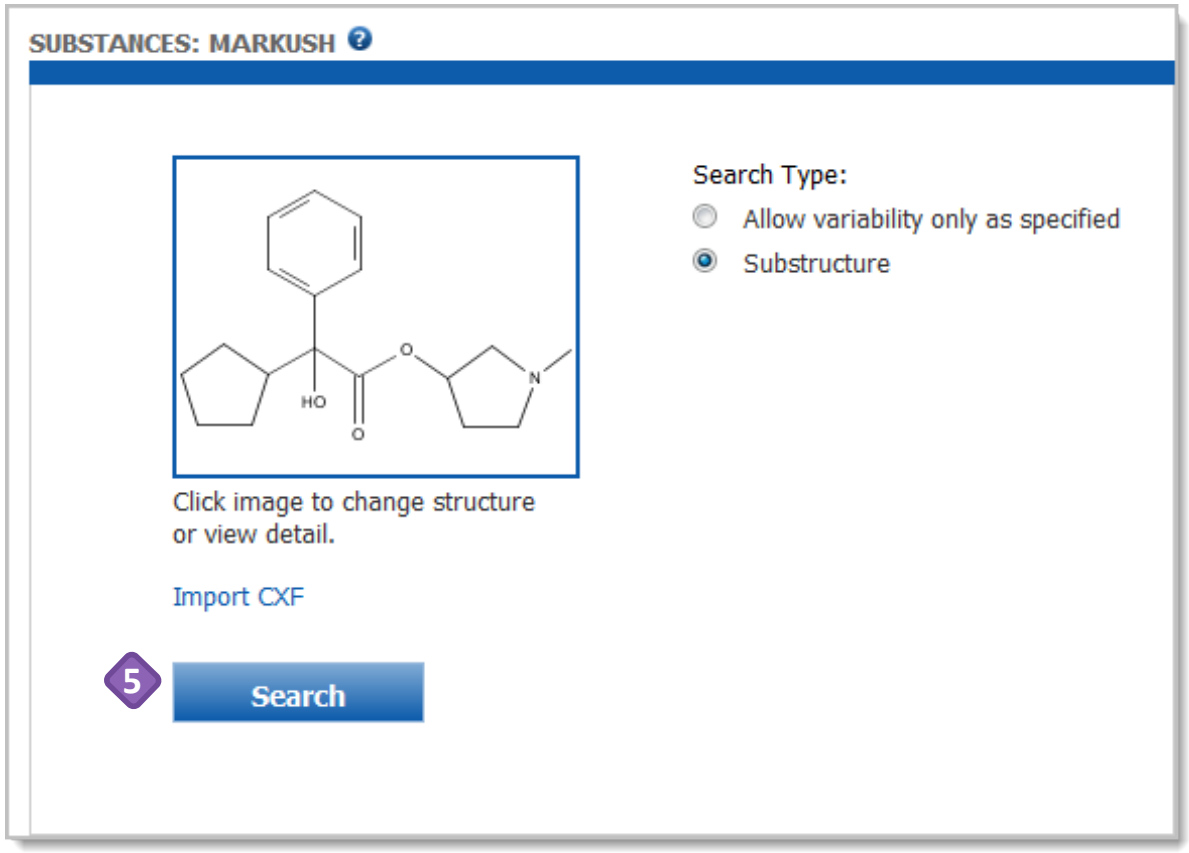


Search by **Markush** to find Markush structures in patents. You begin with a structure search and retrieve patent references that contain those Markush structures.

1. To begin, click **Markush**.
2. Click the picture of the structure drawing window to launch the **Structure Editor**.
3. Draw your structure.
4. Specify the type of structure search and then click **OK** to transfer the structure and type of search to the search page.

SELECT…	IF YOU WANT TO RETRIEVE…
Variable only at the specified positions	Structures in which substitution is only allowed where it is specifically indicated by R-groups or other variable atom or bond features
Substructure of more complex structures	Structures in which substitution is allowed on all positions where it is not explicitly blocked

Continued



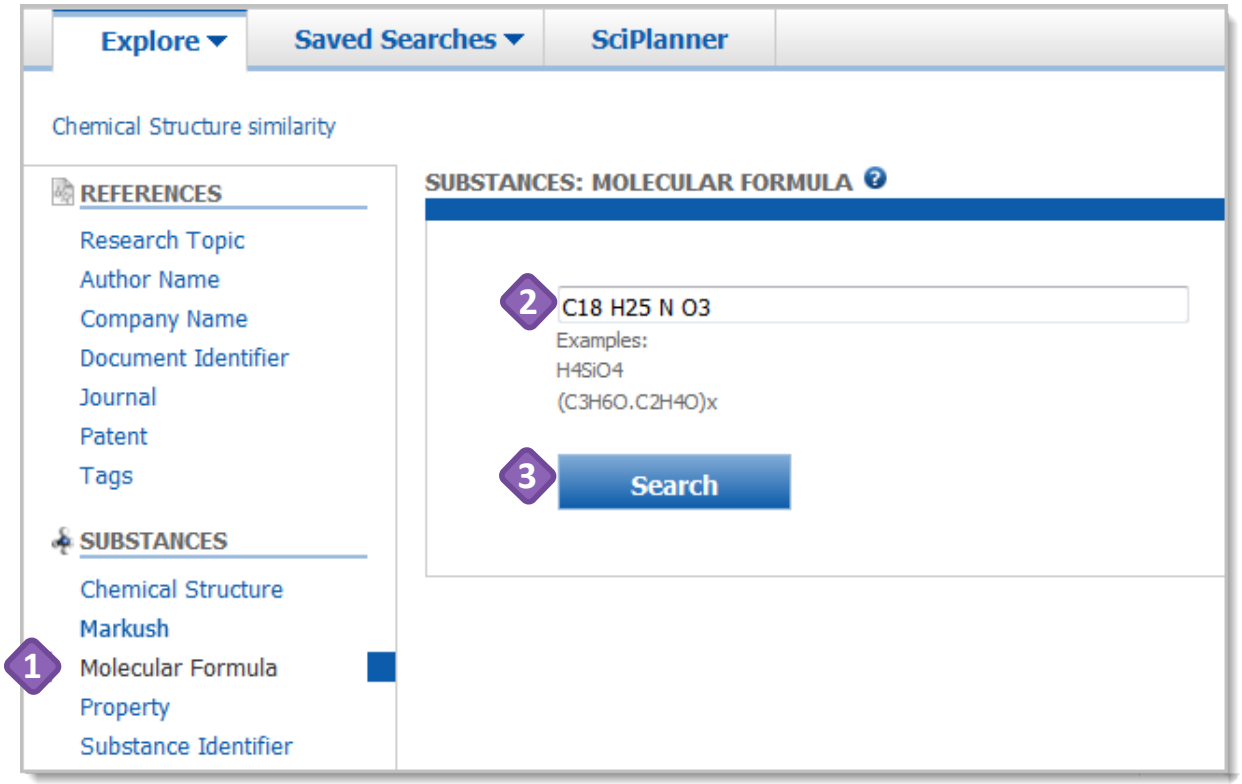
5 Click **Search** to retrieve the answers that meet your query requirements.

SciFinder is useful for a preliminary patentability or freedom to operate search. For a thorough patentability search, consult a patent attorney or informational professional.

Tip
Markush searching is a great way to extend a structure search, especially if you did not find any substances with a structure search and are interested in patentability.

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with a Reference Answer Set."

C. Search by Molecular Formula



1. To begin, click **Molecular Formula**.
2. Enter the molecular formula into the query box.
3. Click **Search.**

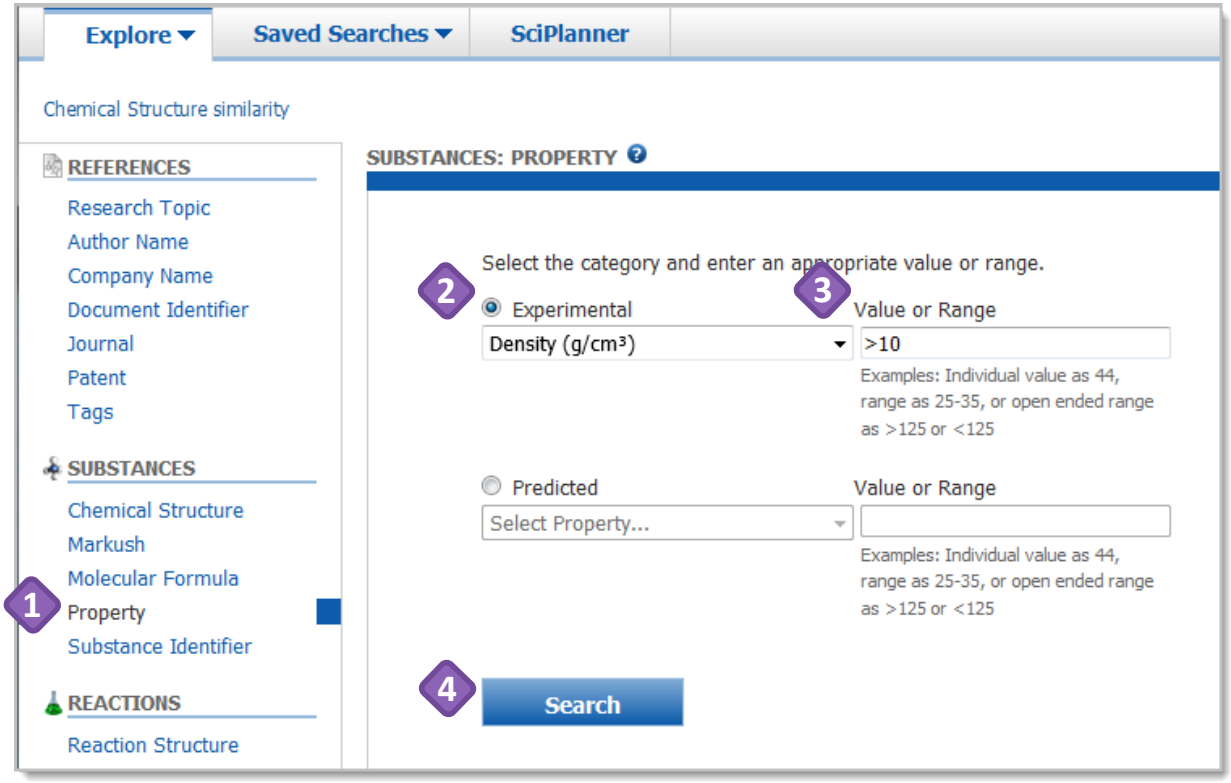
Tip
Click a ? to access context-specific online help. If you click it next to Molecular Formula, the help message provides many examples about how to search Molecular Formulas for polymers, salts, and structure repeating units.

Molecular Formula Query Guidelines

- Specify the full molecular formula, including the hydrogens (Hill Order not required)
- Separate each element symbol and its count with a space
- Capitalize the first character for multi-character symbols, and use lower case for the second letter (i.e., Si, Cl, Fe)
- You can search two isotopes: D = deuterium and T= tritium

Now what?
Molecular Formula searches often retrieve many isomeric substances and it is necessary to narrow answers. To learn about working with the answers, please see the companion document titled, "How to… Work with a Substance Answer Set."

D. Search by Property

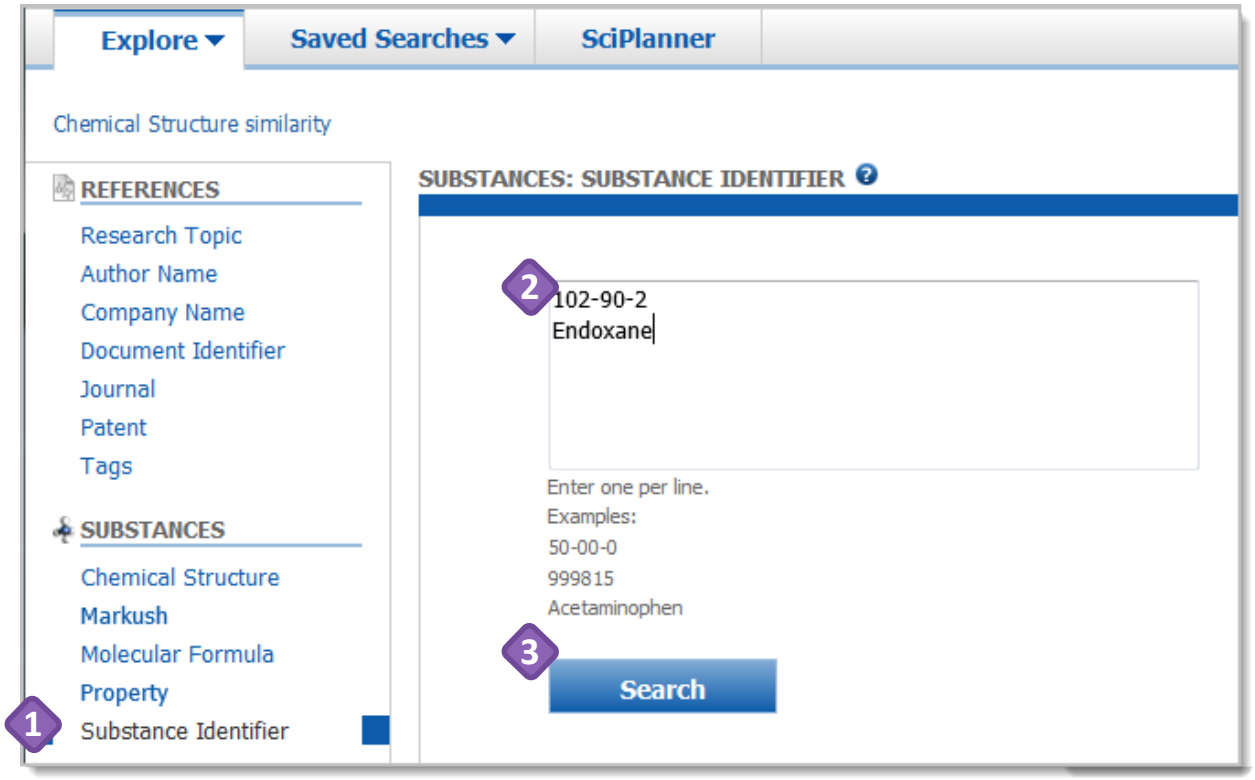


1. To begin, click **Property**.
2. Click the appropriate radio button to select either **Experimental** or **Predicted** property. Next, click the drop-down menu and select the specific type of property you want to search.
3. Enter the **Value or Range**.
4. Click **Search** to retrieve the answers that meet your query requirements.

Tip
If your property search results in a large answer set, you can narrow it by specifying additional criteria using **Refine** or **Analyze**.

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with a Substance Answer Set."

E. Search by Substance Identifier



1. To begin, click **Substance Identifier**.
2. Enter up to 25 substance identifiers, one per line, in the query box.
   - A substance identifier can be a CAS Registry Number® or a chemical name.
   - Simple chemical names, trade names, abbreviations and common names often result in relevant answers.
3. Click **Search** to retrieve the answers which meet your query requirements.

Tip
For complex, systematic names such as some IUPAC names, consider searching by the chemical structure. It is often easier to match a structure rather than all of the chemical nomenclature and punctuation exactly as it is entered into the database.

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with a Substance Answer Set."

Manage Your Searching

1. Start a new references, substances or reactions search.
2. Access **Saved Answer Sets**, **Keep Me Posted** automated alert results, and your search **History**.
3. Open the **SciPlanner** interactive workspace where you can organize your reference, substance and reaction search results.
4. Access **Preferences** and **SciFinder Help** options: **Help**, **Training**, **What's New**, and **Contact Us**.

Tip: Other Ways to Create a Substance Answer Set

- You can also create a substance answer set by starting with a reference search. After you get a reference answer set, click the "**Get Substances**" icon at the top of the page.

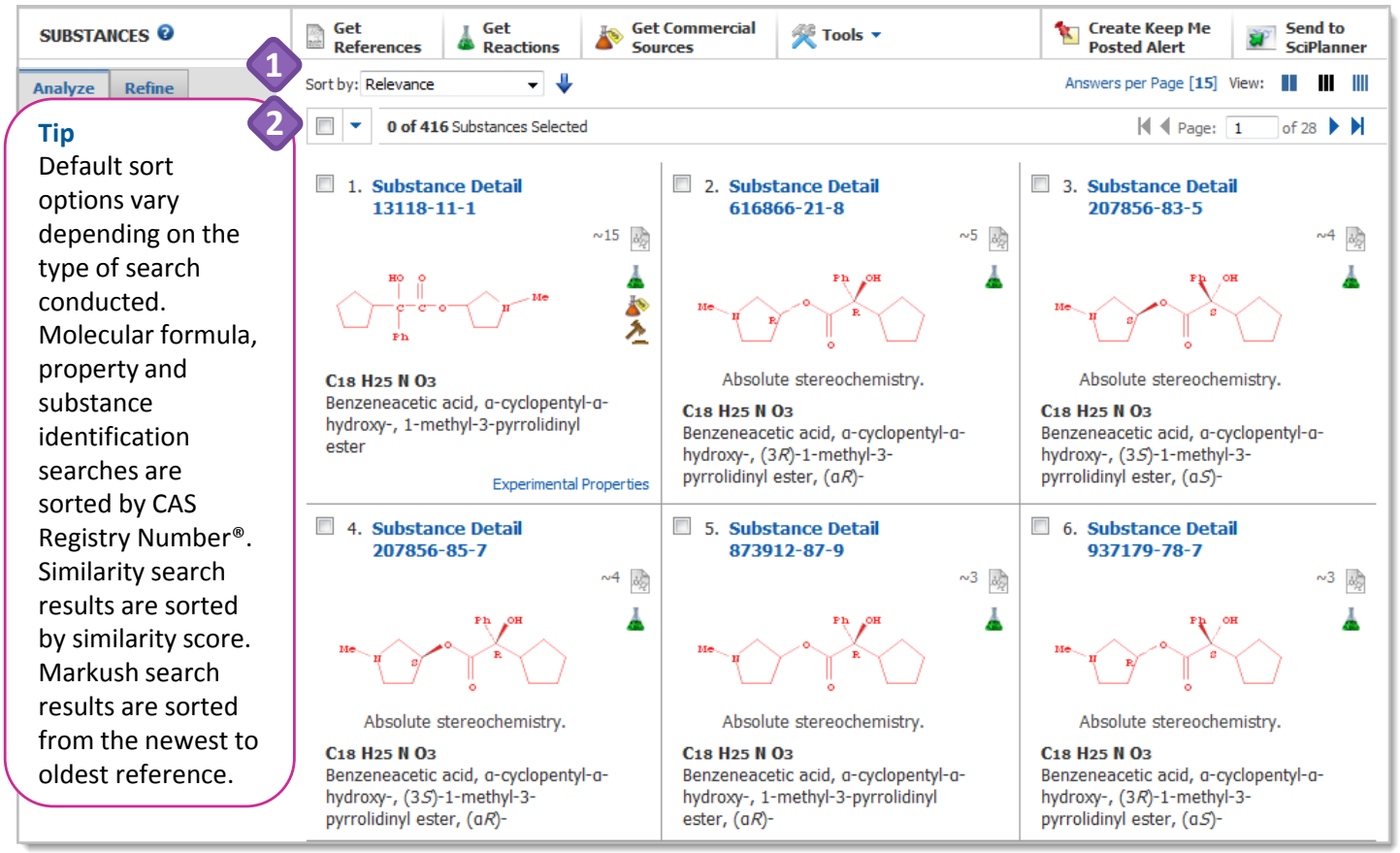
How to Work with a Substance Answer Set

SciFinder®

Easily identify and isolate substances of interest

Quickly retrieve relevant information from the world's largest, publicly available substance database. This guide provides an overview of some of the sort, refine, and analyze tools for confidently evaluating and narrowing even a large answer set. From there, two clicks retrieve references or reactions associated with your substance of interest. For more detailed information and additional training resources, consult the online Help or visit www.cas.org/training/scifinder.

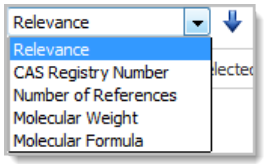
Substance Search Results



Tip

Default sort options vary depending on the type of search conducted. Molecular formula, property and substance identification searches are sorted by CAS Registry Number®. Similarity search results are sorted by similarity score. Markush search results are sorted from the newest to oldest reference.

1 Exact and substructure answer sets are automatically sorted by relevance. Click the drop-down arrow to select another sort option.



- The blue arrow indicates that the results are sorted from most to least relevant. Click the arrow to reverse the sort order.

2 The total number of retrieved substances and the number selected are displayed.

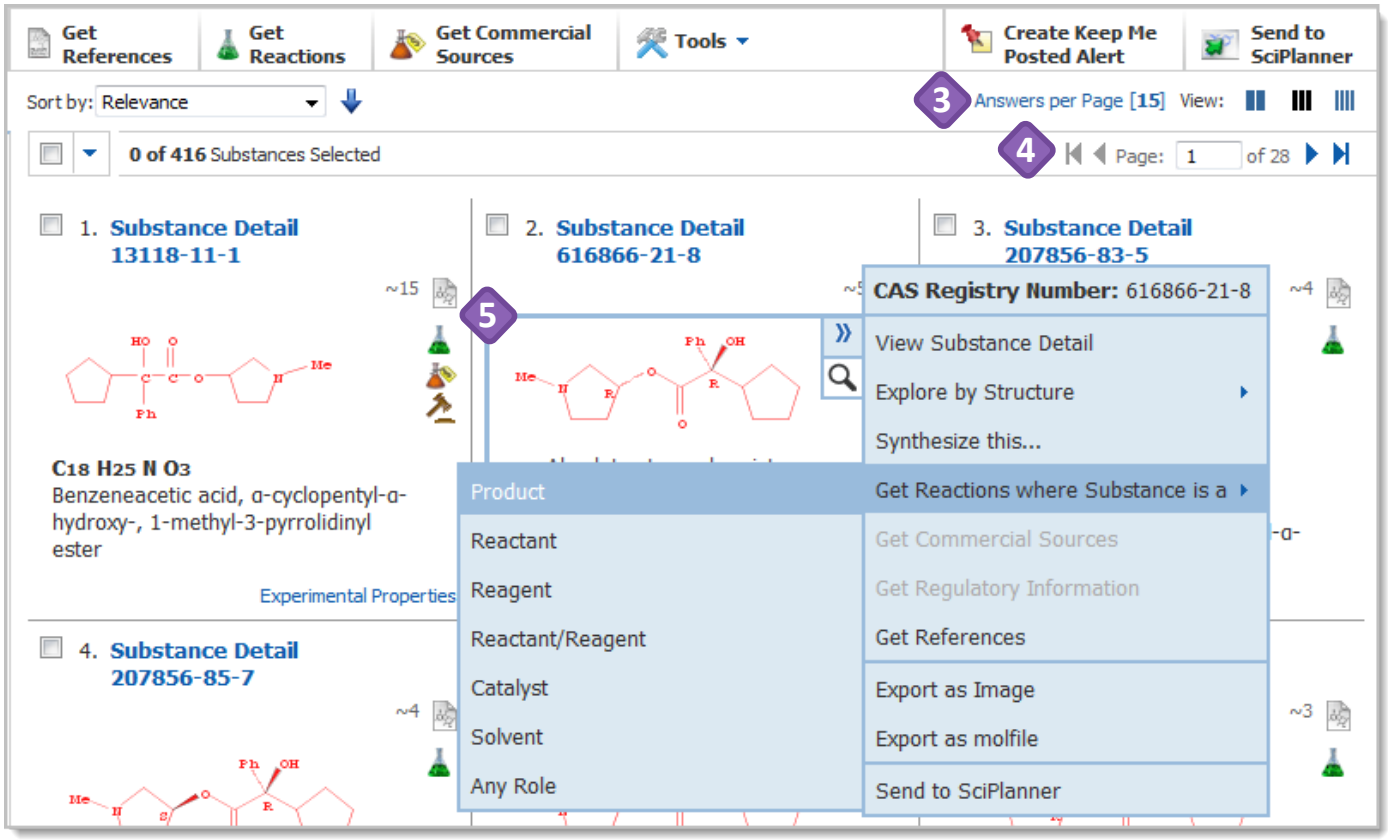
- Click the box to the left of an answer number to select it.
- Click the drop-down arrow for options related to selected answers.

Continued

CAS® | SciFinder®

CAS is a division of the American Chemical Society

www.cas.org



Each answer includes:

- A **Substance Detail** link (see page 3) and the CAS Registry Number™
- Active icons indicate the availability of:
  - References for the substance
  - Reaction data
  - Chemical supplier information
  - Regulated chemical list data
- The chemical structure; the part that matches your query is red
- The molecular formula
- The CA Index Name (useful for government documents)
- Links to **Experimental Properties** and **Spectra**, when available

Tip

Whenever you see a structure in SciFinder, you can mouse over it to access the double blue arrows. Click the arrows to see options for extending your search.

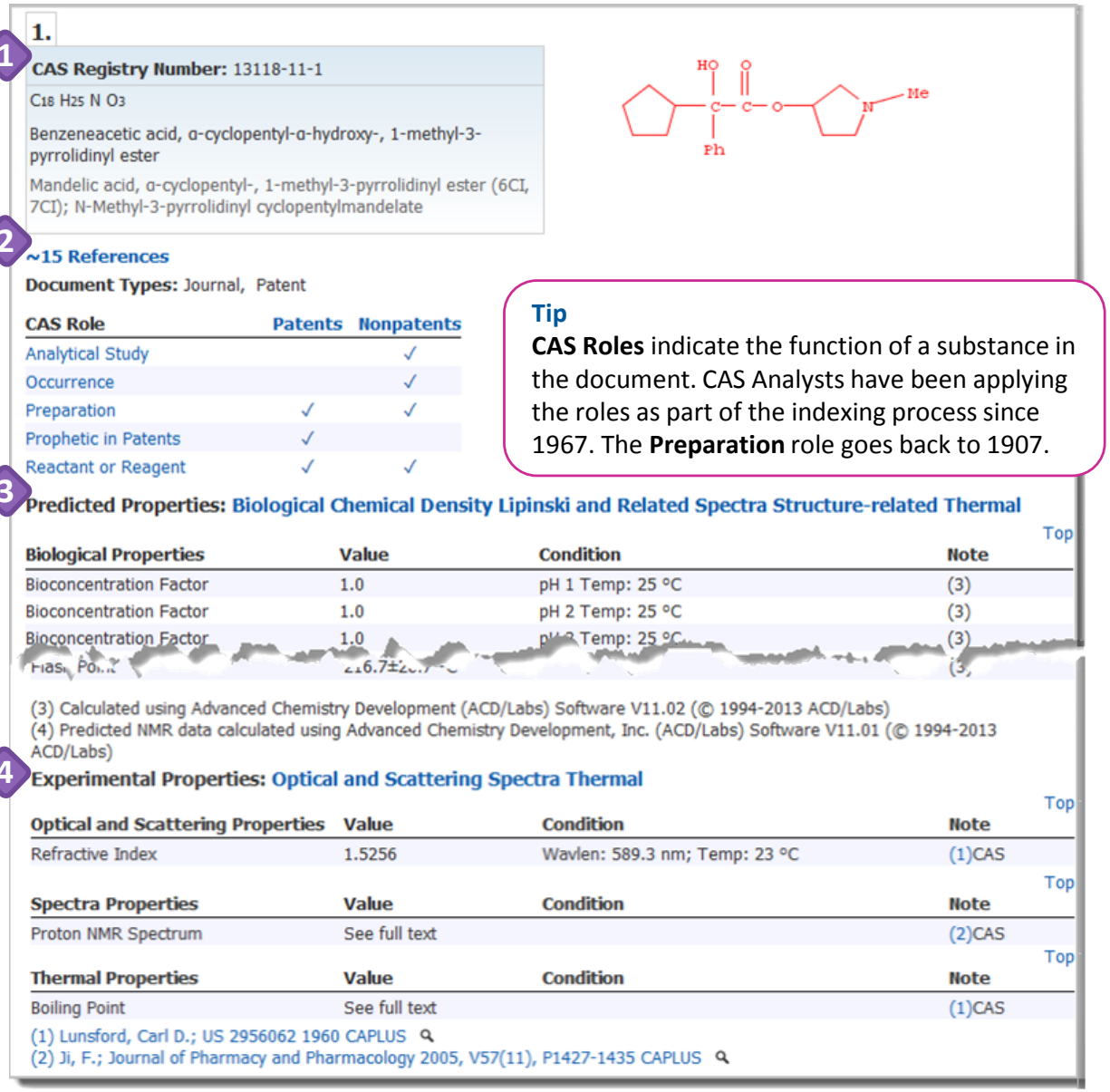
3 Specify the number of answers displayed per page (15, 20, 25 or 50). To the right of **View**, select the number of columns that are displayed.

4 Use the page controls to navigate through your answer set.

5 Mouse over a substance to access additional substance information and tools.

- Click the magnifying glass icon to launch the **Quick View**, a separate window that summarizes data about the substance.
  - Close the **Quick View** window to return to the active session.
- Click the double blue arrow to access the additional search and export options shown here.

Substance Detail



The **Substance Detail** page summarizes the available information for a substance.

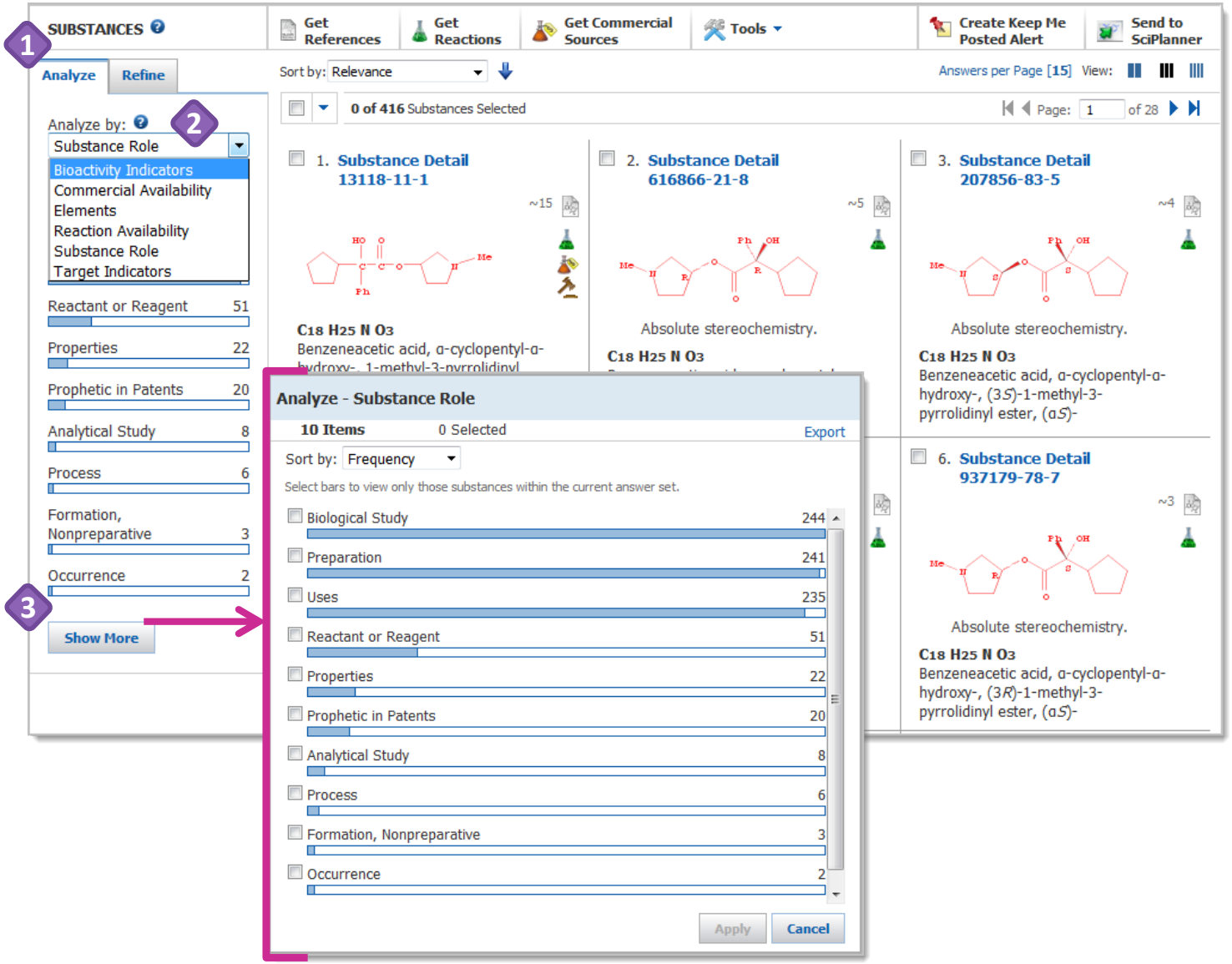
1. The blue box contains the **CAS Registry Number**, molecular formula, CA Index Name, and other names for this substance that CAS analysts found in the literature. The structure is to the right of the blue box; the hit structure is highlighted in red.

2. The number of references for this substance is also a link to those references.
   - Subsets of the references such as **Preparation** or **Patents** are also links.
   - Click a checkmark for more specific subsets such as **Preparation** information from **Patents**.

3. Click a **Predicted Properties** link, such as **Lipinski**, to quickly access that part of the predicted properties table.

4. **Experimental Properties** are reported from specific references.
   - A blue number in the **Note** column indicates that the reference is available in SciFinder. Click the number or the link below the table to see the bibliographic information.
   - Alternatively, click the magnifying glass beside the reference to display the bibliographic information in a separate window (the **Quick View**).

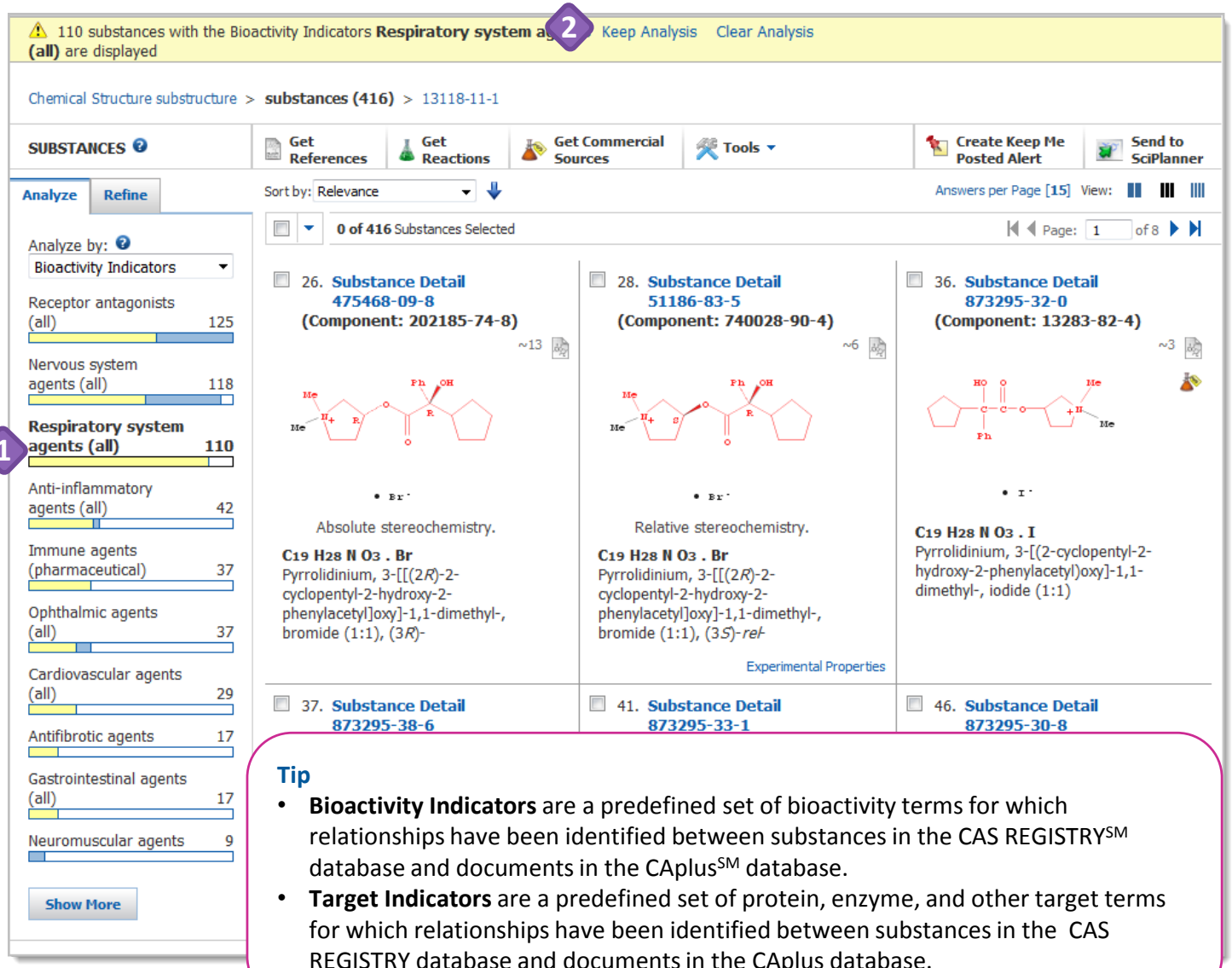
Evaluate Answers with Analysis Options



1. Click the **Analyze** tab. By default, the answer set is analyzed by **Substance Role**.
2. Click the drop-down arrow to see the available **Analyze by:** options.
3. Click **Show More** to see additional data, when available, or to select more than one analysis subset.
   - Click the box to the left of a subset to select it.

Tip
After you select **Show More**, you can **Sort by** either **Frequency** (the default) or **Natural Order** (alphanumeric order).

Narrow an Answer Set after Analysis



Tip

- **Bioactivity Indicators** are a predefined set of bioactivity terms for which relationships have been identified between substances in the CAS REGISTRY℠ database and documents in the CAplus℠ database.
- **Target Indicators** are a predefined set of protein, enzyme, and other target terms for which relationships have been identified between substances in the CAS REGISTRY database and documents in the CAplus database.

1 Click an **Analyze** bar to display that subset of answers. In this example, the answer set has been analyzed by **Bioactivity Indicators** and **Respiratory system agents (all)**.

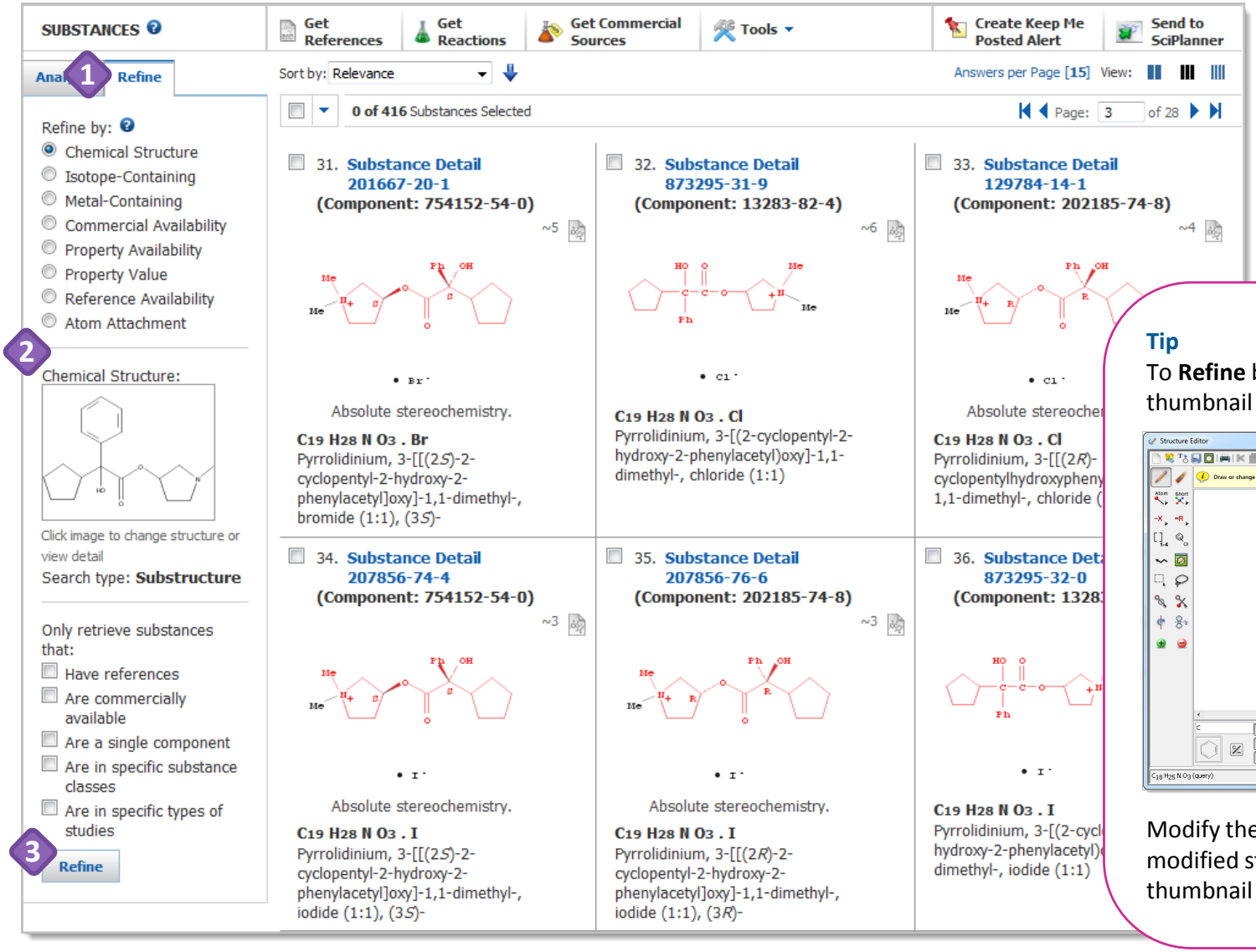
- The analysis bar turns yellow. Other bars can also turn completely or partly yellow to indicate that substances from the selected bar are also present in other subsets.

2 The yellow status bar indicates the answers that are currently displayed.

- Click **Keep Analysis** to make these answers your new answer set.
- Click **Clear Analysis** to return to your original answer set.

Narrow an Answer Set with Refine Options

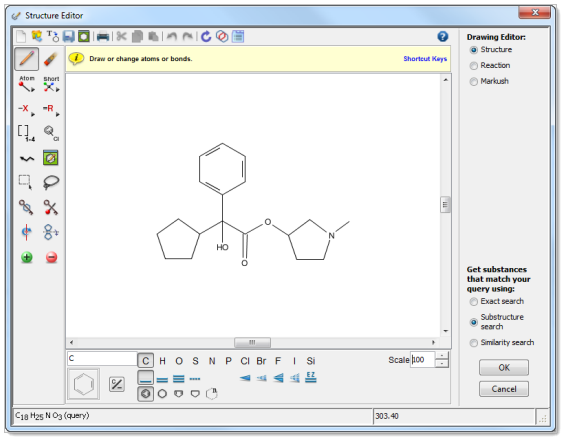
SciFinder®



1. Click the **Refine** tab and select a **Refine by:** option by clicking the radio button.
2. Specify additional criteria below the refine options.
3. Click **Refine**.

Tip

To **Refine** by **Chemical Structure**, click the thumbnail to re-open the **Structure Editor**.



Modify the structure and click **OK**. The modified structure is then displayed in the thumbnail on the **Refine** tab.

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.
   - It is an interactive window where you can store and organize reference, substance and reaction search results.
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 Substances** to retrieve substances for part or all of your answer set.
8. Click **Get Reactions** to retrieve reactions for part or all of your answer set.
9. Click **Get Commercial Sources** to retrieve suppliers for part or all of your substances.
10. Click the **Tools** drop-down arrow to combine this answer set with a previously saved answer set (**Combine Answer Sets**).
11. **Create Keep Me Posted Alert**, when active, allows you to create an automated alert based on the current search strategy.
12. Click **Send to SciPlanner** to send selected answers to the SciPlanner workspace.
    - Use it to gather information for a project, create a report or export research to share with colleagues.

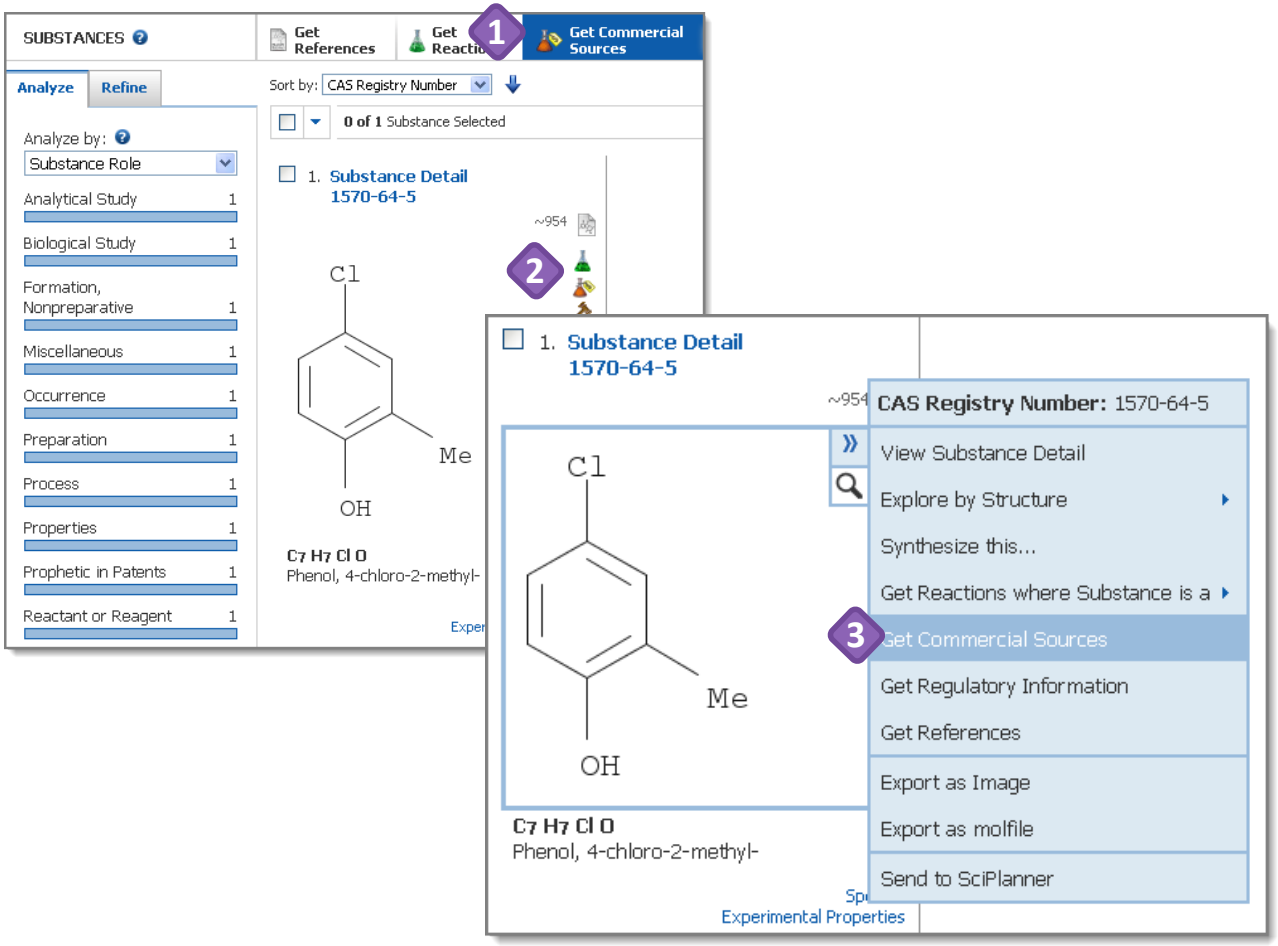
How to Find Commercial Sources

SciFinder®

Need a Source for a Reagent? Let SciFinder® Help Identify Suppliers

Find your substance and then find sources from which to purchase it – all from within SciFinder. You can designate suppliers as preferred or non-preferred, and in many cases link directly to pricing and availability information from a supplier. For additional training resources, consult the online Help or visit [www.cas.org/training/scifinder.](www.cas.org/training/scifinder)

Find Commercial Sources



To find commercial sources for a substance, you can do any of the following:

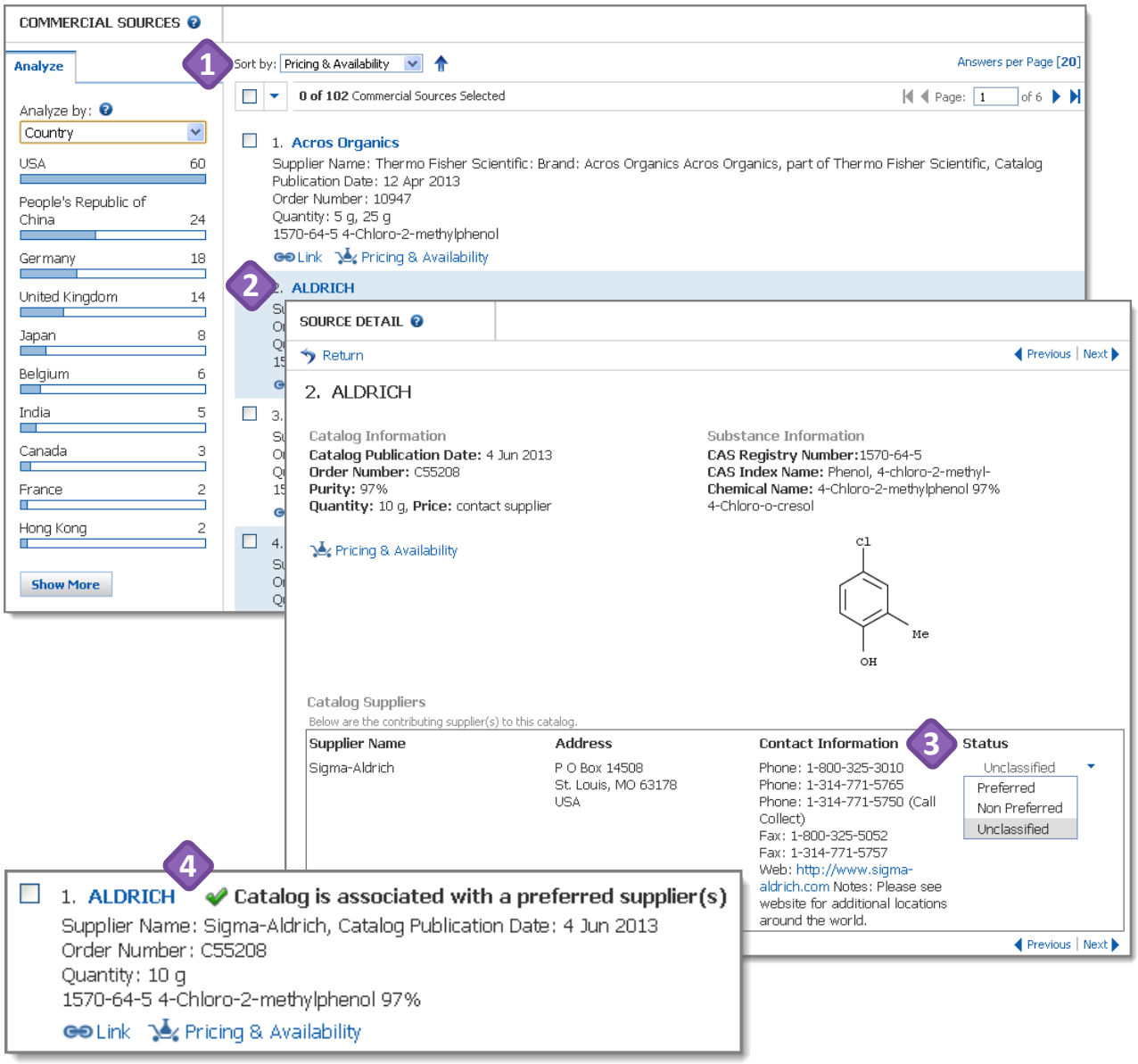
1. Select **Commercial Sources** from the **Tools** menu.
2. Click the **Commercial Sources** icon (red beaker with a yellow price tag).
3. Select **Get Commercial Sources** in the substance context menu.

Tip
Mouse over the structure and click the double blue arrow to see the substance context menu.

CAS® | SciFinder®
CAS is a division of the American Chemical Society

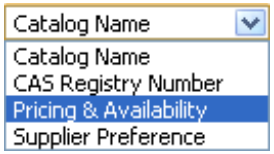
www.cas.org

See Supplier Information



SciFinder returns a list of companies that sell the substance. By default, they are sorted by **Catalog Name**.

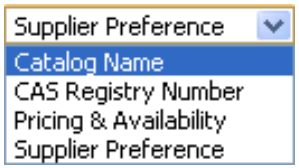
1. Click the drop-down arrow to select a different **Sort by** option. Click the blue arrow to reverse the order.



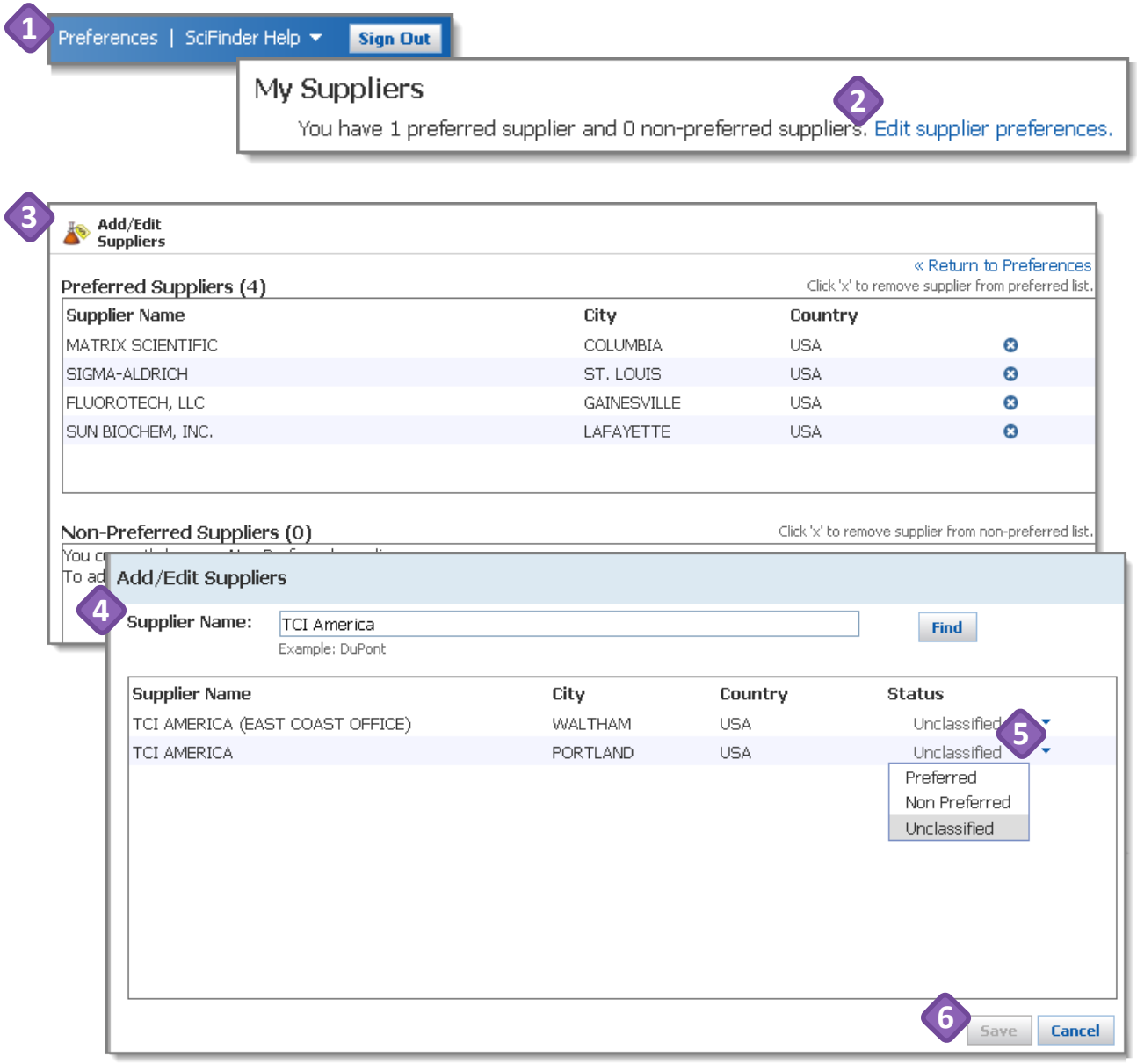
2. Click a company's name to see the **Source Detail** display.

3. The supplier's status is shown in the lower right. Unclassified is the default.
   - Click the drop-down arrow to select a different status: **Preferred** or **Non Preferred**.

4. After you designate a source as **Preferred** or **Non-Preferred**, subsequent commercial source displays will indicate that status and the sort order default becomes **Supplier Preference**.



Manage Preferred Suppliers

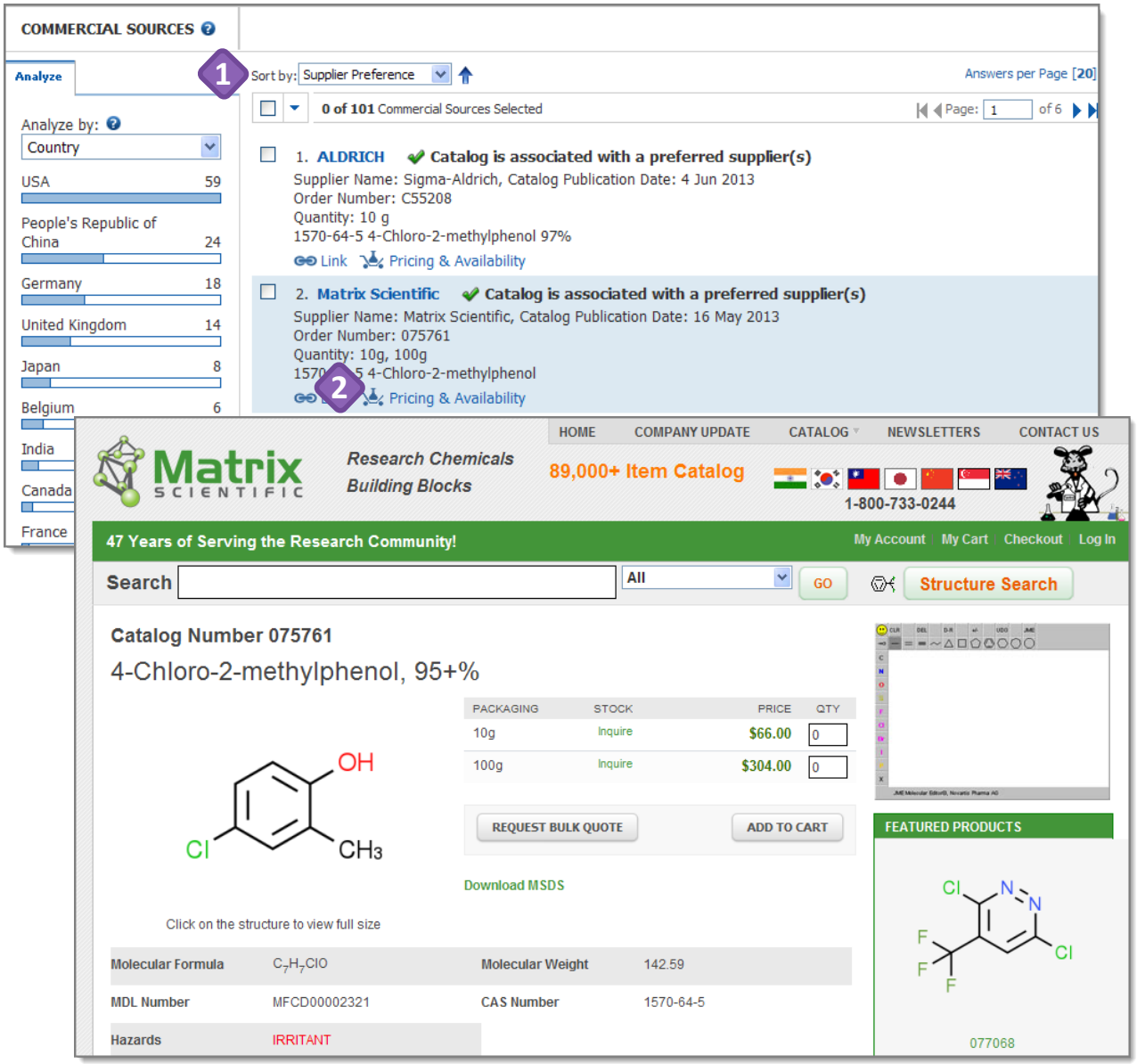


In **Preferences**, you can manage supplier information.

1. Click **Preferences** in the upper right of the any SciFinder window.
2. In the **Preferences** window, click **Edit supplier preferences**.
3. A list of your **Preferred** and **Non-Preferred Suppliers** is displayed in the window.
   - To remove a supplier from the preferred list, click the ⊗ icon.
   - To edit an existing supplier (e.g., changing the designated status), click **Add/Edit Suppliers**.
4. To add a **Supplier Name**, type the name in the text box and click **Find**.
   - Supplier names appear below the text box.
5. Click the drop-down arrow to change the **Status** of a new or existing supplier.
   - After you select a **Status**, the **Save** button becomes active.
6. Click **Save** to keep the changes.

After you create a list of preferred suppliers, they will be displayed at the top of subsequent answer sets and will be the default setting for **Sort** and **Analyze**.

Check Pricing and Availability



Preferred suppliers are displayed at the top of answer sets and are the default setting for **Sort** and **Analyze**.

1. To see **Pricing & Availability** information, use either **Sort** or **Analyze by** to identify suppliers who make pricing information available online.

2. Click the **Pricing & Availability** link to access the supplier's website.

Tip
Some suppliers require you to create a login ID before they give you access to the information.

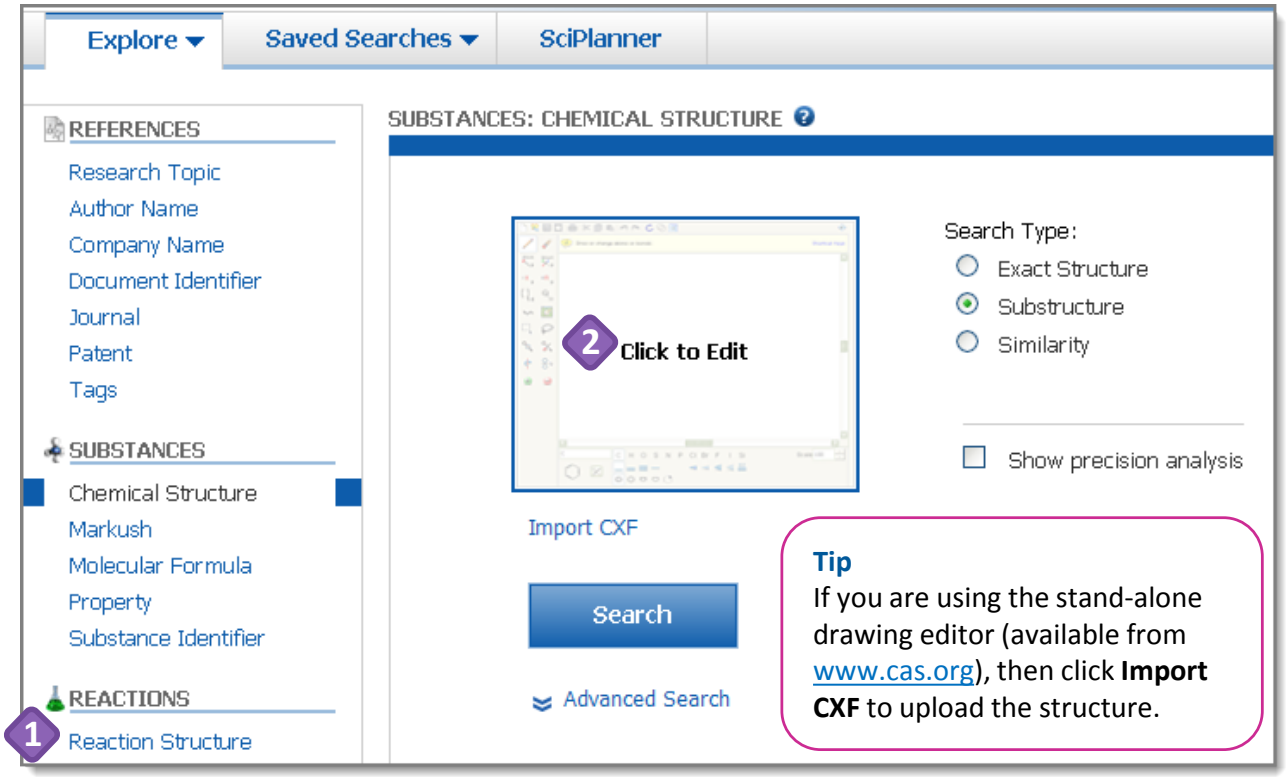
How to Create a Reaction Answer Set

SciFinder®

Find all relevant reactions based on criteria you specify

Search the world's largest, publicly available reaction database and quickly find highly relevant results, no matter the size of your answer set. This How to Guide explains a variety of ways to design your reaction search. Refer to "How to… Work with a Reaction Answer Set" to learn about tools and techniques to easily sort, organize and narrow your results and find the most relevant answers. For more training resources, consult the online Help or visit [www.cas.org/training/scifinder.](www.cas.org/training/scifinder)

Begin a Reaction Search

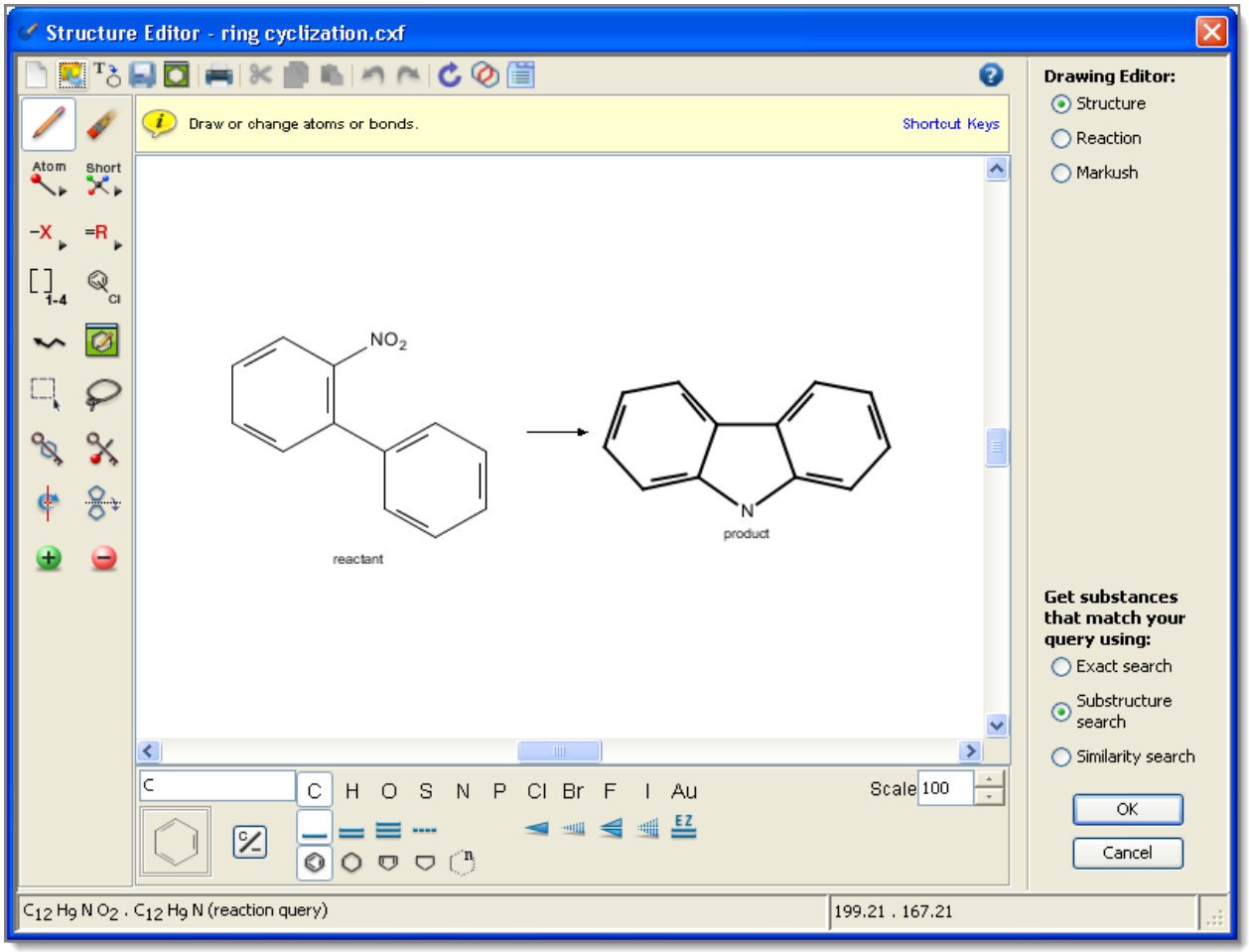


Tip
If you are using the stand-alone drawing editor (available from www.cas.org), then click **Import CXF** to upload the structure.

1. To begin, go to the left navigation pane and click **Reaction Structure**.
2. Click the picture of the reaction drawing window to launch the **Reaction Editor**.

Tip
Click ? to access context-specific online help.

Draw the Reaction



1. Draw your reaction.

   Learn about drawing in the **Reaction Editor** with the following tutorials, available in the online **SciFinder Help**:
   - "Introduction to the SciFinder Drawing Editor"
   - "Introduction to Reaction Searching"

2. Select the type of reaction search that you want to conduct.

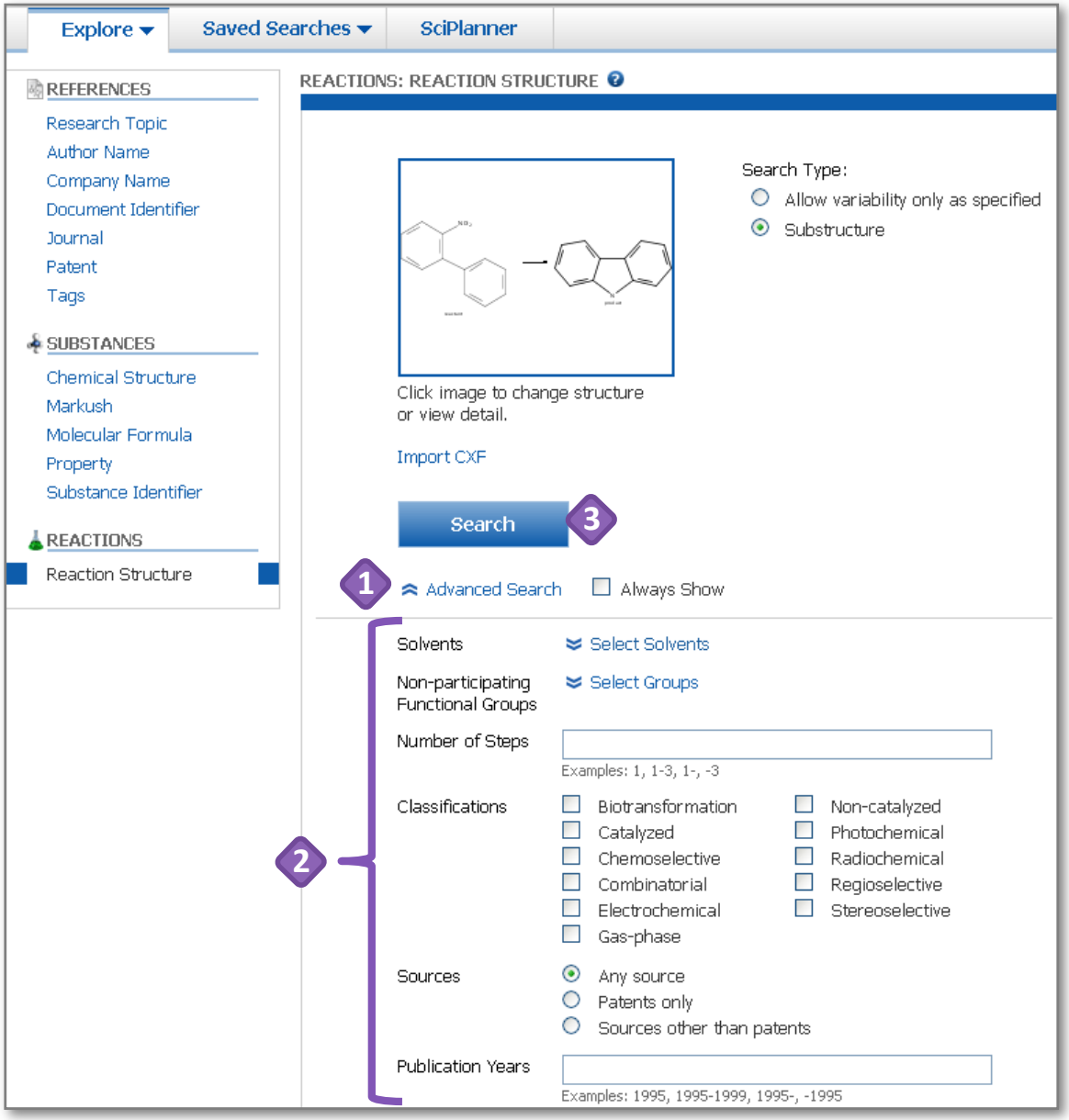
SELECT…	IF YOU WANT TO…
Variable only at the specified positions	Prohibit substitution at all atoms (except variables and R-groups) and prohibit additional ring fusion.
Substructure of more complex structures	Allow additional substitution and ring fusion.

3. Click **OK** to transfer the reaction and type of search to the search page.

Tip on Stereo Searching

CAS scientists apply structure data to a record by reporting the information in the original document. If no stereo is identified, then the molecule is listed as a "flat" (2-dimensional) structure. If you search stereo bonds, you can miss relevant data that was listed in the literature only in a 2-dimensional format, whereas searching the flat structure will retrieve both 2-dimensional and 3-dimensional (stereo) structures.

Search the Reaction



When you click **OK** in the **Reaction Editor**, your reaction and **Search type** are transferred to the reaction search page.

1. (optional) Click **Advanced Search** to see additional search options.
2. (optional) Select limiters, such as **Number of Steps**, to further restrict your search.
3. Click **Search**.

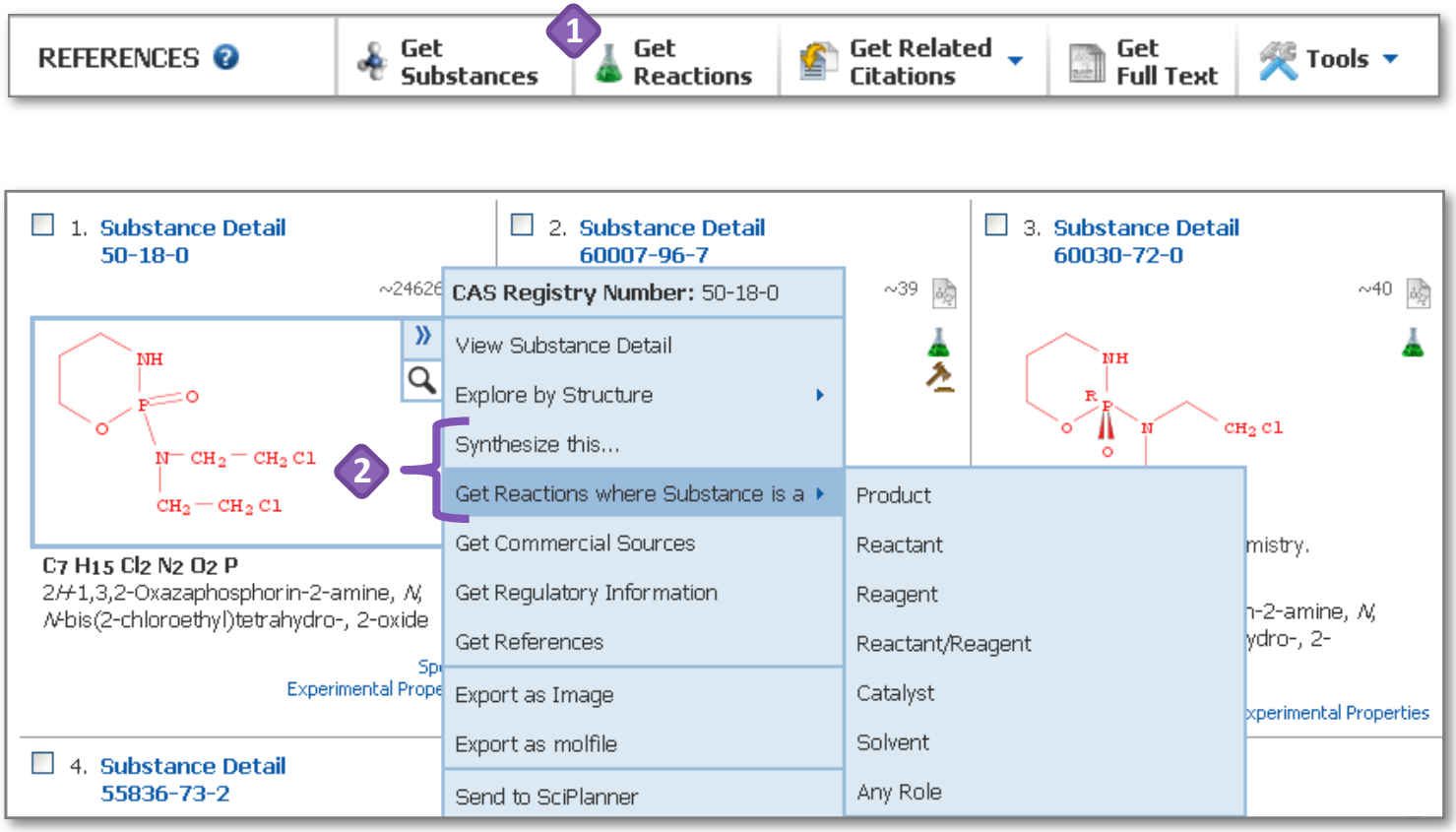
Tip

The limiters are available as part of the **Refine** and **Analyze** functions, so it is often advantageous to start with a broad search and narrow the answer set later.

Now what?

After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reaction Answer Sets."

Other Ways to Create a Reaction Answer Set

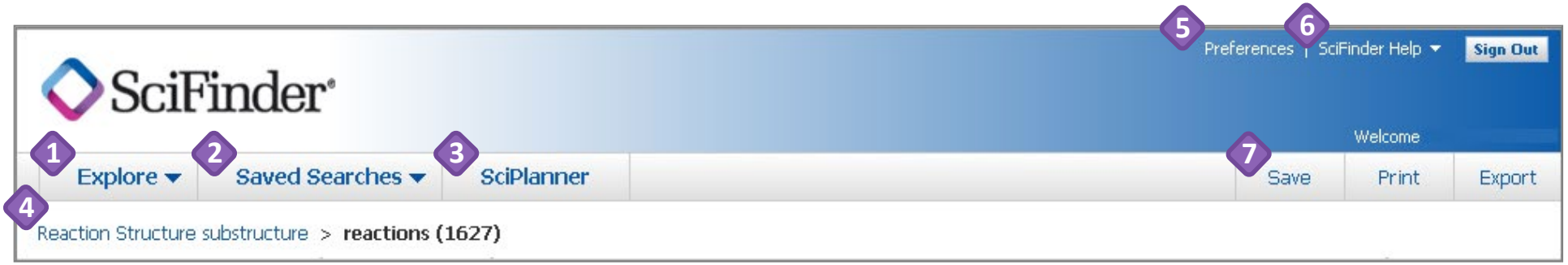


You can also create a reaction answer set by starting with either reference or substance answers.

1. After you get a reference or substance answer set, click **Get Reactions** on the toolbar.

2. After you get a substance answer set, mouse over a substance until a blue box appears around it. Click the double blue arrows in the upper right, and then select either **Synthesize this…** or **Get Reactions where Substance is a >** and select the reaction role for the substance.

Manage Your Searching



1. Start a new **References**, **Substances** or **Reactions** search.
2. Access **Saved Answer Sets**, **Keep Me Posted** automated alert results, and your search **History**.
3. Open the **SciPlanner** interactive workspace where you can organize your reference, substance and reaction search results.
4. The breadcrumb trail shows each step in your current search history. Hover over a step to see more information about it. Click a step to return to that part of your search.
5. Click **Preferences** to customize your search options.
6. Click the **SciFinder Help** drop-down arrow to access online **Help**, **Training**, **What's New** and **Contact Us**.
7. Click **Save**, **Print** or **Export** to open a dialog window and initiate these procedures.

Now what?

To learn about working with the reaction answer set, please see the companion document titled, "How to… Work with Reaction Answer Sets."

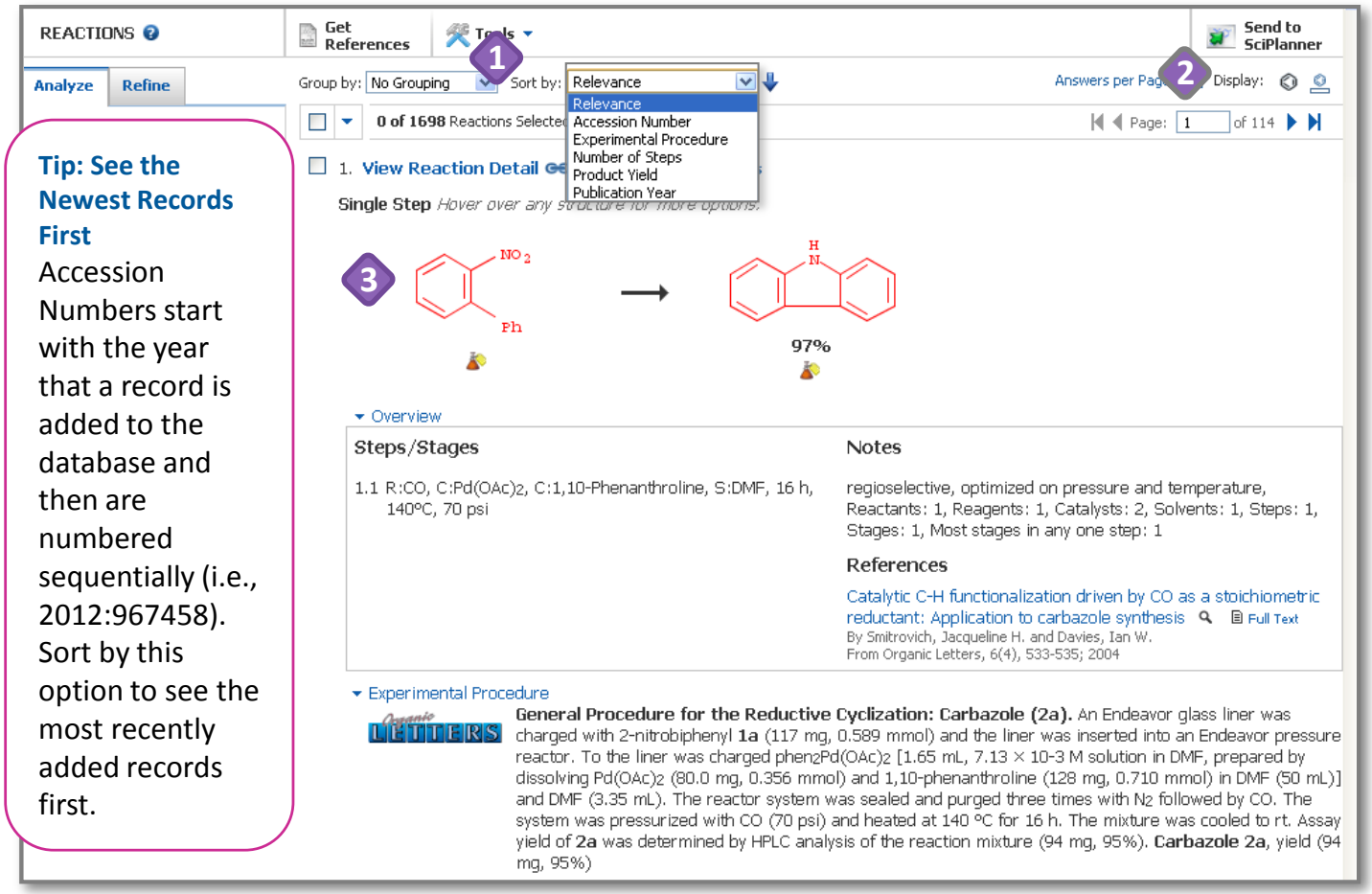
How to Work with a Reaction Answer Set

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.

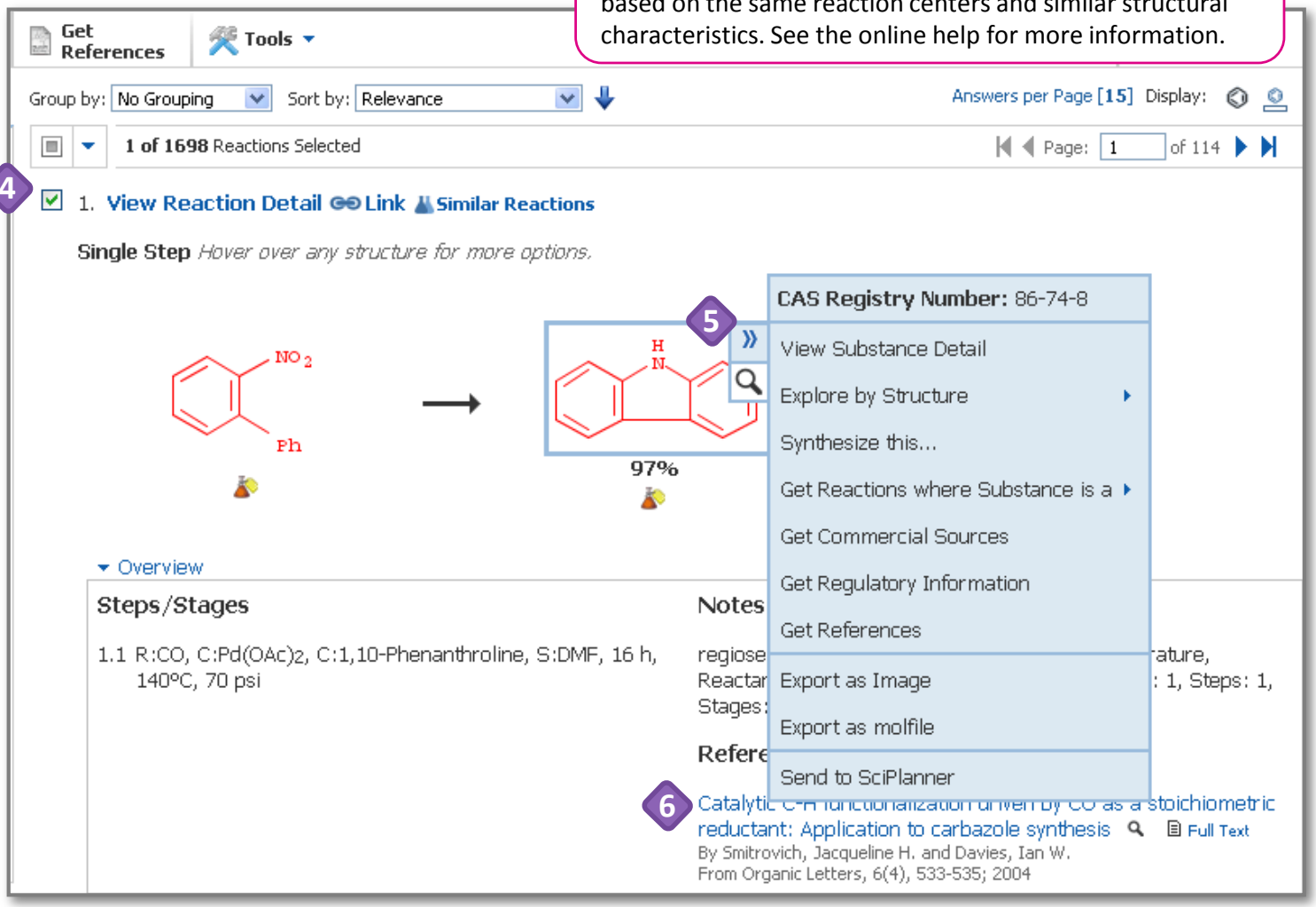
1. By default, answers are sorted from most to least relevant.
   - Click the drop-down arrow to select other sorting criteria.
   - Click the blue arrow to reverse the sort order.

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.

Continued

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.



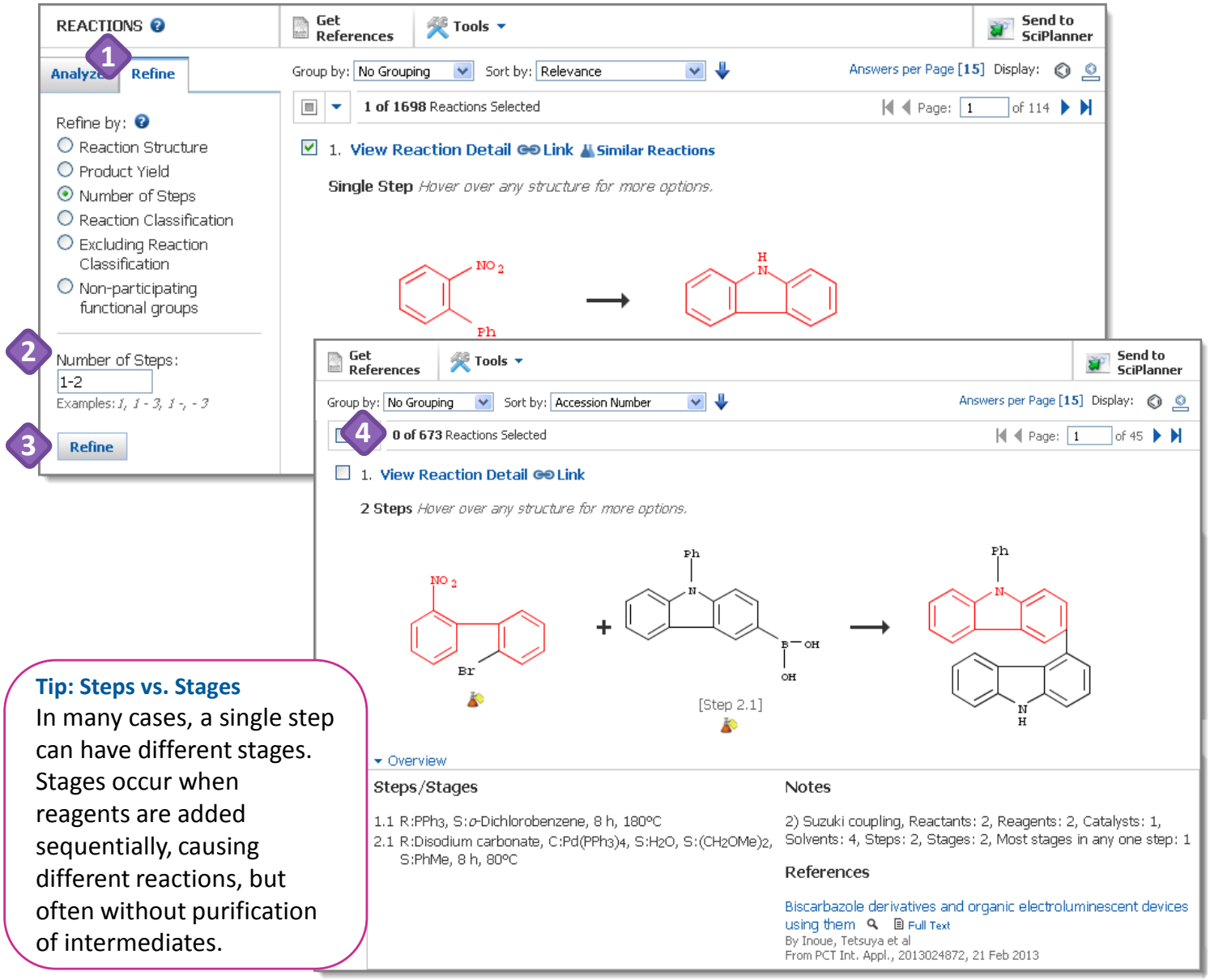
4 Click the box beside an answer number to select it. You can work with selected items several ways, such as saving them or getting references for them.

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

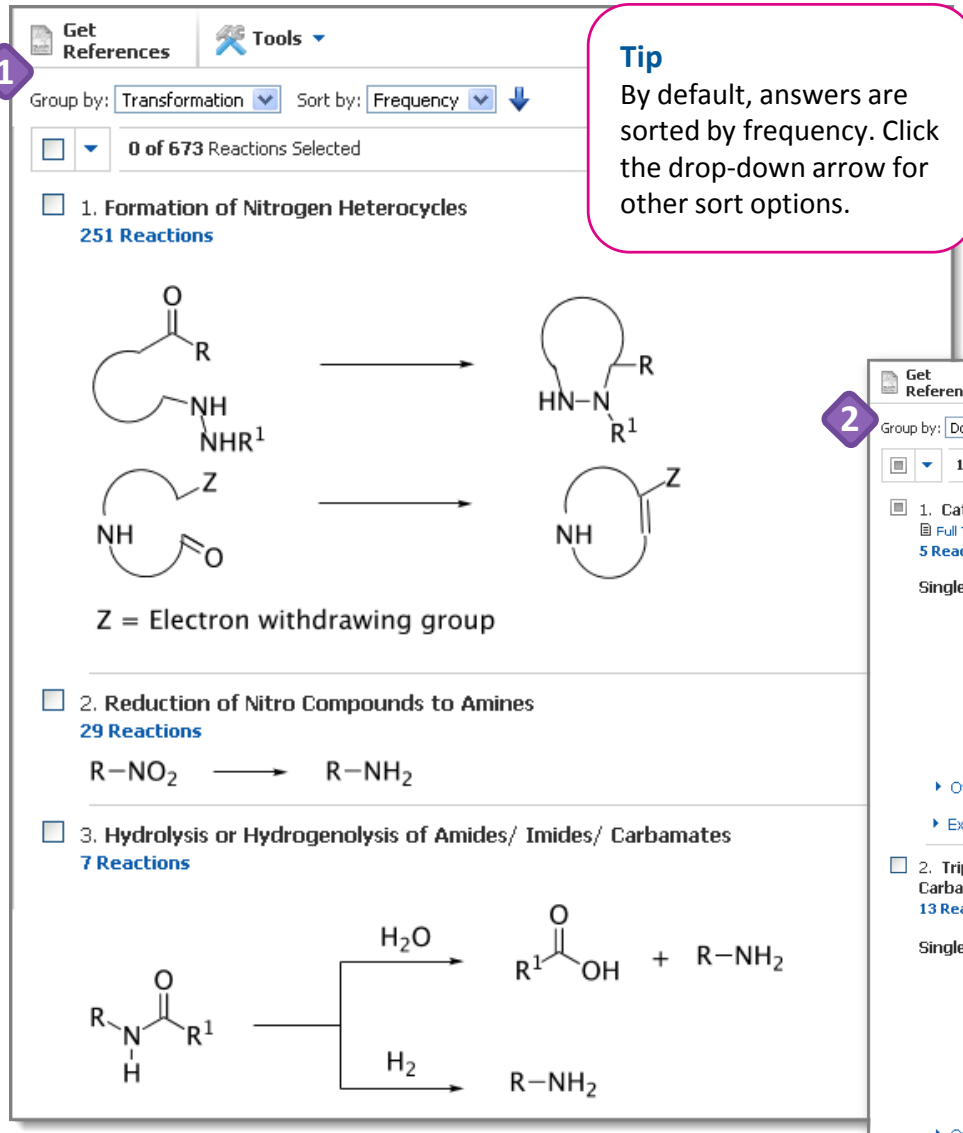


1. On the **Refine** tab, click a radio button to select a **Refine by:** option.
2. Below the radio buttons, further define the criteria by which you want to refine.
3. Click **Refine**.
4. The answer set is narrowed according to the criteria you specified.

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

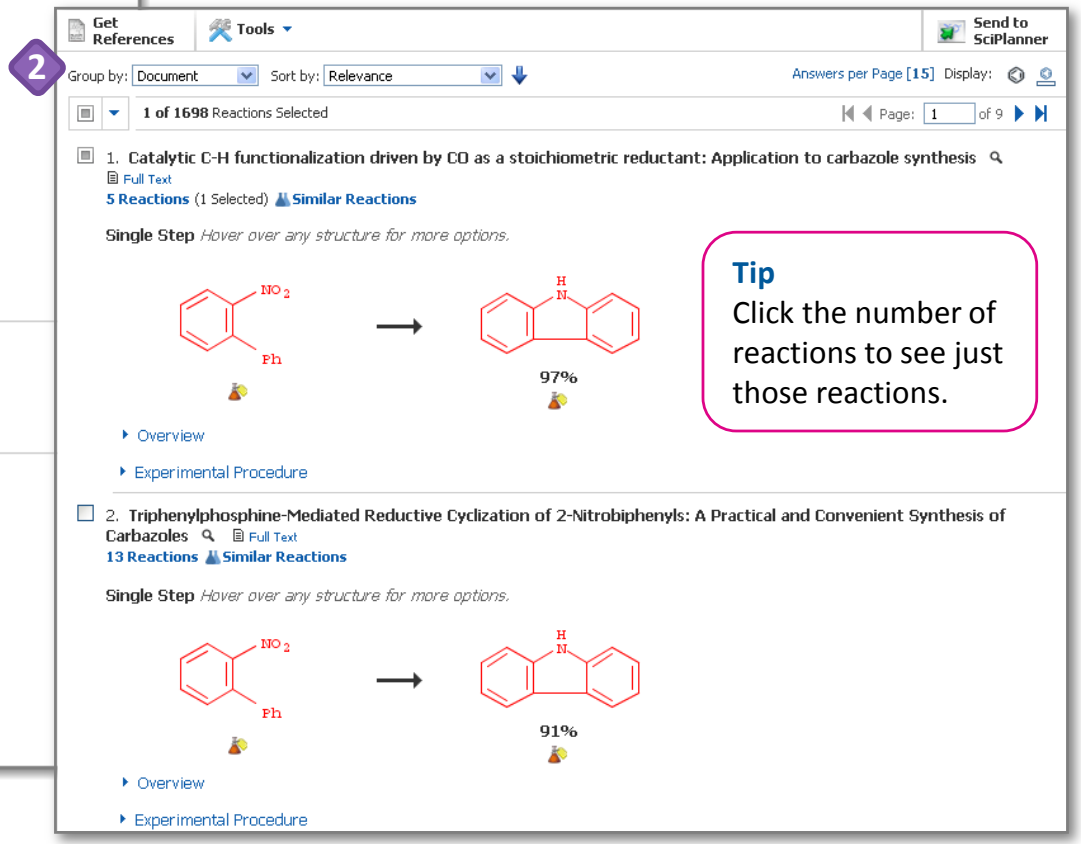


Tip
By default, answers are sorted by frequency. Click the drop-down arrow for other sort options.

1 **Group by: Transformation** groups single-step reactions based on transformation types so you can quickly evaluate synthesis options and preferred pathways.

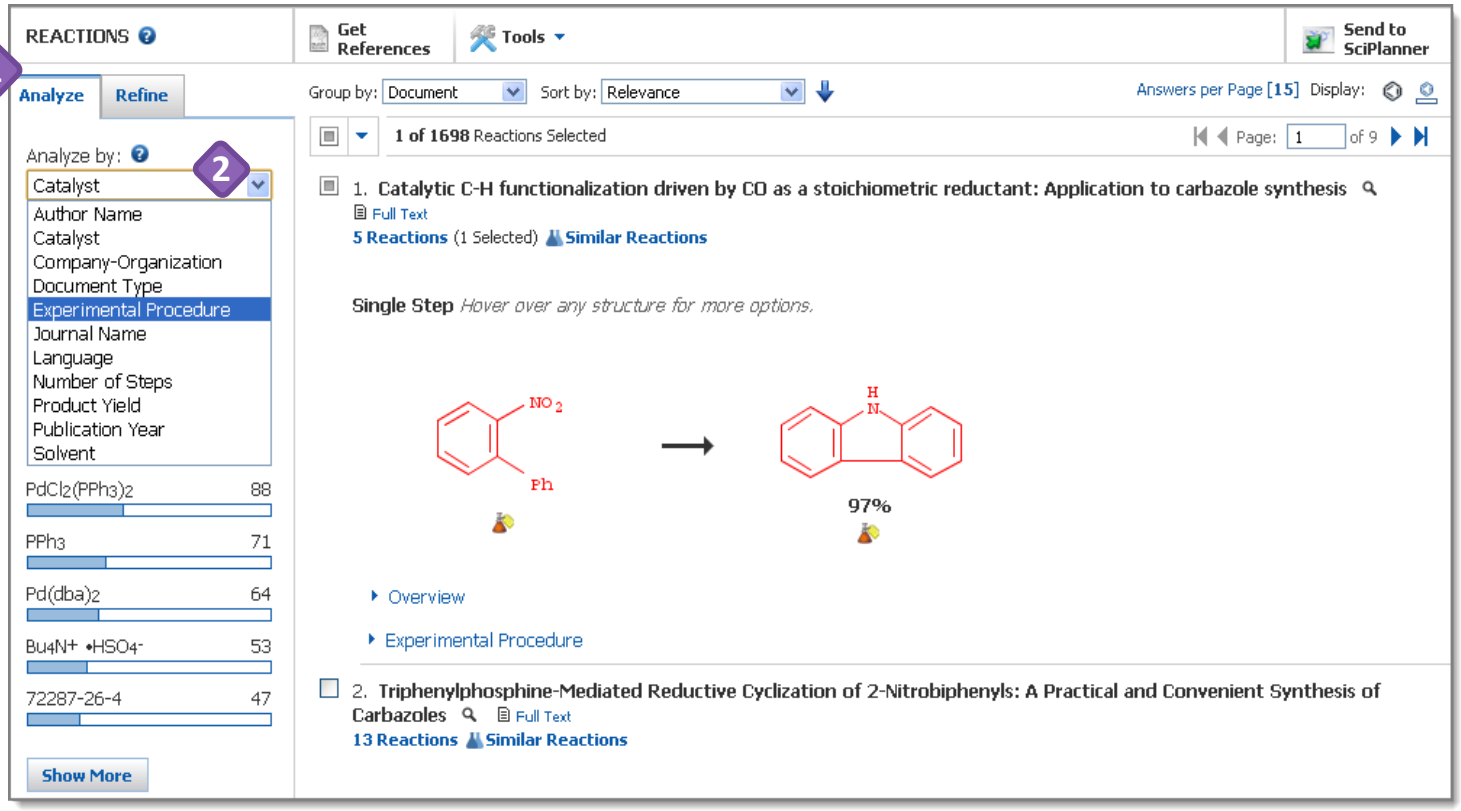
- Reactions can fall into more than one category.
- Unclassified single- and multi-step reactions (if any) appear at the end of the answer set.

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



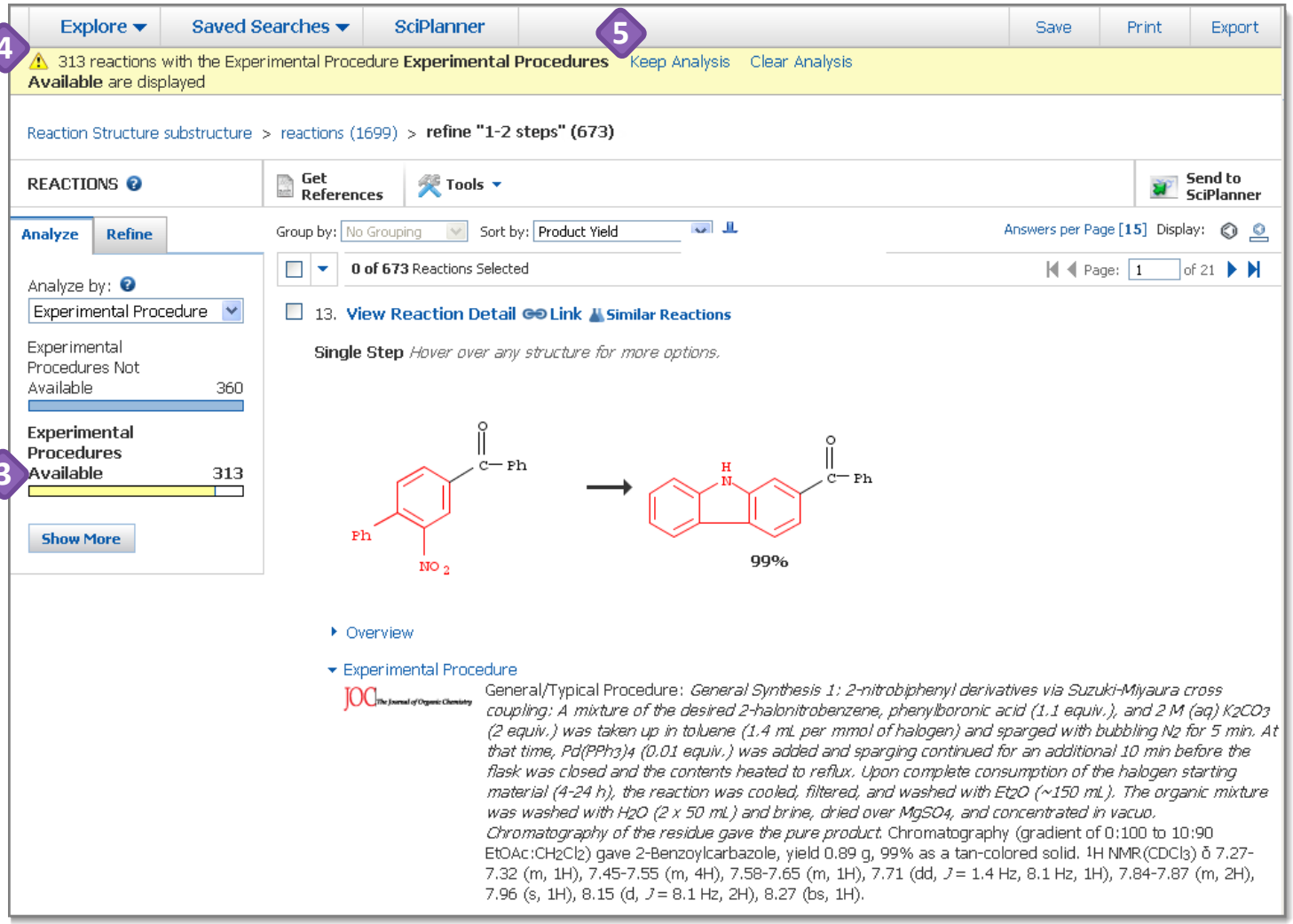
1. Click the **Analysis** tab.
2. Click the drop-down arrow to select an **Analyze by:** option.

- 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.

Continued



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

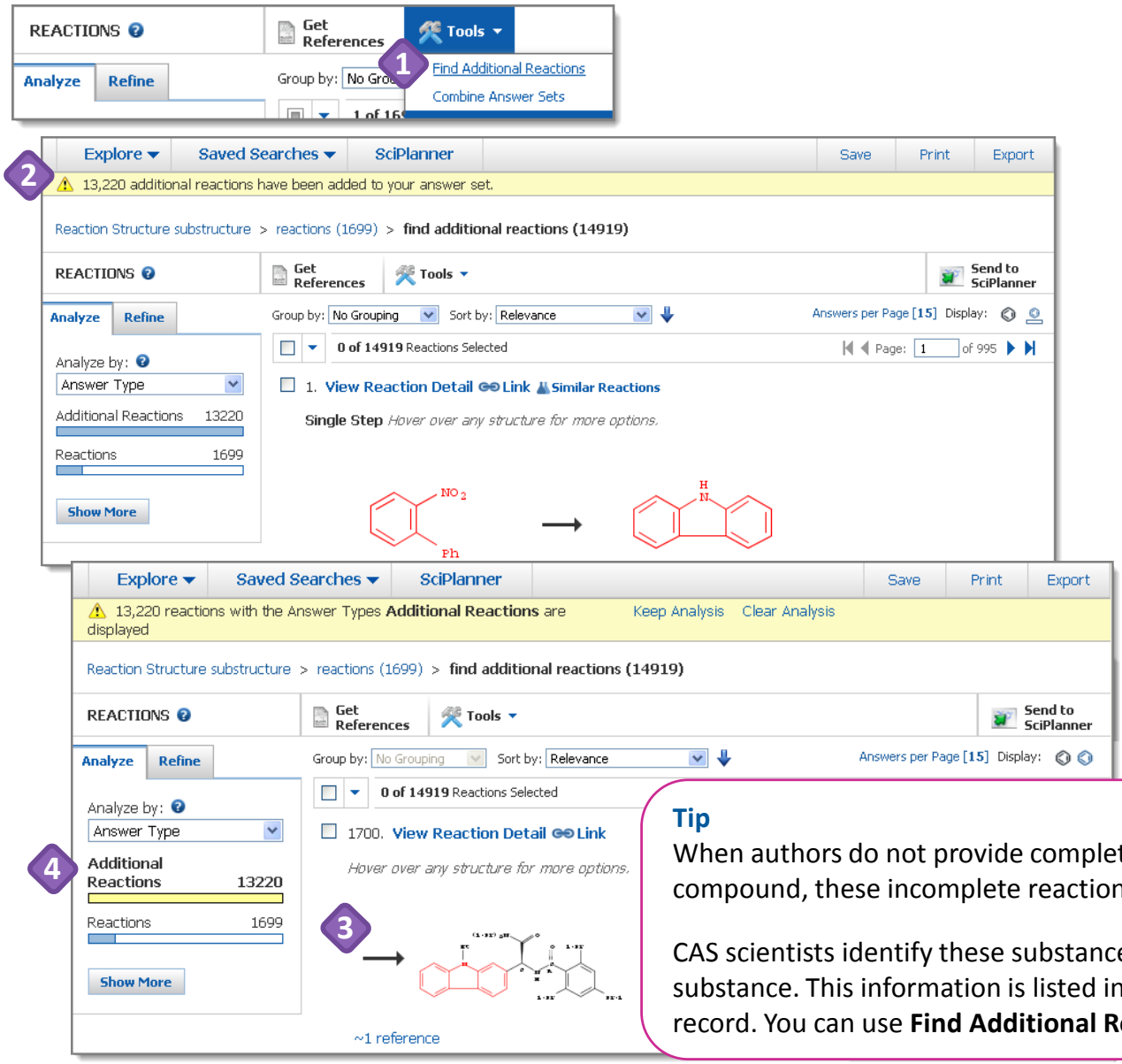
3. Click an analysis bar to display only the answers in a subset. The selected bar turns yellow.

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.

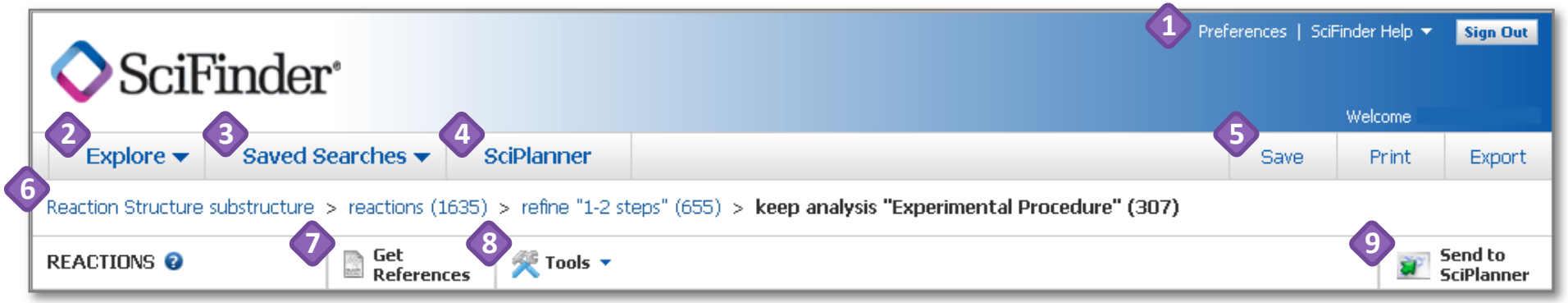
4. The default **Analyze** of the new answer set is **Answer Type**.
   - Select **Additional Reactions** to see only the newly added reactions.

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.

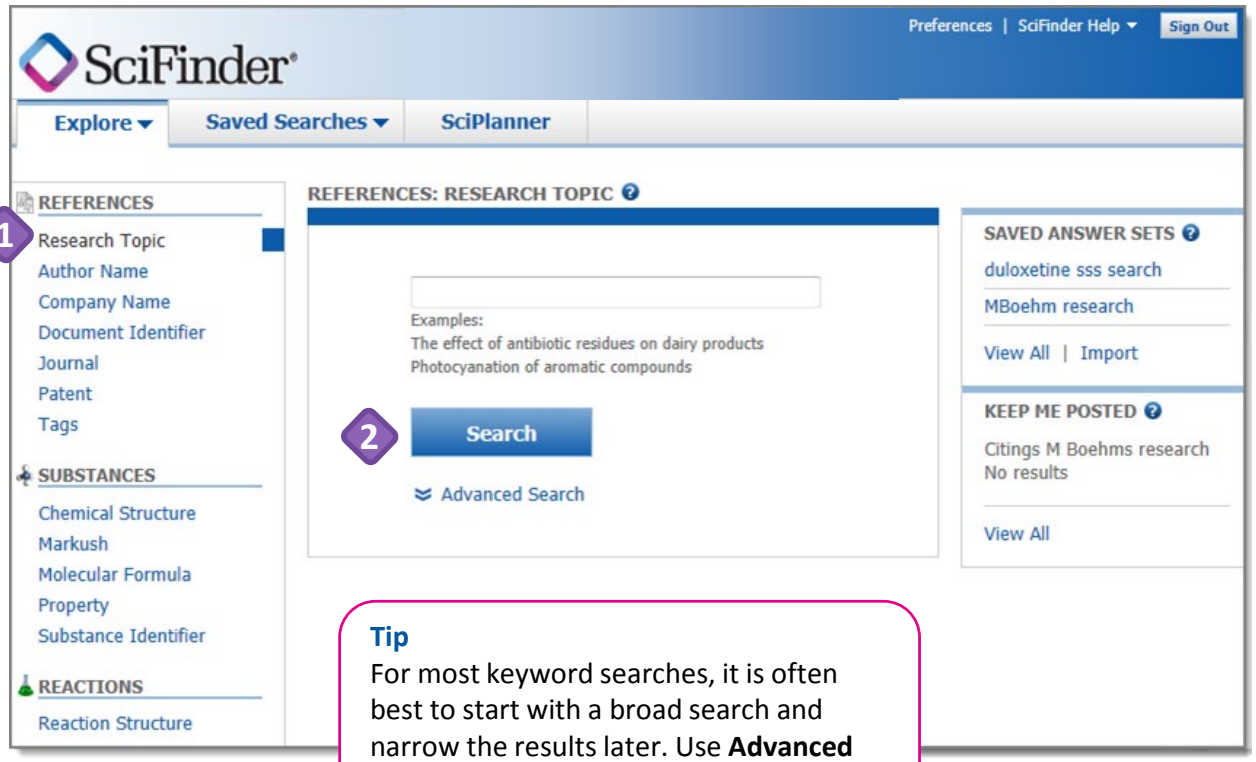
How to Create a Reference Answer Set

SciFinder®

Find references quickly and easily

In SciFinder, you are searching the world's largest, publicly available reference database for chemistry and related sciences as well as MEDLINE® (the National Library of Medicine® (NLM®) journal citation database). Select from various reference search options, based on the information at hand and your research needs. This guide explains how to conduct each type of reference search. When you have your answer set, refer to "How to … Work with Reference Answer Sets" for ways to evaluate the results and target the most relevant answers. For more detailed information about SciFinder, consult the online help or visit www.cas.org/training/scifinder.

Types of Reference Searches

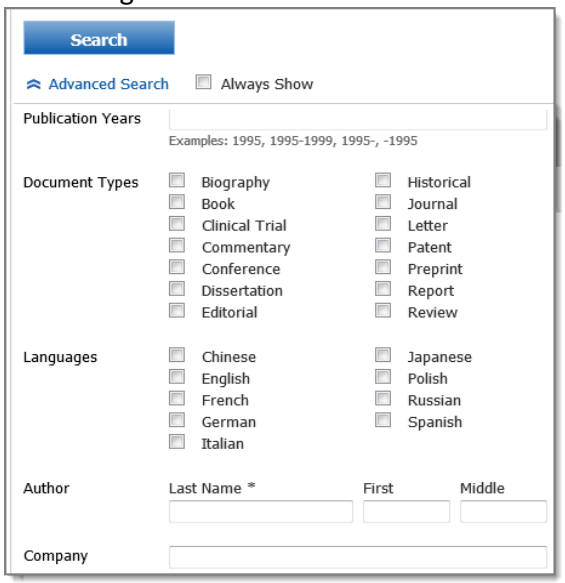


Tip

For most keyword searches, it is often best to start with a broad search and narrow the results later. Use **Advanced Search** criteria to find specific references.

1. On the **Explore** tab, under **REFERENCES**, you can search by any of the seven options.

2. Click **Advanced Search** to see criteria for narrowing a search:



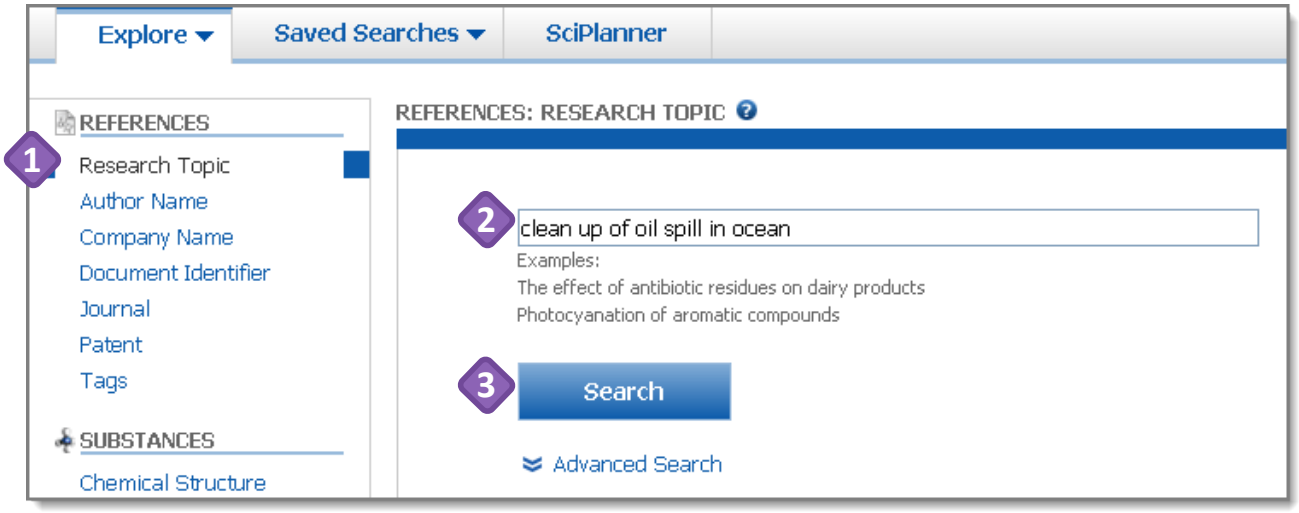
- These search limiters are available as part of the **Refine** and **Analyze** functions, so you can also apply them later in your search process.

CAS® | SciFinder®

CAS is a division of the American Chemical Society

www.cas.org

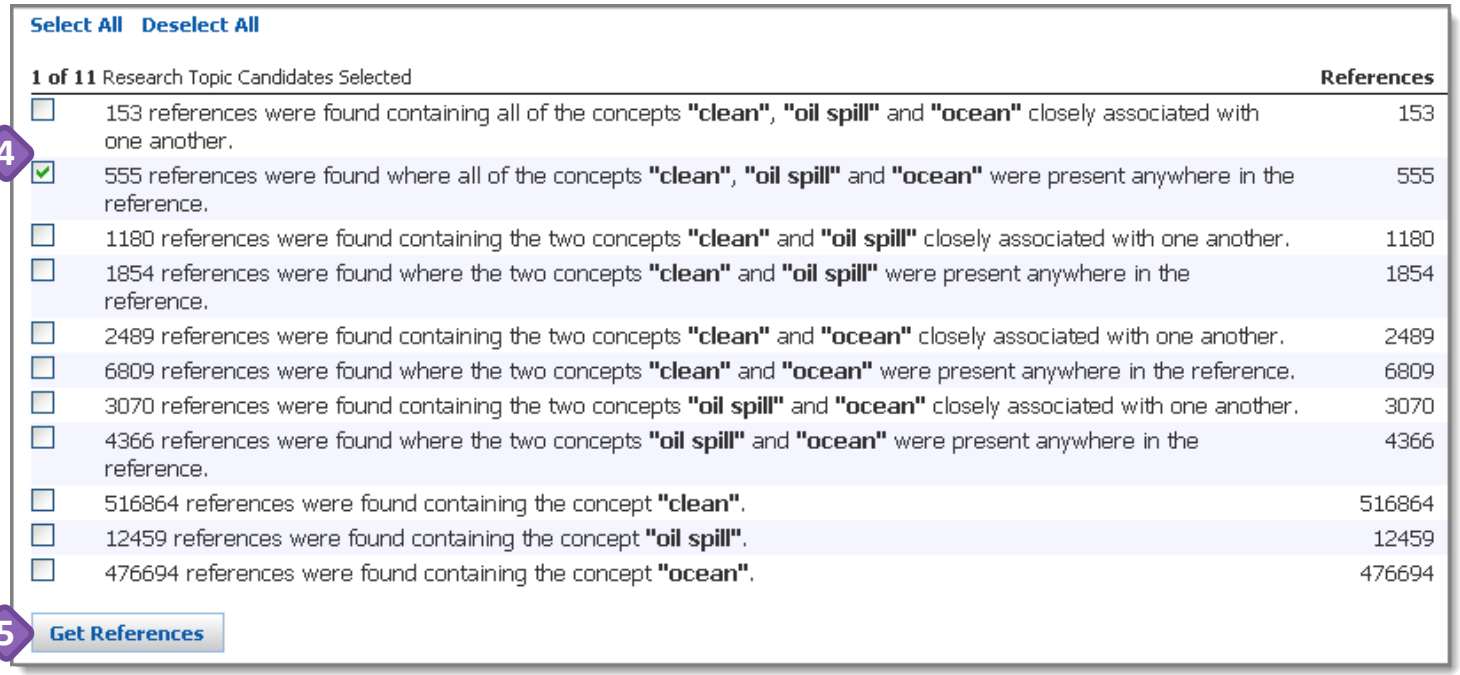
Search by Research Topic



1. To begin, click **Research Topic**.
2. Enter your search concept(s) in the query entry text box.
   - A search concept, or keyword, is a term or phrase relevant to your topic of interest.
   - Enter up to seven concepts, separated by prepositions, in English.
     - Recommendation: enter two or three concepts, separating each concept with a preposition. Use additional concepts to refine your answer set later.
   - Use "not" or "except" to exclude a term.
3. Click **Search**.

Continued

Tip
You can include up to three synonyms or acronyms for a concept. Place them in parentheses immediately following the concept and separate them with commas. E.g., cat (kitten, feline, felis catus)



SciFinder returns a set of **Topic Candidates**.

4 Select the answer set that you want to use from the list.
- Click the box to select an option. A green checkmark indicates it has been selected.

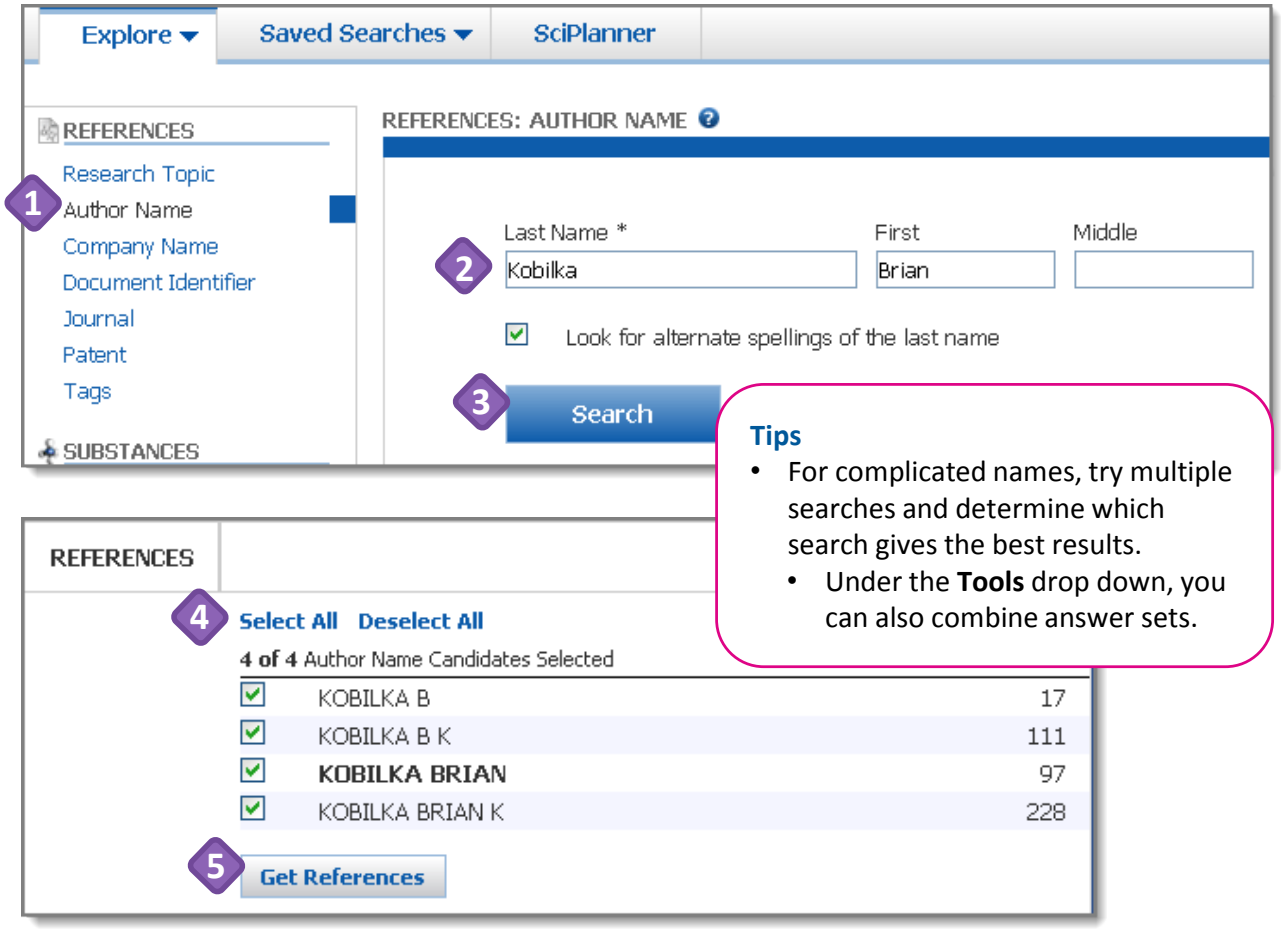
5 Click **Get References**.

SCIFINDER CONSIDERS TERMS TO BE...	WHEN THE TERMS ARE FOUND...
"As entered"	Exactly as you have entered them.
"Closely associated with one another"	Within the same sentence or title.
"Present anywhere within a reference"	Anywhere (perhaps widely separated) within a record's title, abstract, or indexing.
"Containing the concept"	Somewhere in the record.

Tip
All concepts "present anywhere in the reference" is often a good starting point. If the number of references is too large or you find many non-relevant references, consider selecting the narrower option in which all of the concepts are "closely associated with one another."

Now what?
After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Search by Author Name



Tips

- For complicated names, try multiple searches and determine which search gives the best results.
  - Under the **Tools** drop down, you can also combine answer sets.

1. To begin, click **Author Name**.
2. Enter as much of the name as you know.
   - Only the **Last** name is required. Include the **First** and **Middle** names or initials to improve the search results.
   - Enter punctuation (spaces, hyphens, etc.) as if you were writing the name.
   - Replace special characters with equivalent character(s), e.g., ae replaces ä. Consult the online help for more information about special characters.
   - For optimal retrieval, "Look for alternative spellings of the last name" is selected by default.
3. Click **Search**.
4. SciFinder returns a list of authors. The number of references associated with each name appears on the right.
   - Click the box next to any name(s) you want to select. A green checkmark appears.
5. Click **Get References**.

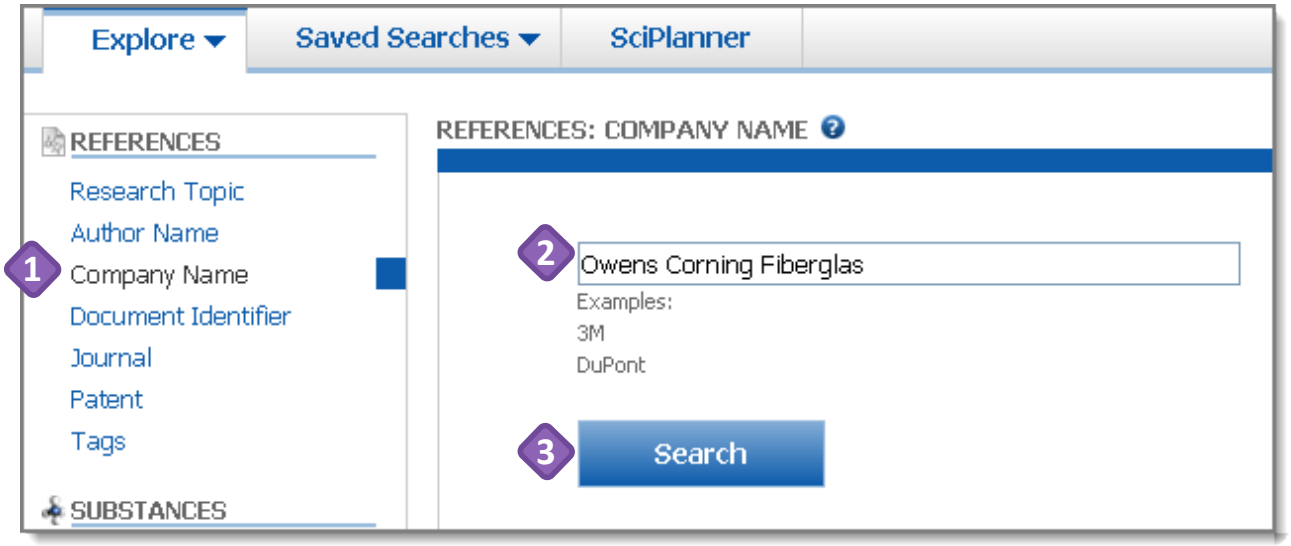
Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Tip

Create a Keep Me Posted (KMP) automatic alert if you want to know when new records for this author are added to the database. See the "Create and Manage Alerts (KMPs)" guide for more information.

Search by Company Name



1. To begin, click **Company Name**.
2. Enter the name of one organization into the query entry text box.
3. Click **Search**.

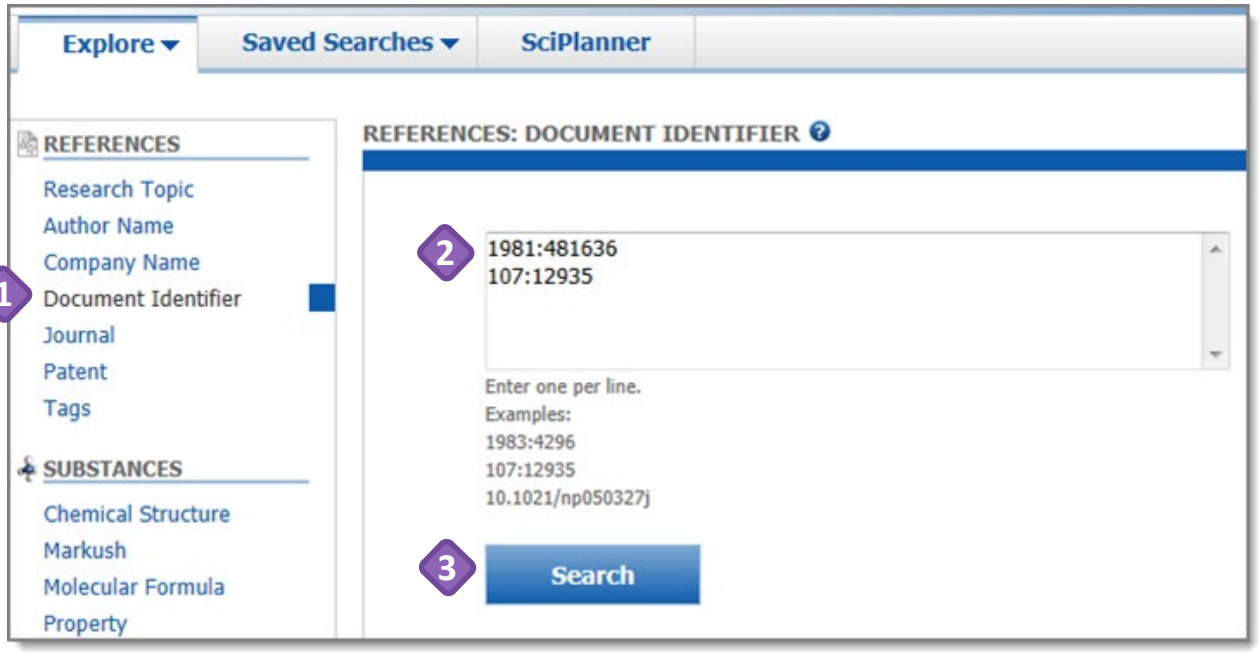
Tip
To see all of the name variations that SciFinder considered, analyze the answer set by Company/Organization. See "How to … Work with Reference Answer Sets" for more details.

Company Name Searching Guidelines

- SciFinder considers various spellings, acronyms, abbreviations, and related terms when retrieving results. It does not consider mergers and acquisitions.
- SciFinder automatically searches common synonyms and abbreviations. For example, entering "Company" or "Co." returns the same results.

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Search by Document Identifier



1. To begin, click **Document Identifier**.
2. Enter up to 25 identifiers, one per line, in the query entry text box.
3. Click **Search**.

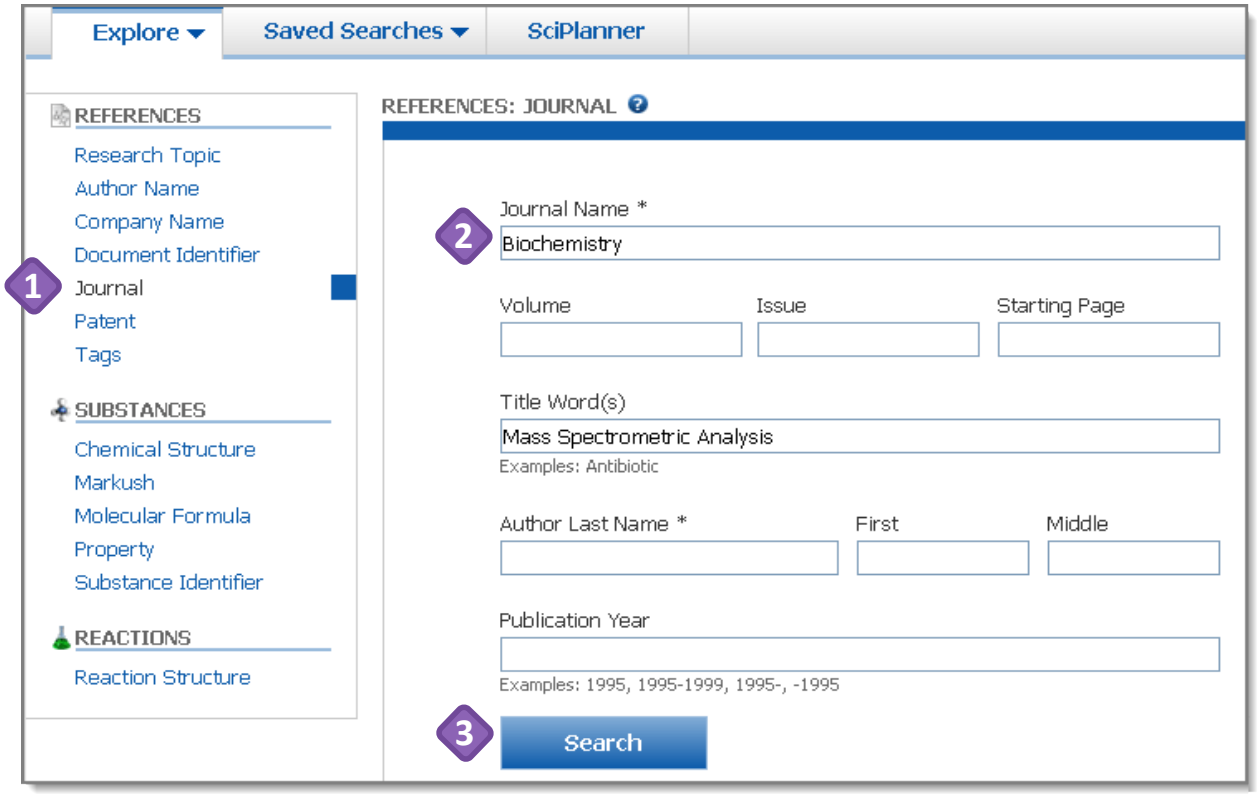
Tip
SciFinder ignores punctuation and accepts both two-digit and four-digit formats for years. Therefore, the search term 1983:4296 will retrieve both the PubMed ID 834296 and the CAplus Accession Number 1983:4296. Select the document of interest when you review the answers.

Searchable Document Identifiers

TYPE OF IDENTIFIER	EXAMPLE
Accession number: A unique number applied to a record when it is put into the database. It begins with the year that the document entered the database.	CAplus: 2012:1527010 MEDLINE: 1998010009
Document number: A sequential identification number that is assigned to a document (before the document enters the database).	CAplus: 107:12935 Medline: 22893704 (also called a PubMed ID number)
Digital object identifier (DOI): an alphanumeric character string that uniquely identifies an electronic document over the course of its lifetime.	10.1021/jp204843r

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Search by Journal



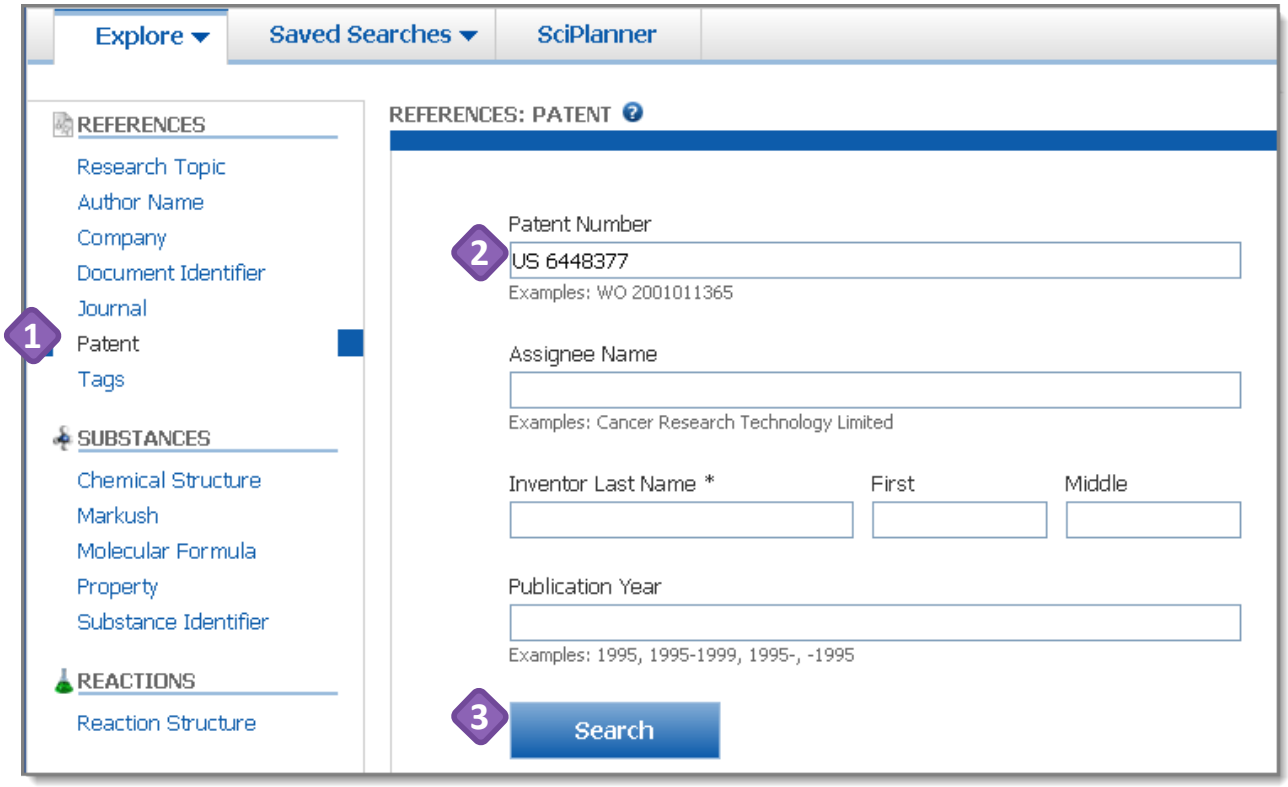
1. To begin, click **Journal**.
2. Enter a **Journal Name** (required).
   - Enter data in the additional fields to retrieve more specific answers.
3. Click **Search**.

Tip
Create a broad search by using title words, only a journal name or only a last name. Narrow search results by using a full title, the journal name, issue and starting page, the author's full name, or a combination of these items.

FIELD	DATA ACCEPTED
Journal Name	• Full name, abbreviation, or acronym • Abbreviations or acronyms must not contain spaces or punctuation • Maximum of 30 characters
Volume	Number (38) or alphanumeric string (45a) • A Journal Name must be specified before a Volume, Issue, or Starting Page can be recognized
Issue	Number (16) or month (June)
Starting Page	Number (46), letters (iii), or alphanumeric string (m287)
Title Word(s)	Key words, a partial title or a full title

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Search by Patent



1. To begin, click **Patent**.
2. Enter a **Patent Number**.
   - Acceptable patent numbers include any number that identifies a patent, such as patent application numbers, priority application numbers, and patent numbers.

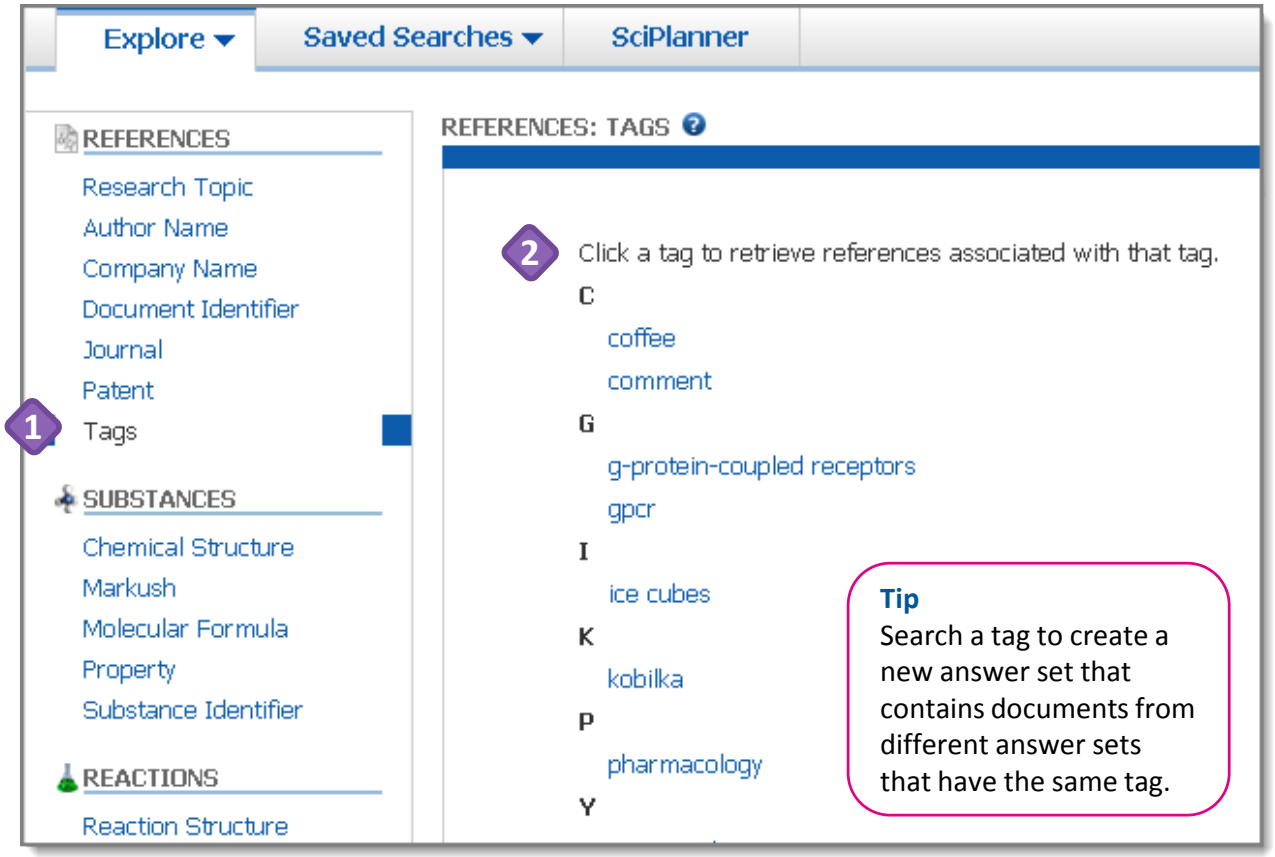
TYPE OF IDENTIFIER	EXAMPLE
Patent Application Number	WO 2012-US29090
Priority Application Number	US 1996-15450P
Patent Number	JP 2001519650

   Alternatively, you can enter an **Assignee Name** or **Inventor Name**.
   - Enter data in several fields to create a narrower search.
3. Click **Search.**

Tip
One number can retrieve both a granted patent and an unrelated patent application. You can easily select the record of interest while reviewing the search results.

Now what?
After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Search by Tags



A tag is a user-defined keyword that you can apply to references in one or more answer sets. When you save an answer set, the tag is saved with the associated reference. Search a tag to retrieve any references to which the tag was applied.

1. To begin, click **Tags**.
2. From the displayed list, select the tag that you want to search.

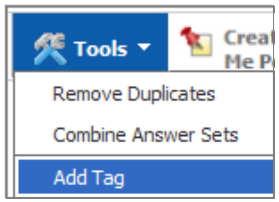
SciFinder retrieves all of the records to which that tag has been applied. This feature allows you to pull references from several different answer sets and place them all into a new answer set .

Now what?

After you click a keyword, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to… Work with Reference Answer Sets."

Tip

When reviewing your search You can apply tags to records results by selecting **Add Tag** from the **Tools** menu. In the dialog box, enter the key word(s) that you want to apply as a tag. After they are created, tags become searchable.

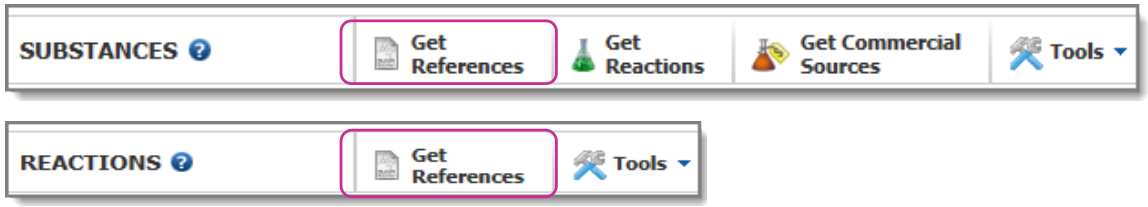


Manage Your Searching

1. Start a new **References**, **Substances** or **Reactions** search.
2. Access **Saved Answer Sets**, **Keep Me Posted** automated alert results, and your search **History**.
3. Open the **SciPlanner** interactive workspace where you can organize your reference, substance and reaction search results.
4. Access **Preferences** and **SciFinder Help** options: **Help**, **Training**, **What's New** and **Contact Us**.
5. Click **Save**, **Print** or **Export** to open a dialog window and initiate these procedures.

Tip: Other Ways to Create a Reference Answer Set

- You can also create a reference answer set by starting with a reaction or substance search. After you get a reaction or substance answer set, just click the "**Get References**" icon at the top of the page.



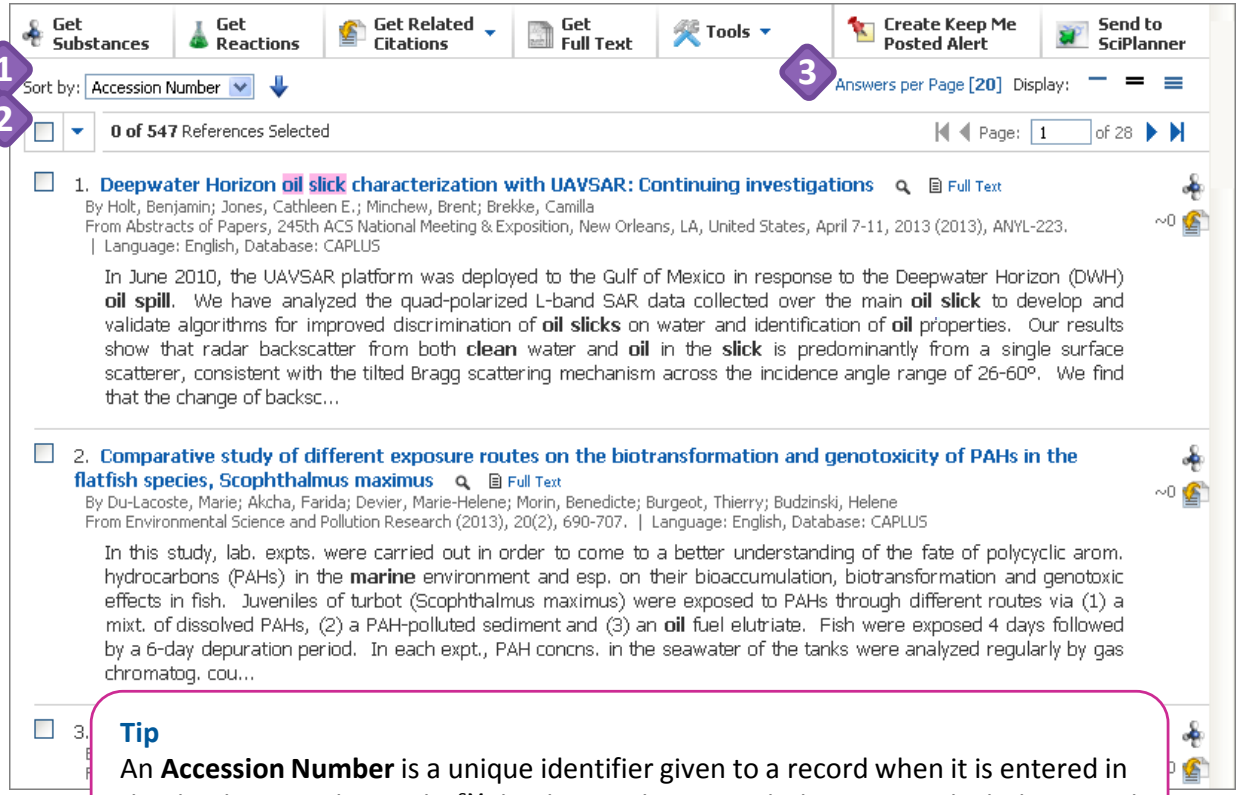
How to Work with a Reference Answer Set

SciFinder®

Easily identify and isolate references of interest

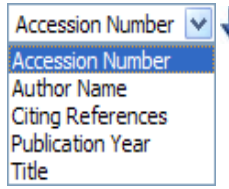
Quickly retrieve relevant information from the world's largest, publicly available reference database for chemistry and associated sciences. This guide provides an overview of some of the sort, refine, and analyze tools for confidently evaluating and narrowing even a large answer set. From there, a single click retrieves substances or reactions associated with your references. For more detailed information and additional training resources, consult the online help or visit www.cas.org/training/scifinder.

Reference Search Results



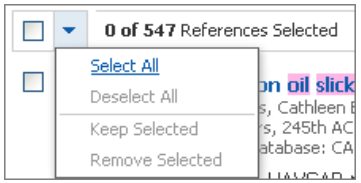
Tip
An **Accession Number** is a unique identifier given to a record when it is entered in the database. In the CAplus[SM] database, it begins with the year in which the record is put into the database, followed by a colon and sequential numbering.

1. By default, references in your answer set are sorted by **Accession Number**. Click the drop-down arrow for other sort options.



   - The blue arrow indicates the sort order (e.g., newest to oldest or alphabetical). Click the arrow to reverse the order.

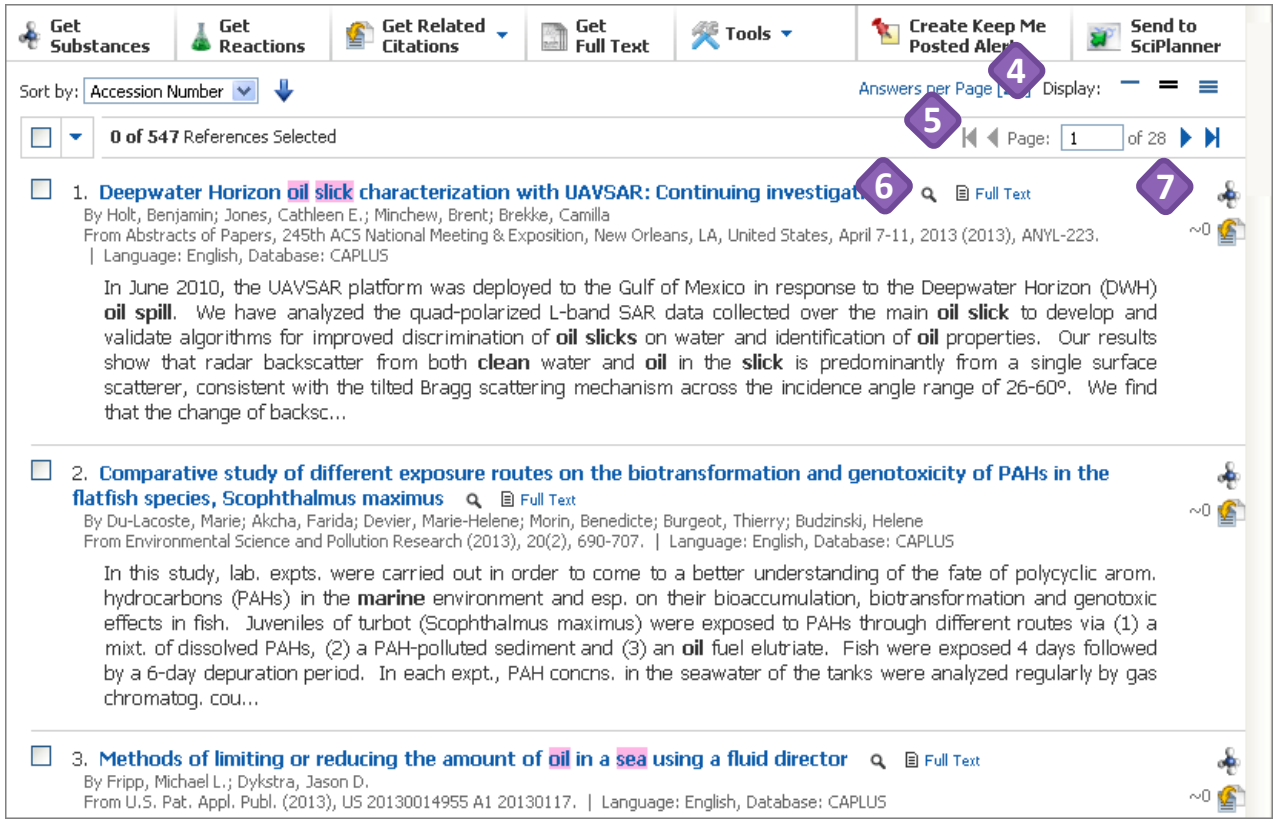
2. Below the **Sort by** options, the number of references in the answer set and the number that have been selected are displayed.
   - Click the blue drop-down arrow to select all of the answers.



   - To select individual answers, click the box to the left of an answer number.

3. Specify the number of answers displayed per page.

Continued



Tip

With the **Full Text** link, European and US patents are often immediately available via Espacenet. If your company purchases journal subscriptions, your Knowledge Center or SciFinder Administrator can set up the CAS Full Text Options page to let you immediately access records from those journals from your desktop.

4 Three **Display** options are available:

- One bar shows the bibliographic information.
- Two bars shows the bibliographic information and a partial abstract. It is the default, shown here.
- Three bars shows the bibliographic information and the full abstract.

5 Use the page controls to navigate through your answer set.

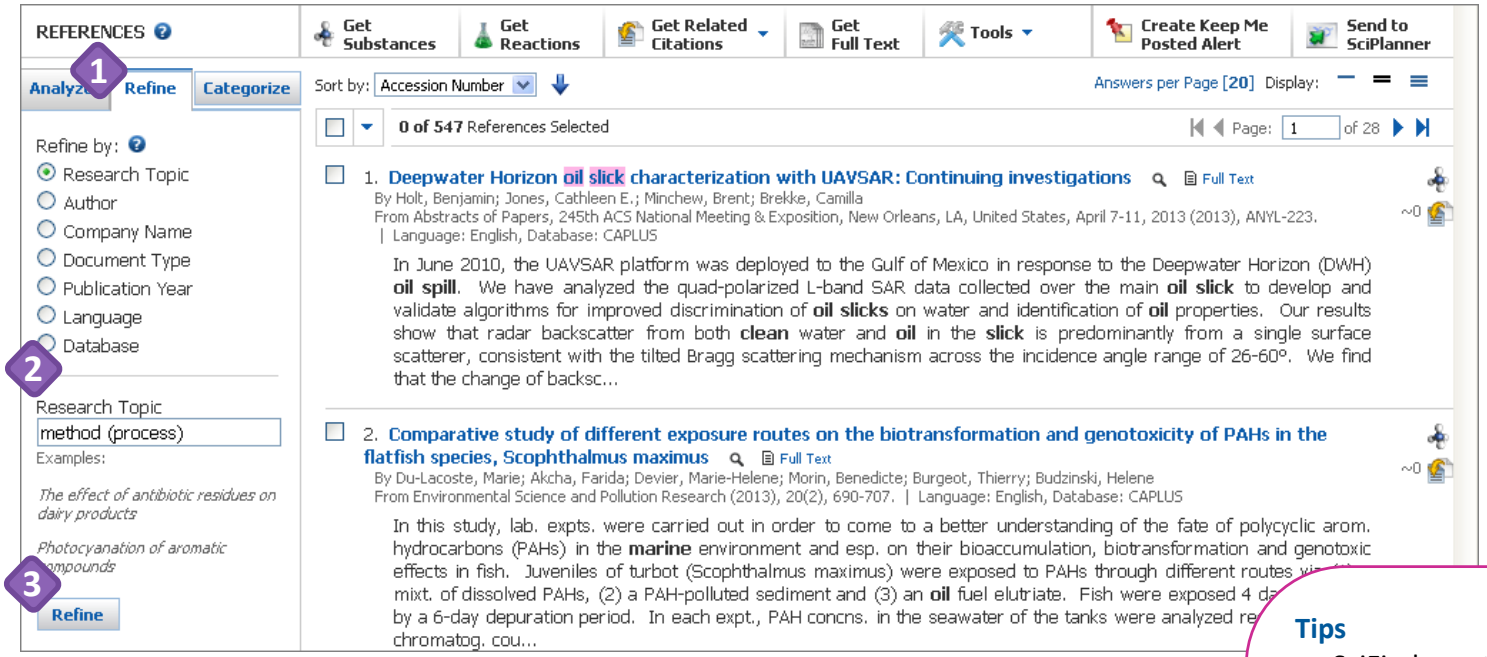
6 The magnifying glass is a link to a "**Quick View**." Click it to open a new window that contains the reference details. Close the window to return to your active session.

Click the **Full Text** link to launch the **CAS Full Text Options** page (not shown).

7 Click the molecule icon to see the **Substances** indexed for a document (not shown). CAS analysts identified these substances as being important to the science reported in the document.

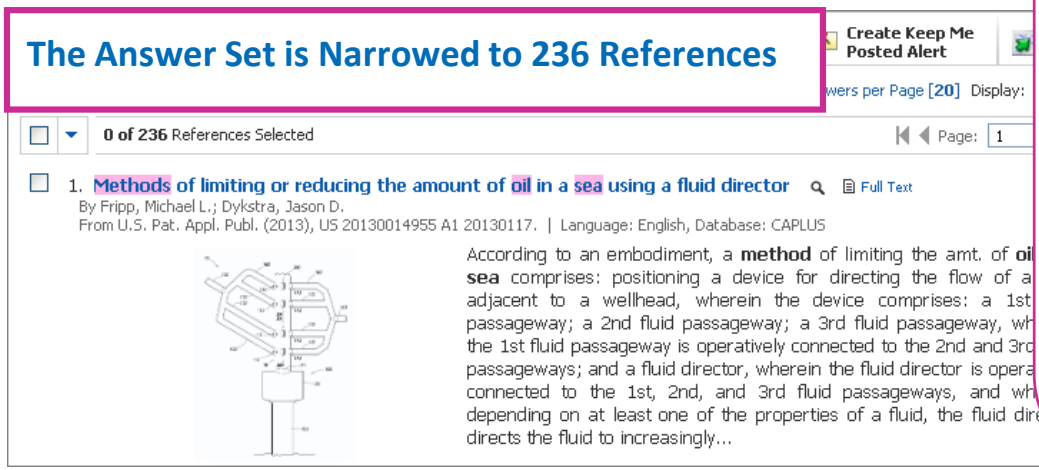
Click the **Citings** icon to retrieve the documents that have cited this reference.

Narrow an Answer Set with Refine Options



1. Click the **Refine** tab and click a radio button to select a **Refine by:** option.
2. Specify additional criteria below the refine options.
   - Here, the answer set is refined to include answers with two additional concepts.
   - A synonym is included in parentheses.
3. Click **Refine**.

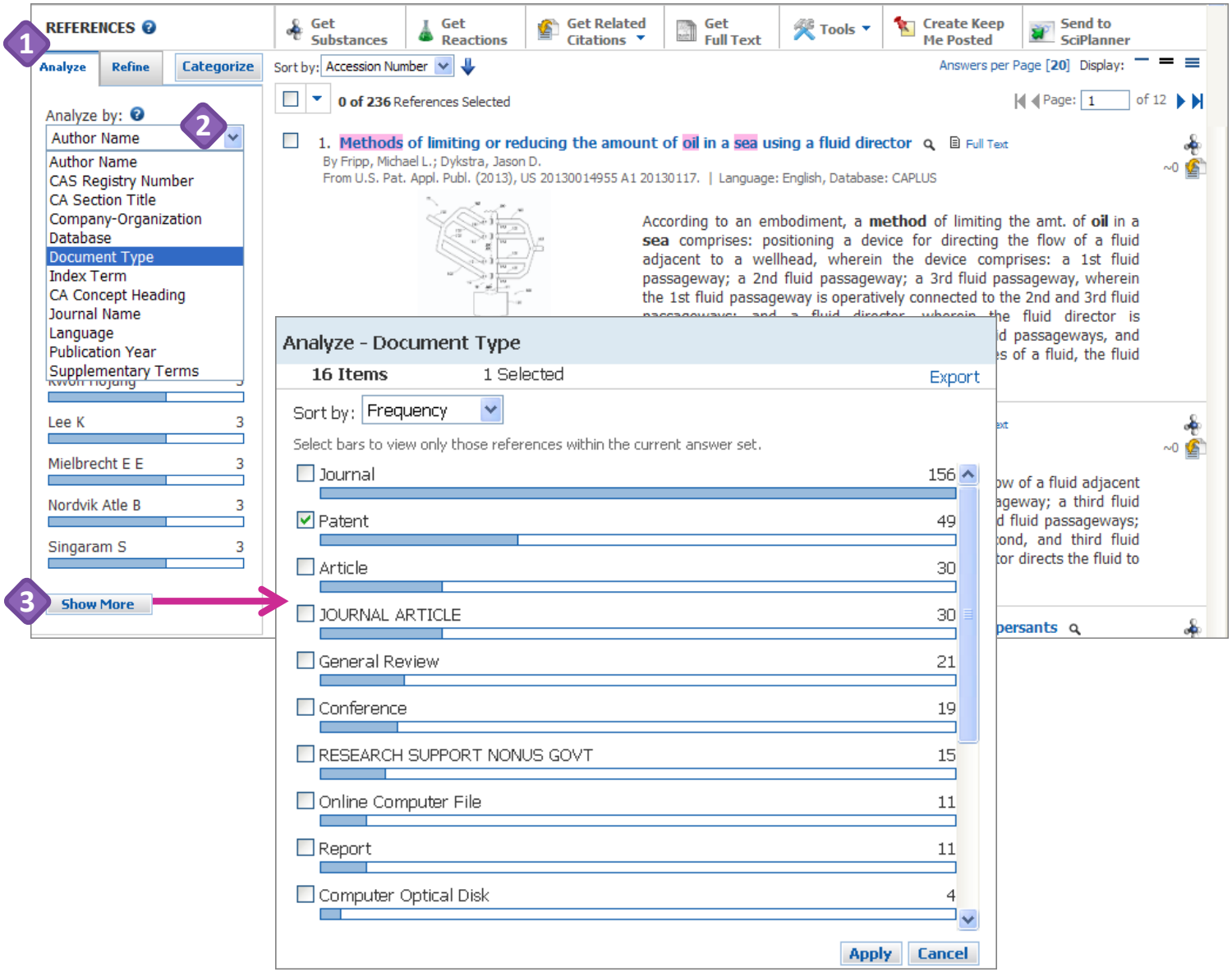
The Answer Set is Narrowed to 236 References



Tips

- SciFinder automatically searches for both singular and plural forms of a word (**method**; **methods**), alternate word endings and forms (**clean**; **cleaning**), and common synonyms (**ocean**; **sea**; **marine**) to save you time and increase comprehensiveness.
- When searching or refining by **Research Topic**, you can include up to three synonyms, separated by commas and enclosed in one set of parentheses.
- When you refine by **Research Topic**, both the old and new hit terms are highlighted in the title and are bolded in the abstract.

Evaluate Answers with Analyze Options



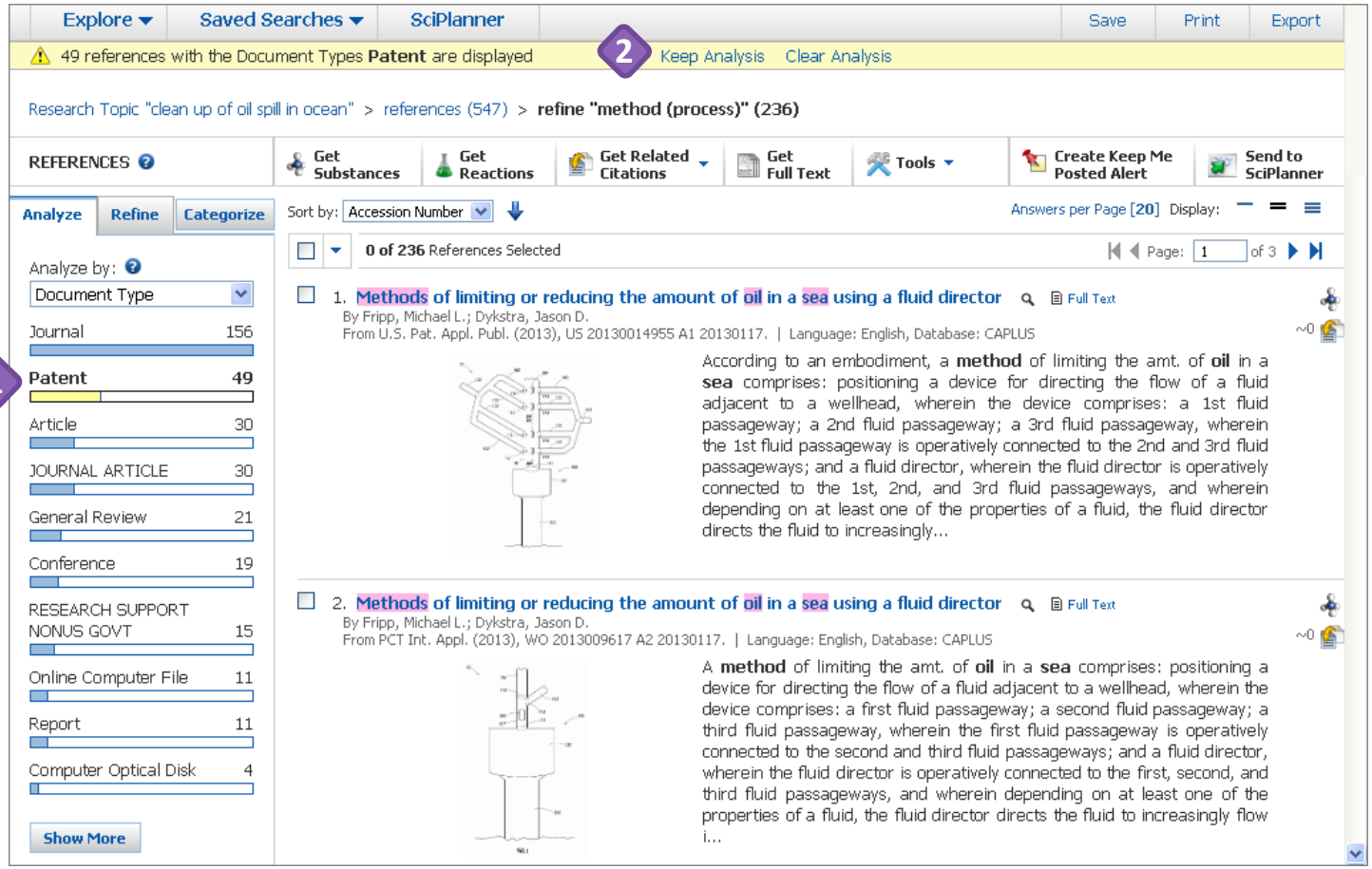
1. Click the **Analyze** tab. By default, the answer set is analyzed by **Author Name**.
2. Click the drop-down arrow to see the available **Analyze by:** options.
3. Click **Show More** to see additional data when it is available (see inset), or to select more than one analysis subset.
   - E.g., it is useful when you want to select several variations of an author's name.

Continued

Tip

Some document types are listed in all capital letters. These subsets are unique to MEDLINE® (aka PubMed). The 30 **JOURNAL ARTICLE(s)** in MEDLINE are also included in the **Journal** subset which contains the documents from both MEDLINE and CAplus.

Narrow an Answer Set after Analyzing



Here, the answer set has been analyzed by **Document Type**.

1. Click an analysis bar to display that subset of answers.
   - Parts of other analysis bars turn yellow if any records fall into more than one subset.

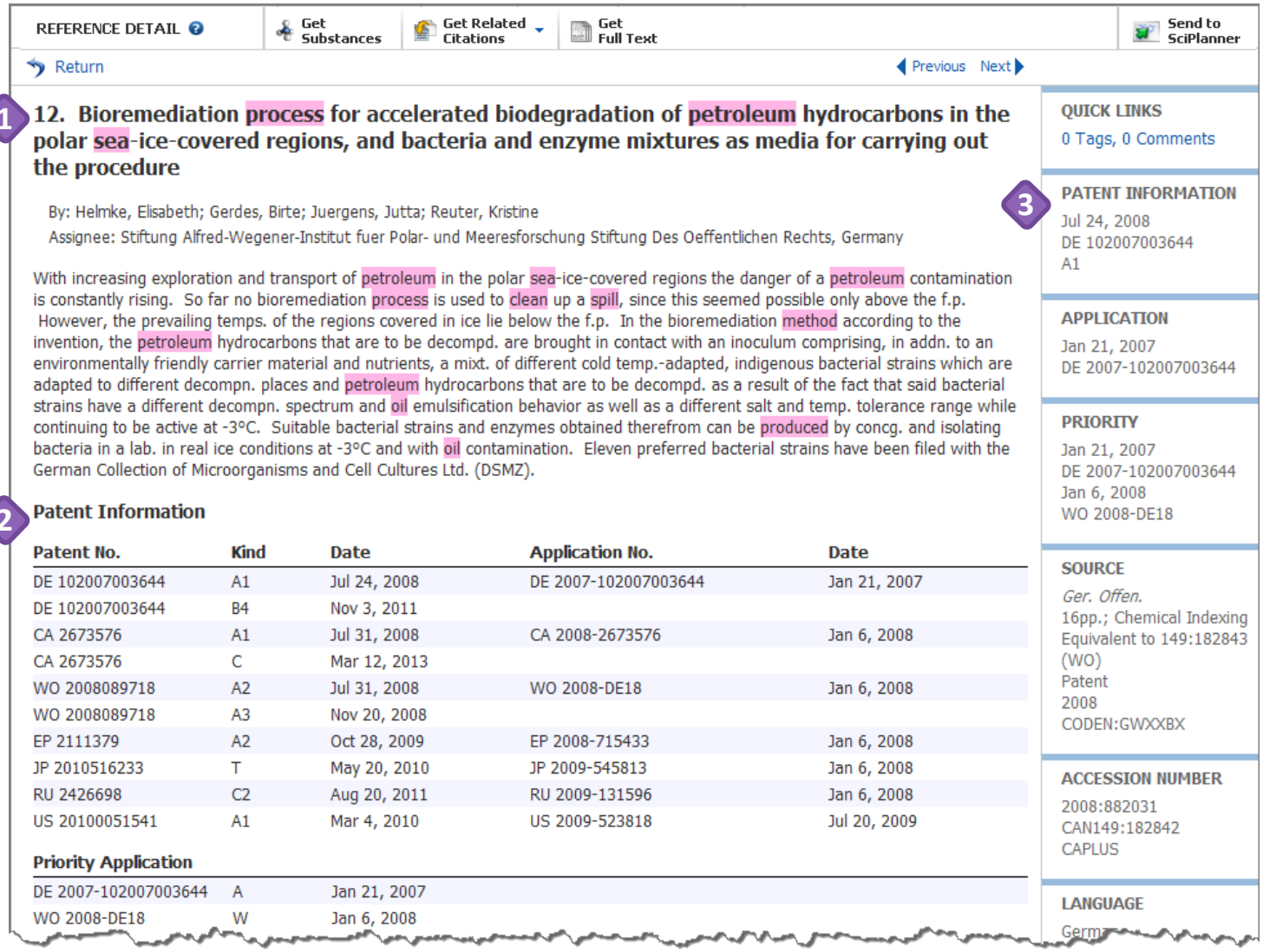
2. The yellow status bar indicates the answers that are currently displayed.
   - Click **Keep Analysis** to make these answers your new answer set.
   - Click **Clear Analysis** to return to your original answer set.

Or, select a different subset on the **Analyze** tab to view those records.

Tip

The **Analyze** capability is an effective way to learn more about your results because you can use **Clear Analysis** to return to the original answer set. After you have explored the answer set several ways, you can then decide how you want to narrow it, make that selection, and then click **Keep Analysis** or choose to narrow the answer set using other techniques.

Reference Detail



When you click the blue title of a reference in your answer set, the **Reference Detail** is displayed.

1 At the top, the title, authors, and abstract are shown.

2 For patents, below the abstract you will see the **Patent Information** table.
- The **Priority Application** is the first application filed with a patent office.
- WIPO patents will always list the WO patent application number as well as the first country where the patent application was filed.

3 On the right are details about the publication **Source**, the associated **Company/Organization**, the **Accession Number**, the **Publisher** and the original **Language** (after 1967).

Continued

5 CAS scientists extract key scientific terms and concepts from each document. This **Indexing** is added to each reference.

- Each of the 80 Chemical Abstracts **Section** codes covers one broad scientific discipline.
- The **Concepts** are standardized, uniform index terms.
- **Substances** are the chemical compounds critical to the science of the document.
- **Supplementary Terms** are relevant keywords for that document. They are not controlled vocabulary.

6 Below the **Indexing** are the **Citations** for the document.

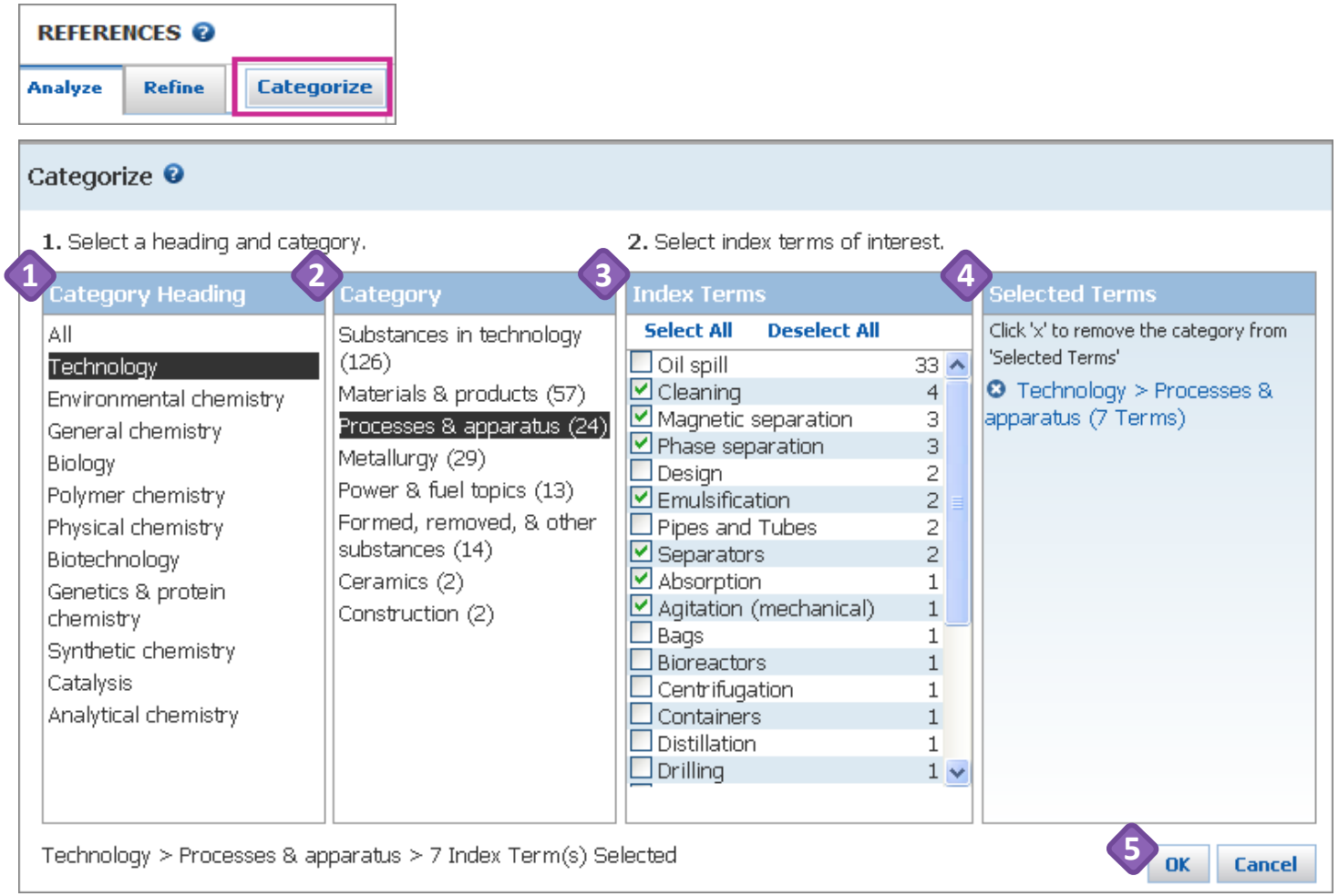
- If the citation is blue, you can click it to see the database record for that reference.

7 You can apply or **Edit Tags** to documents here.

- You can search **Tags**. This feature allows you to combine records from many answer sets into one answer set.
- You can also add a tag (up to 500 records) under the **Tools** button on the toolbar.

8 You can add **Comments** to individual records as reminders about important information or as project identifiers.

Use Categorize to Identify Specific Records



Tip

Add **Index Terms** to your search query. Begin with a broad research topic search. In the answer set, find a couple records that are very relevant. Look at the index terms for those documents. Then, re-run the search with these index terms added to your search query.

CAS scientists identify key terms and concepts that they include in the indexing of each database record. These index terms are standardized and uniform to describe the science in the original document.

Categorize lets you find the references associated with selected indexing.

Click the **Categorize** button to launch the **Categorize** window.

1. Select a **Category Heading**.
2. Select a **Category** of interest.
3. Select one or more **Index Terms** by clicking the box to the left of a term.
4. In the **Selected Terms** summary box, click the blue circle with the white "X" to delete a term.
5. Click **OK** to narrow your search based on the selected index terms.

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.
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 Substances** to retrieve substances for part or all of your answer set.
8. Click **Get Reactions** to retrieve reactions for part or all of your answer set.
9. Click **Get Related Citations** to **Get Citing** or **Get Cited** references.
10. Click **Get Full Text** to launch **CAS Full Text Options**.
11. Click the **Tools** drop-down arrow to access **Remove Duplicates**, **Combine Answer Sets** and **Add Tags**.
12. **Create Keep Me Posted**, when active, allows you to create an automated alert based on the current search strategy.
    - See "How to… Create and Manage KMP Alerts" for more information.
13. Click **Send to SciPlanner** to send selected answers to the SciPlanner workspace.
    - Use it to gather information for a project, create a report or export research to share with colleagues.

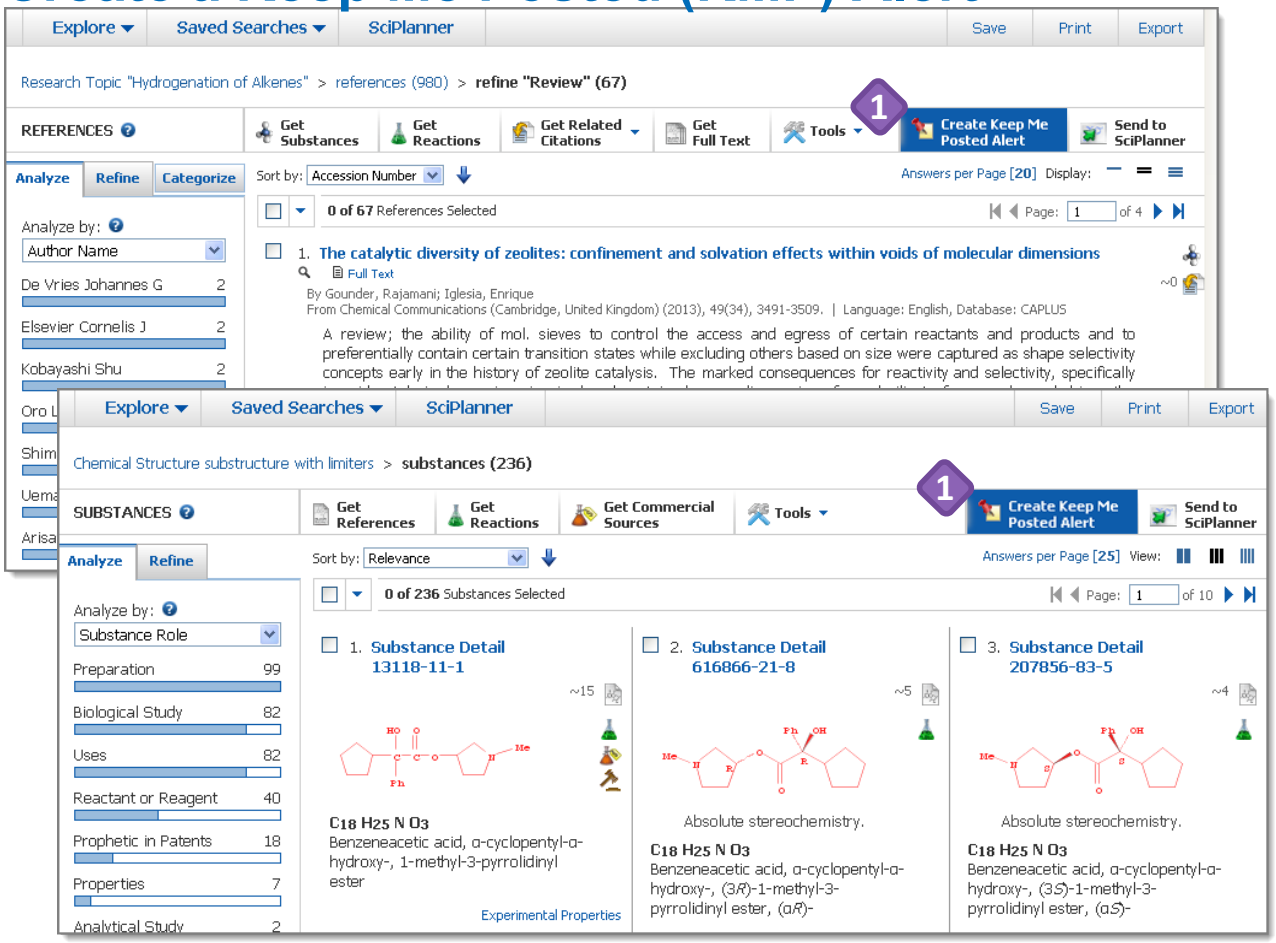
How to Create and Manage Alerts

SciFinder®

Automatic notifications keep you up-to-date on the latest developments in your field.

After you create a substance or reference answer set, you can be notified automatically when new records on your search topic are added to the database. Track competition, monitor patents or conduct business analysis with this convenient feature. Additional information about Keep Me Posted alerts is available in the online help or in additional training materials at [www.cas.org/training/scifinder.](www.cas.org/training/scifinder)

Create a Keep Me Posted (KMP) Alert



SciFinder searches databases that are updated daily. You can set up a KMP alert so that you never miss important, new information. To begin, conduct a search on your topic of interest.

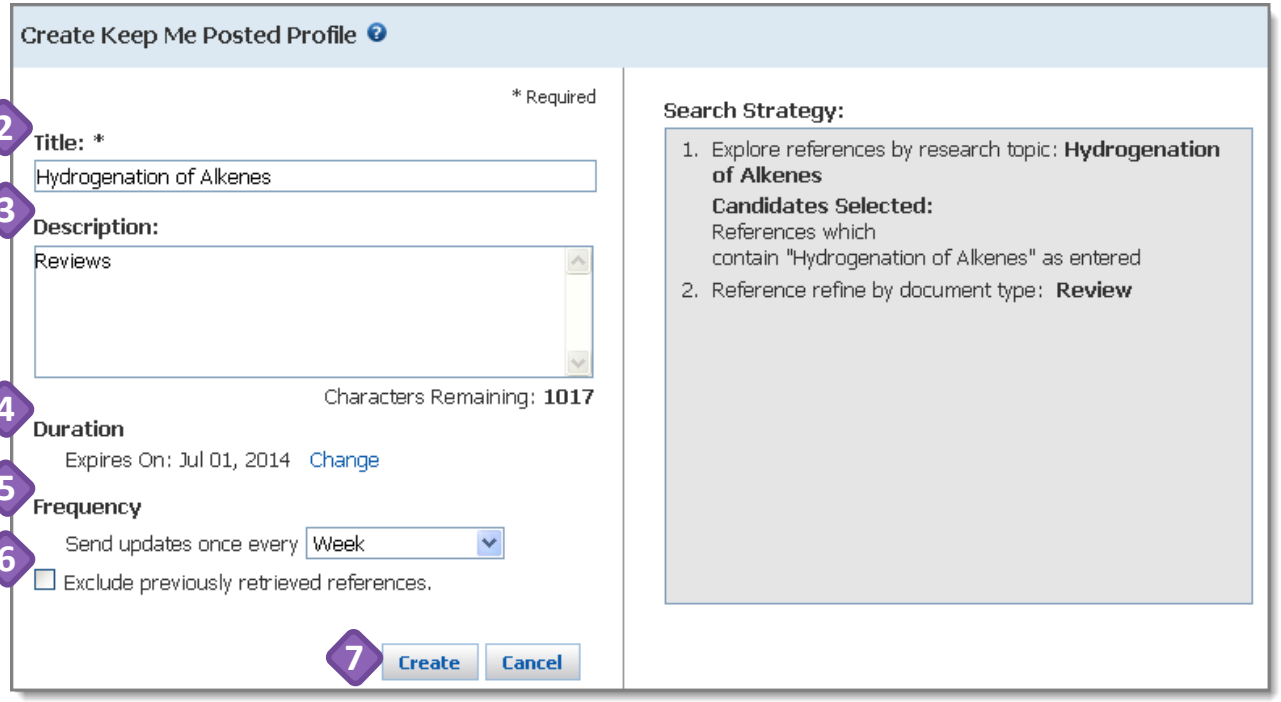
1 When the **Create Keep Me Posted Alert** button is present, you can create an automated KMP alert based on your search.

In the following example, the alert is created for a reference search. The same **Create Keep Me Posted Alert** option is also available if you want to be notified about new data related to substance searches.

Continued

Tips

The KMP button will not be active if your search strategy includes steps that cannot be included in a KMP. Such steps include **Analyze** and **Categorize**. Consult the online help (?) for details.

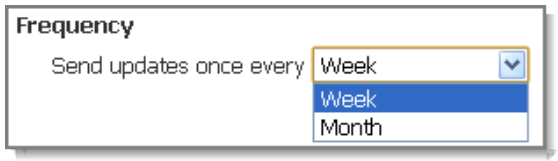


2 Enter a **Title** for your KMP profile.

3 (optional) Enter a **Description**.

4 The **Duration** of the profile is automatically set to one year from the date it is created. To change the duration, click **Change** and select the desired timeframe.

5 Specify how often you would like notifications to be sent: weekly or monthly.



6 If you select weekly, you will be notified when the bibliographic information for the record is first entered into the database and again when the indexing (substances and scientific vocabulary) is added.

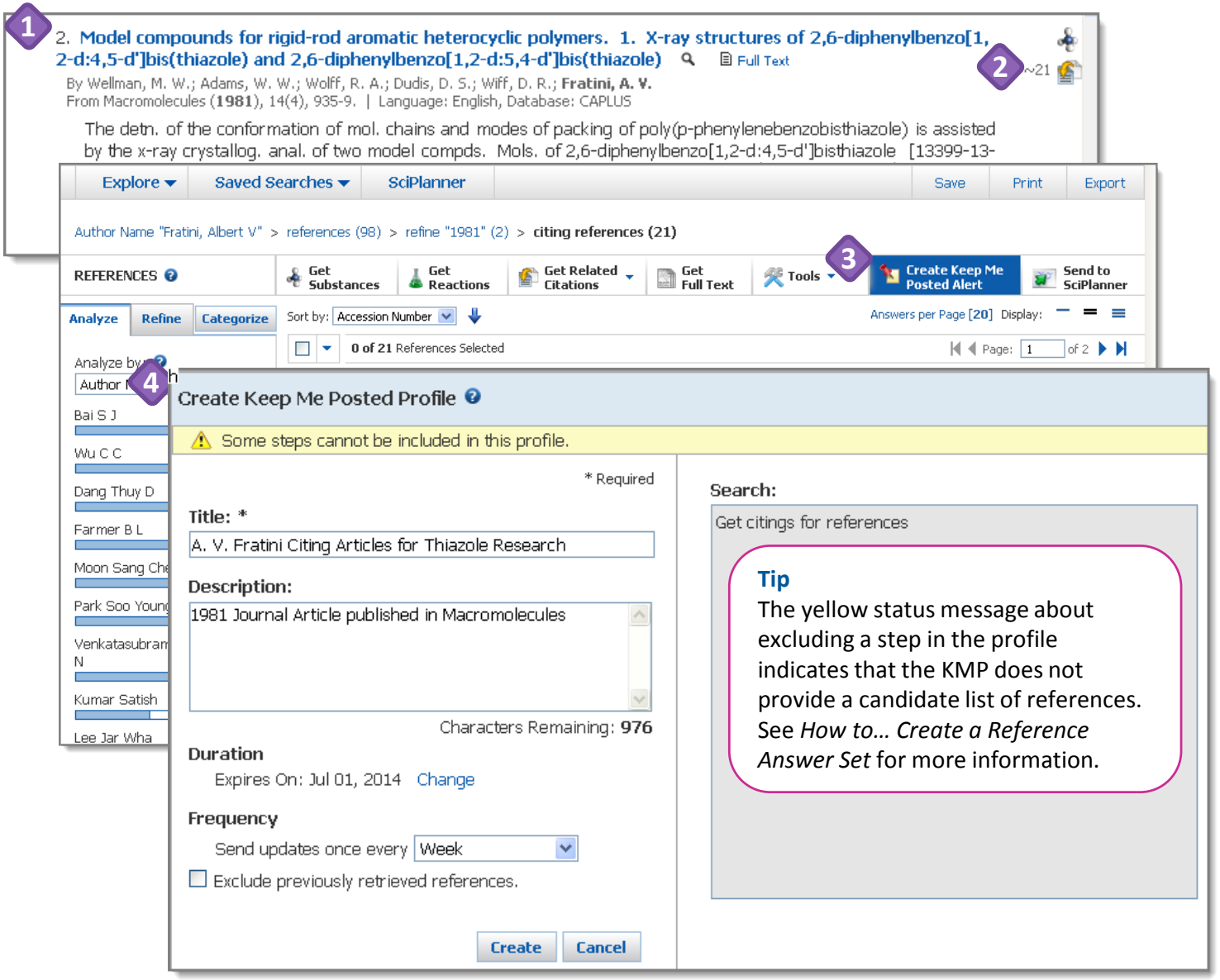
- Click the checkbox to **Exclude previously retrieved references** if the indexing is not relevant to your research needs.

7 Click **Create**. You are then returned to your active session.

Tips

- If you are interested in timely patent information, then a SciFinder KMP can help to keep you updated. Bibliographic information from nine major patenting authorities is entered into the CAplus[SM] database within two days of being issued. CAS scientists have up to 27 days to add the keyword and substance indexing to the record.
- Substance alerts do not include stereo, precision or similarity candidates.

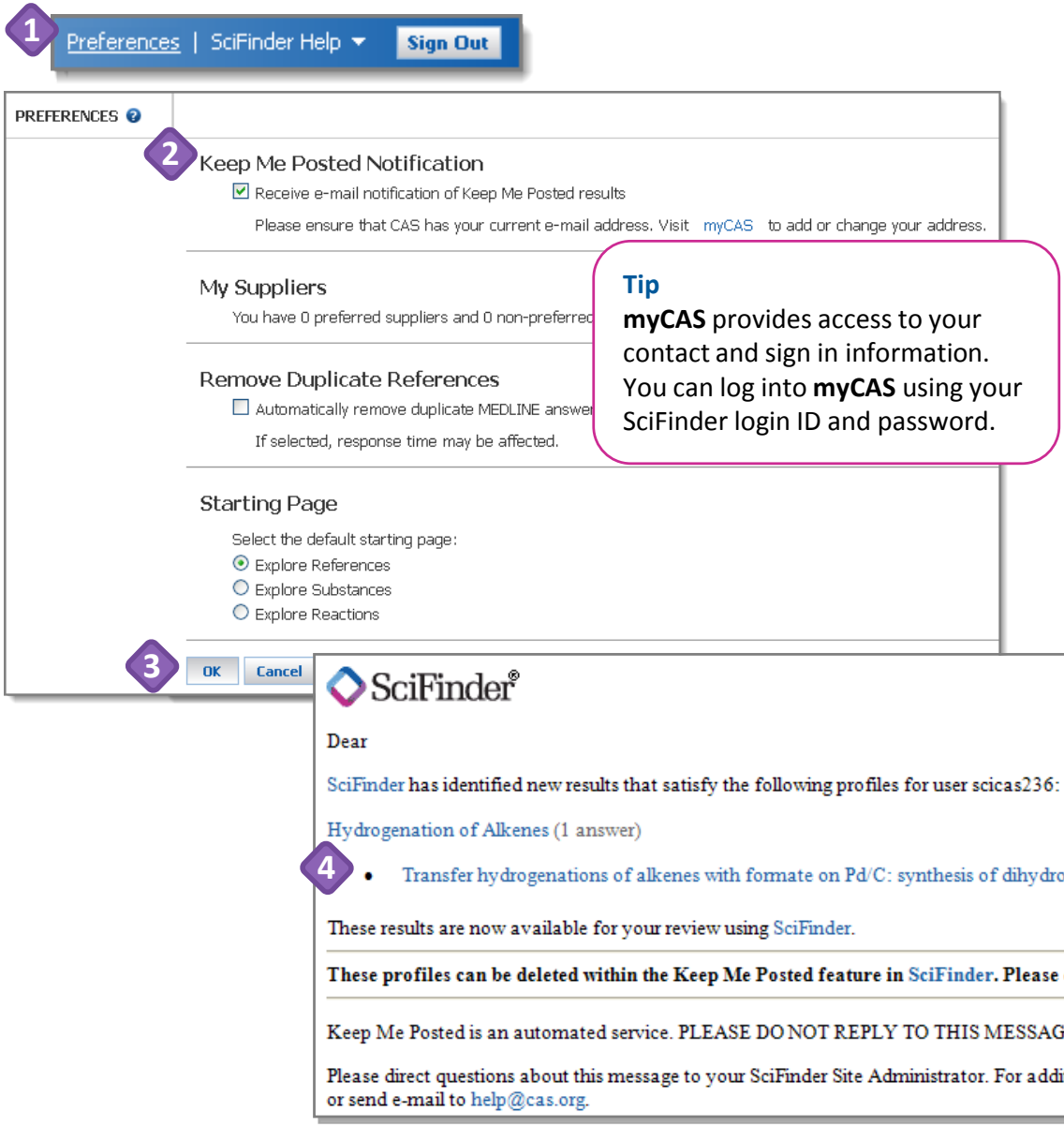
Follow Citings Using a KMP Alert



You can create a KMP alert to automatically receive a notification whenever a specified document is cited.

1. Find the document of interest.
2. Click the **Citings** icon located to the right of the title.
3. After the citing references appear, click **Create Keep Me Posted Alert**.
4. Complete the **Create the Keep Me Posted Profile**.
   - Whenever the original document is cited, then you will get an alert about it.
   - After you complete the profile, you are returned to your active session.

Set KMP Preferences



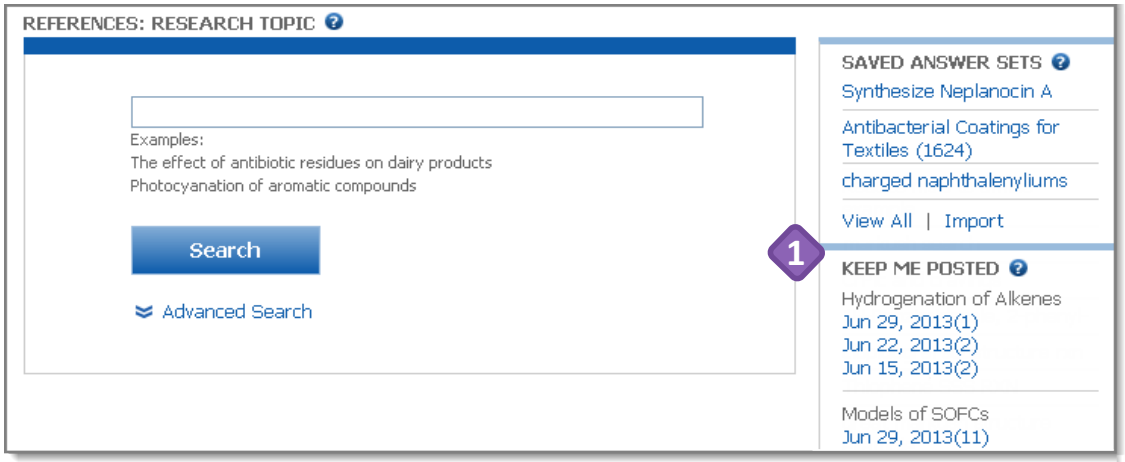
Tip
myCAS provides access to your contact and sign in information. You can log into **myCAS** using your SciFinder login ID and password.

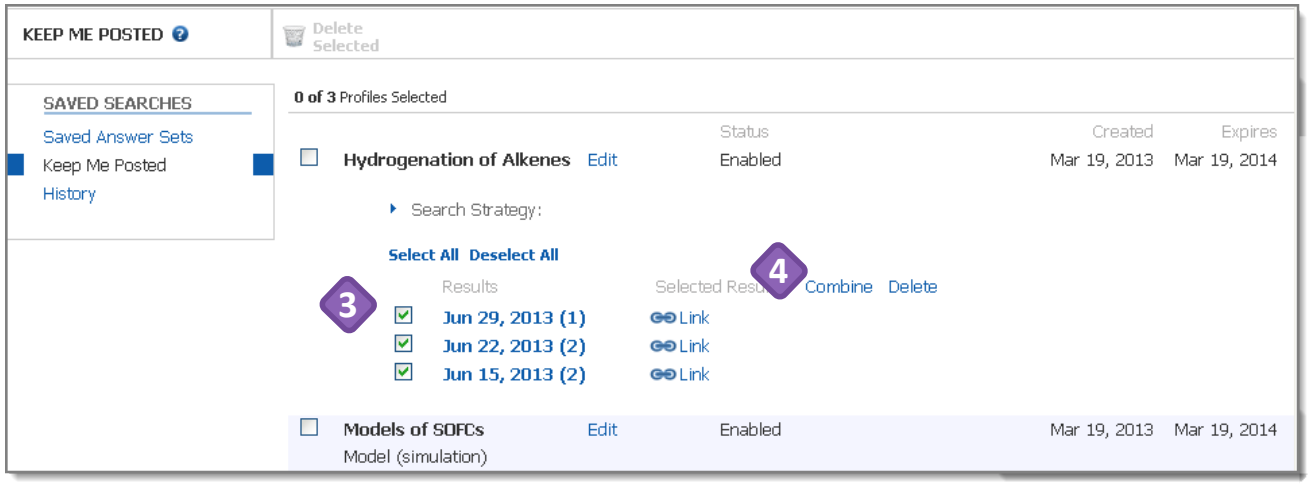
Tip
If your alert finds more than ten results, sign in to SciFinder to see all of them.

You can set your **Preferences** to receive an e-mail whenever a new KMP result is available or an existing alert is about to expire.

1. Click **Preferences** in the upper right corner of the SciFinder window.
2. Check the box to receive e-mail notifications.
   - Make sure your e-mail address is correct by clicking the **myCAS** link.
3. Click **OK** to save your **Preferences**.
4. The KMP results e-mail will contain hyperlinks for up to the first ten new titles or substances. Click a hyperlink to sign into SciFinder and open the record.

Access KMP Results





You can access KMP results in two ways.

1. On the right side of any Explore window:
   - Click a date to open the answers received on that date.
   - The number of records found on that date is shown in parentheses.

2. Click **Keep Me Posted** on the **Saved Searches** tab.
   - Click a date to open the answers received on that date.

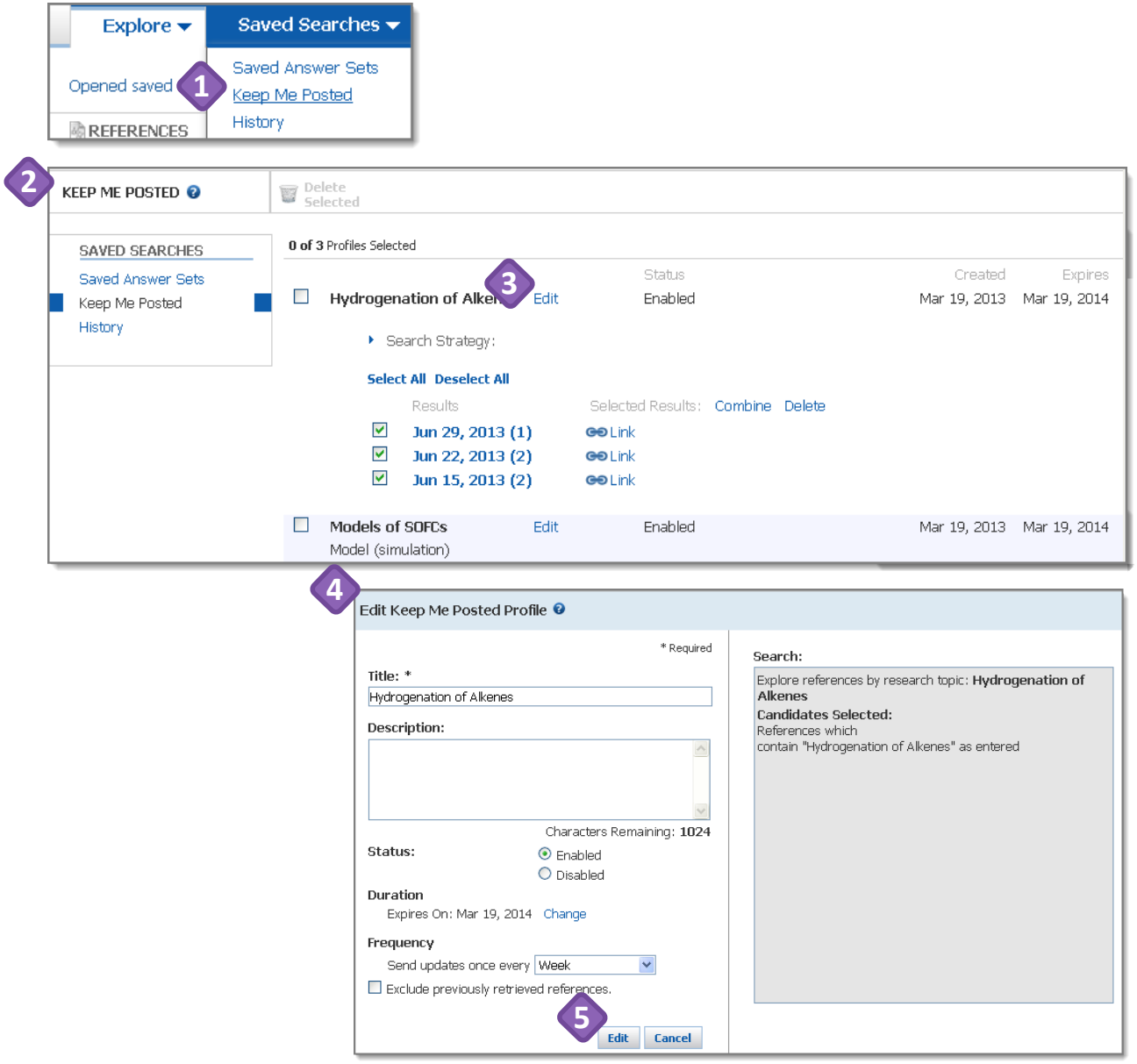
To review answers found on multiple dates simultaneously, merge them into a single answer set.

3. In the **Keep Me Posted** window, select the answer sets you want to merge together.

4. Click **Combine** and in the dialog window, select the combine both sets option.

The combined answer set will open in SciFinder so that you can review the answers.

Edit KMP Alerts



1. To review your current awareness profiles and results, go to the **Saved Searches** drop-down menu and select **Keep Me Posted**.
2. In the **Keep Me Posted** window, you can see the status of all your alerts.
3. To change a profile, click **Edit**, located to the right of the profile title.
4. Change the title, description, status, duration and/or frequency of your alert.
5. Click **Edit** at the bottom of the dialog box to save the changes.

Tip

To change the expiration date of an alert that is about to expire, use **Edit**. On the Keep Me Posted page, SciFinder also sends you a yellow status message when an alert is about to expire. This message includes a link that says **Extend 12 Months**.

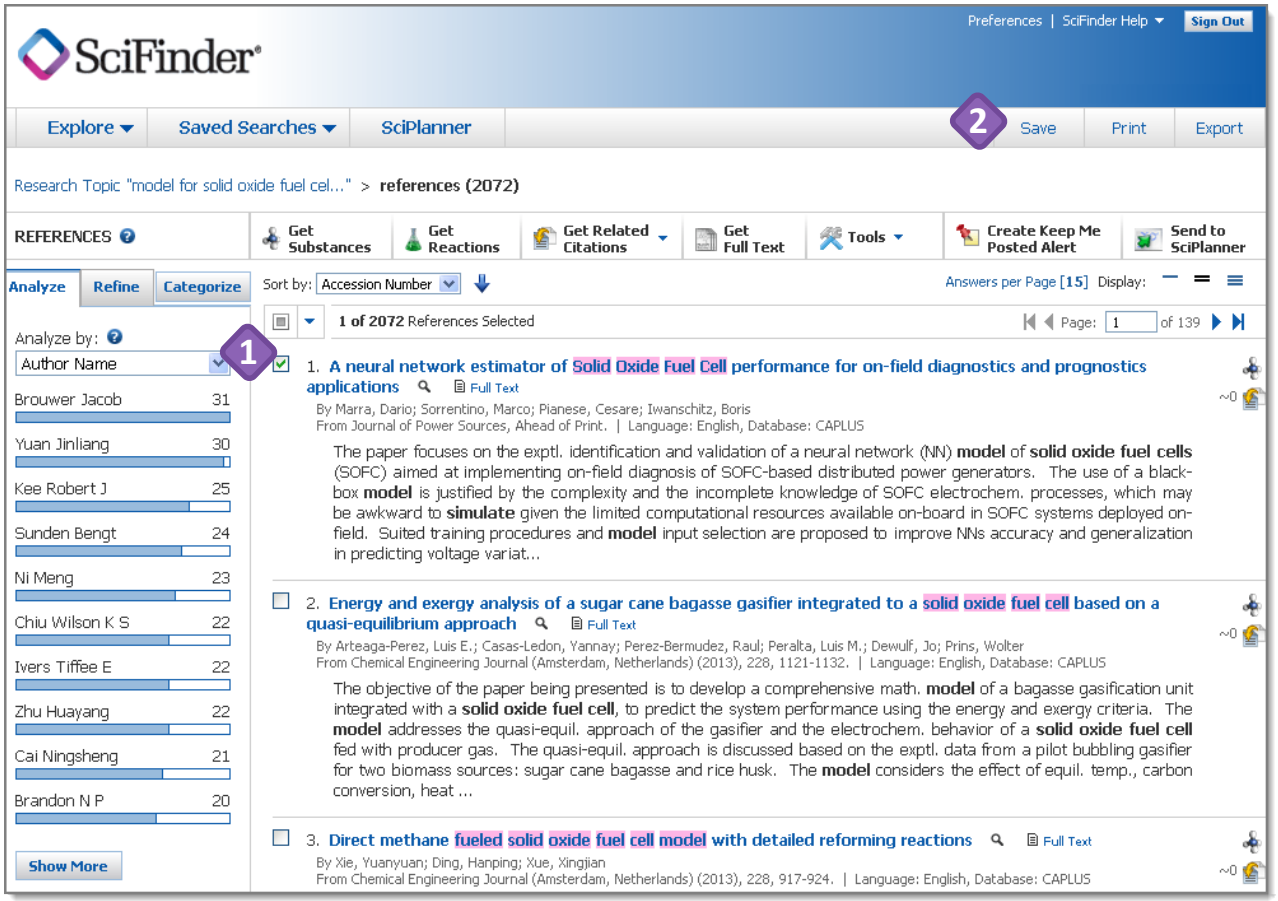
How to Save, Print and Export Answers

SciFinder®

Keep your SciFinder answers for future use

Keep answer sets for future use with print, save, and export capabilities. To generate a hardcopy of part or all of your answer set, use Print to create a .pdf file that can be viewed, saved and printed. Save your answers to the SciFinder server for future use or Export answers to your computer to use with other software applications or to share with colleagues. To access additional training resources on this and other topics, consult the online Help or visit [www.cas.org/training/scifinder.](www.cas.org/training/scifinder)

Save, Print and Export: General Information



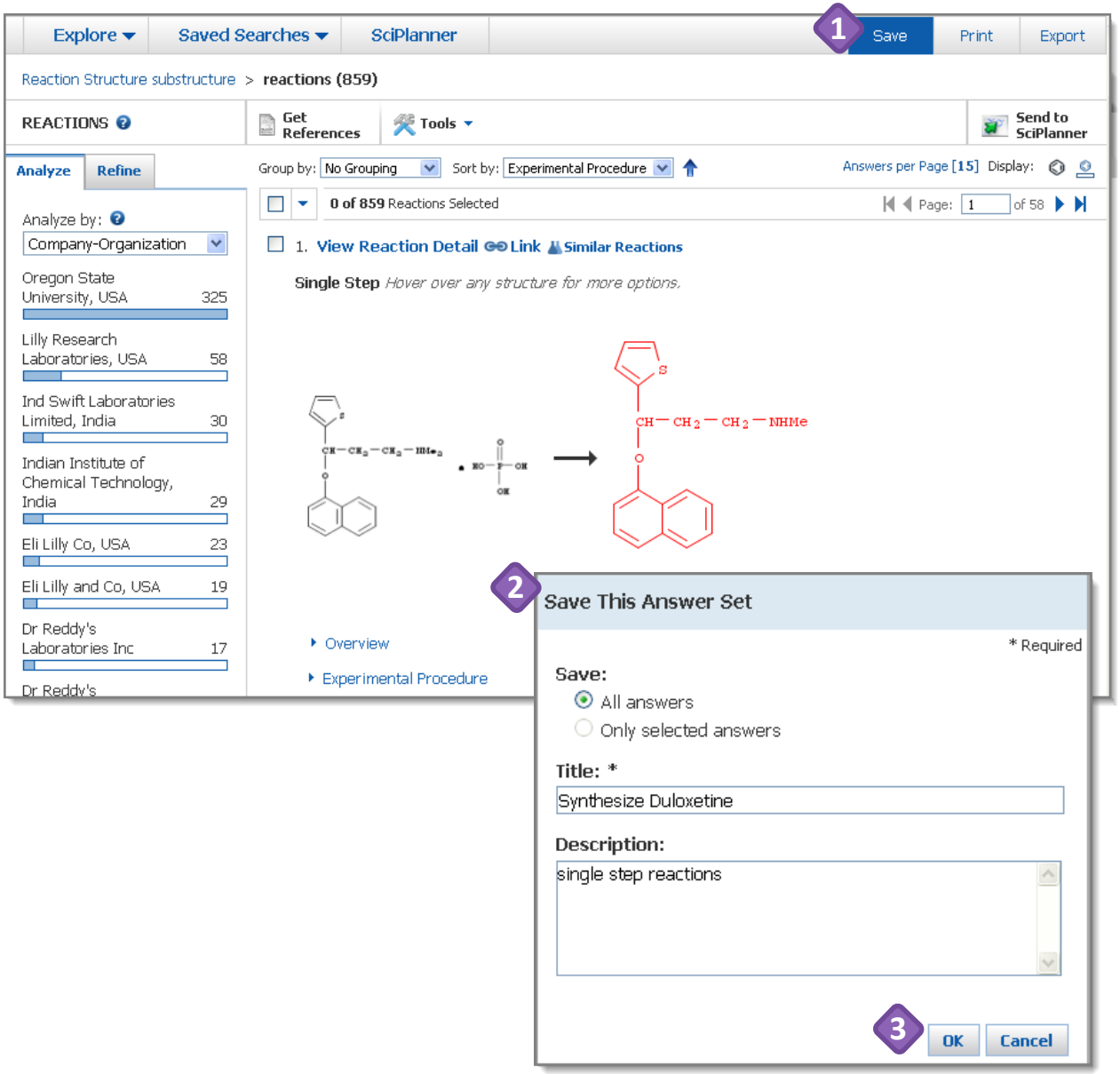
Save, Print or **Export** reference, substance and reaction answer sets.

1. By default, all answers are saved, printed or exported.
   - An option to save, print or export only selected answers is available.
   - To select answers, click the box to the left of an answer number.

2. In the upper right , click **Save**, **Print** or **Export** to launch a dialog window.
   - The options in the dialog window will vary depending on the type of answer set and whether you are saving, printing or exporting.

The following pages show examples of printing, saving and exporting answer sets.

Save Reactions Example



Use **Save** to place a file of your reference, substance or reaction answers on the SciFinder server. The answers are saved with your SciFinder login ID so that you can access them from any computer.

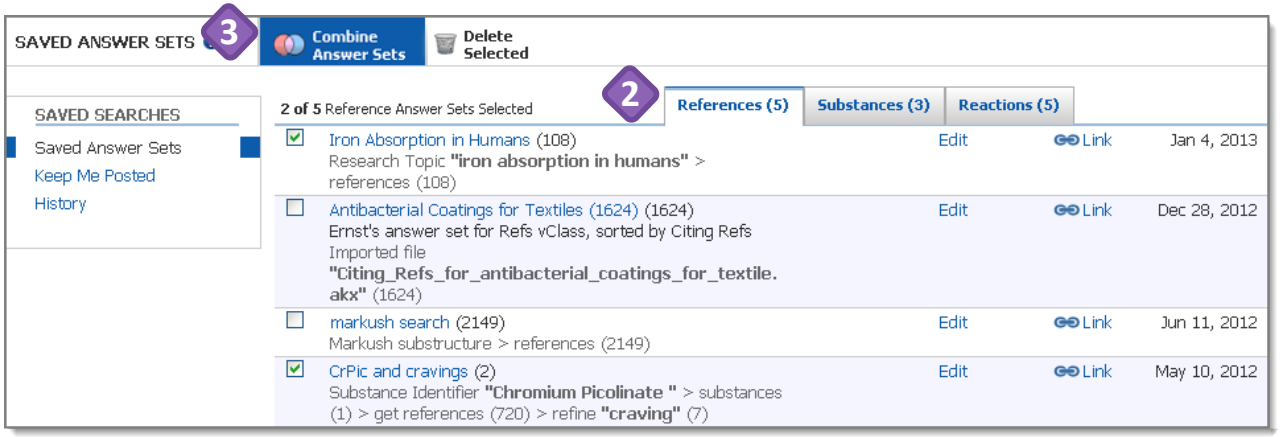
1. Click **Save**, located in the upper right.
2. In the **Save This Answer Set** window, select the answers to save, enter a **Title** and enter an optional **Description**.
3. Click **OK** to save the answers.

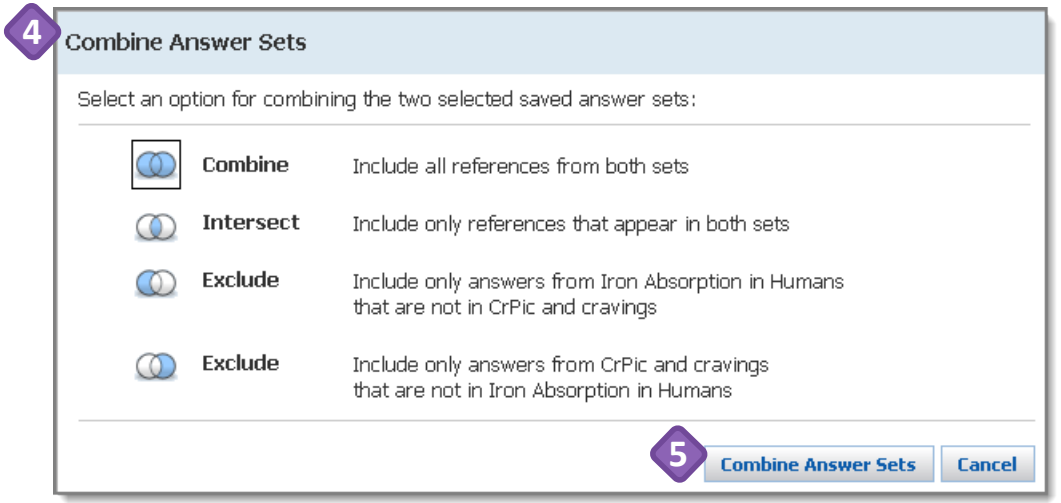
The **Save This Answer Set** dialog window closes and you are returned to your active session. To place answers on your own computer or network, use **Export**.

Tip
For a single answer set, you can save up to 20,000 answers of any type.

Work with Saved Answer Sets

Click the drop-down arrow on the **Saved Searches** tab to access all of your **Saved Answer Sets**, **Keep Me Posted** alert results, and your search **History**.





1. On the top navigation bar, click **Saved Answer Sets** to open the **Saved Answer Sets** dialog window.

2. Saved reference, substance and reaction answer sets are available on separate tabs. You can click:
   - A title to re-open the answer set.
   - **Edit** to make changes to the title or description.
   - **Link** to create a link that you can bookmark for quick access or send to colleagues who can open the answer set in SciFinder.
   - A checkbox and then **Delete Selected** to remove a saved answer set.

3. If you select two or more answer sets, then the **Combine Answer Sets** button becomes active. Click it to open the corresponding window.

4. You can combine two answer sets in one of four ways. Select the combine option of interest.
   - If you select more than two answer sets, then only the **Combine** and **Intersect** options are available.

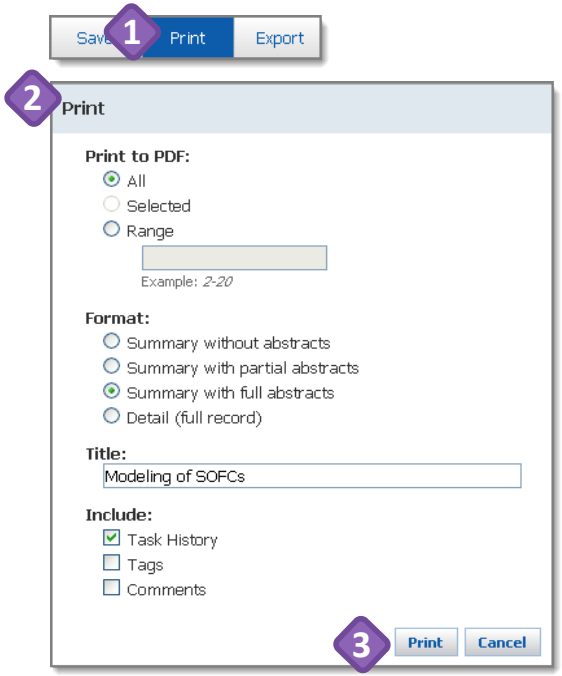
5. Click the **Combine Answer Sets** button. The answers are merged and become your active session.

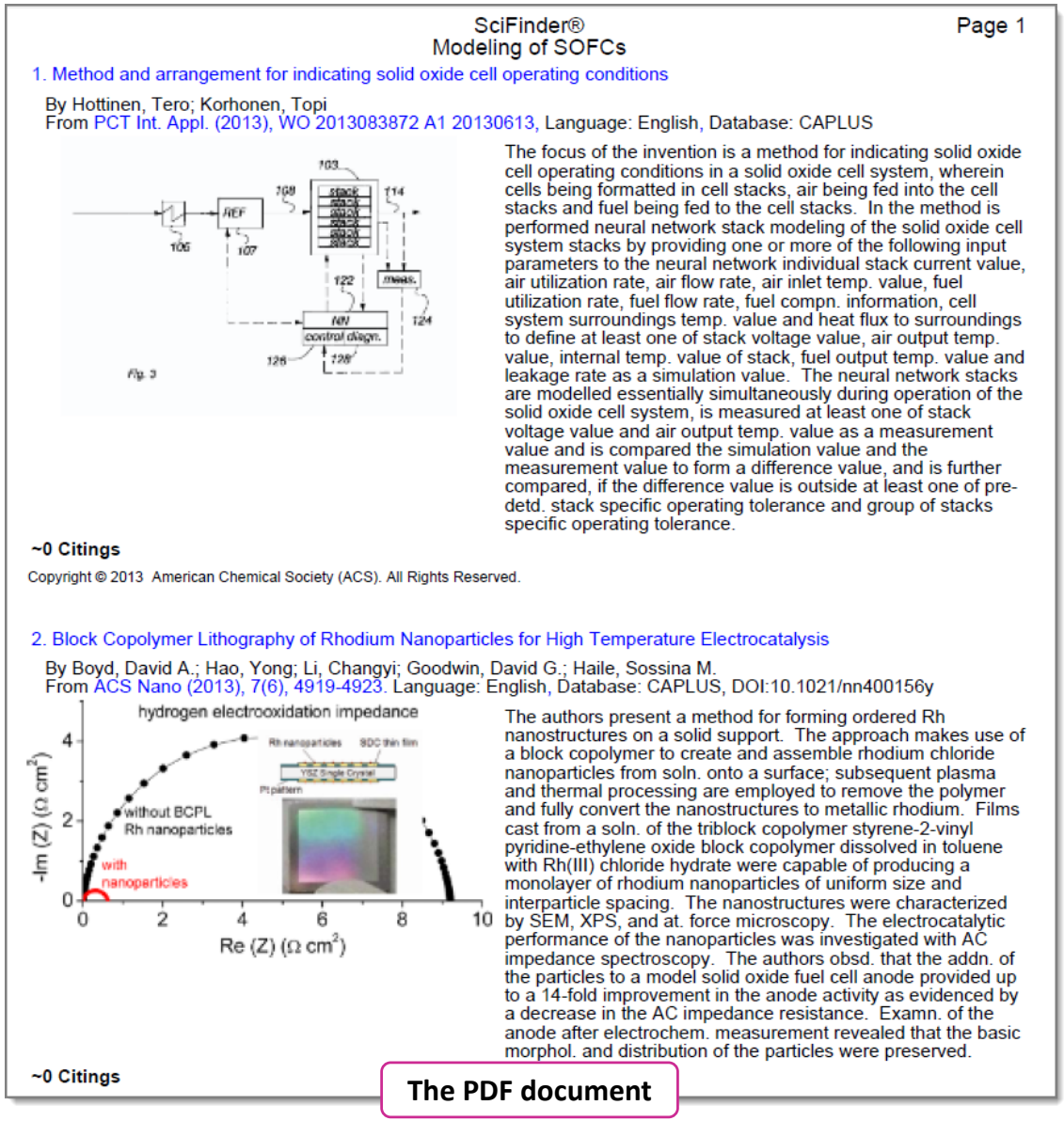
Print References Example

1. You can print references, substances and reactions. To begin, click **Print** in the upper right.

2. In the **Print** dialog window:
   - Select the answers you want to print: **All**, **Selected**, or a **Range.**
   - In the **Format** section, click a radio button to select the parts of the record that you want to print.
   - Enter a **Title.**
   - If desired, specify additional information to **Include** with your answer set (options vary depending on the type of answer set).

3. Click **Print** to generate a .pdf file that downloads or opens in a separate window, depending on browser settings.




SciFinder®
Modeling of SOFCs
Page 1

1. Method and arrangement for indicating solid oxide cell operating conditions

By Hottinen, Tero; Korhonen, Topi
From PCT Int. Appl. (2013), WO 2013083872 A1 20130613, Language: English, Database: CAPLUS

The focus of the invention is a method for indicating solid oxide cell operating conditions in a solid oxide cell system, wherein cells being formatted in cell stacks, air being fed into the cell stacks and fuel being fed to the cell stacks. In the method is performed neural network stack modeling of the solid oxide cell system stacks by providing one or more of the following input parameters to the neural network individual stack current value, air utilization rate, air flow rate, air inlet temp. value, fuel utilization rate, fuel flow rate, fuel compn. information, cell system surroundings temp. value and heat flux to surroundings to define at least one of stack voltage value, air output temp. value, internal temp. value of stack, fuel output temp. value and leakage rate as a simulation value. The neural network stacks are modelled essentially simultaneously during operation of the solid oxide cell system, is measured at least one of stack voltage value and air output temp. value as a measurement value and is compared the simulation value and the measurement value to form a difference value, and is further compared, if the difference value is outside at least one of pre-detd. stack specific operating tolerance and group of stacks specific operating tolerance.

~0 Citings

Copyright © 2013 American Chemical Society (ACS). All Rights Reserved.

2. Block Copolymer Lithography of Rhodium Nanoparticles for High Temperature Electrocatalysis

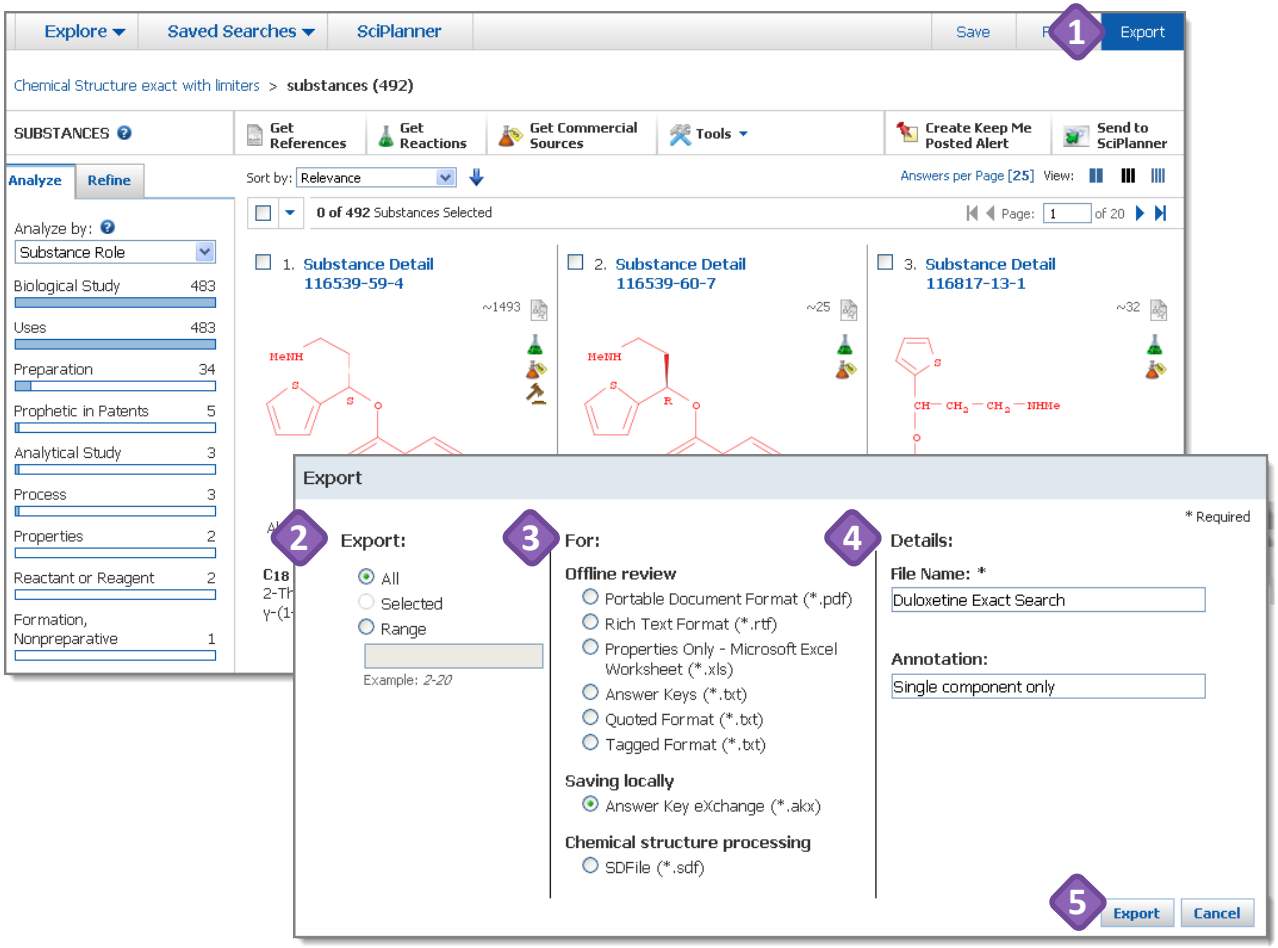
By Boyd, David A.; Hao, Yong; Li, Changyi; Goodwin, David G.; Haile, Sossina M.
From ACS Nano (2013), 7(6), 4919-4923. Language: English, Database: CAPLUS, DOI:10.1021/nn400156y

The authors present a method for forming ordered Rh nanostructures on a solid support. The approach makes use of a block copolymer to create and assemble rhodium chloride nanoparticles from soln. onto a surface; subsequent plasma and thermal processing are employed to remove the polymer and fully convert the nanostructures to metallic rhodium. Films cast from a soln. of the triblock copolymer styrene-2-vinyl pyridine-ethylene oxide block copolymer dissolved in toluene with Rh(III) chloride hydrate were capable of producing a monolayer of rhodium nanoparticles of uniform size and interparticle spacing. The nanostructures were characterized by SEM, XPS, and at. force microscopy. The electrocatalytic performance of the nanoparticles was investigated with AC impedance spectroscopy. The authors obsd. that the addn. of the particles to a model solid oxide fuel cell anode provided up to a 14-fold improvement in the anode activity as evidenced by a decrease in the AC impedance resistance. Examn. of the anode after electrochem. measurement revealed that the basic morphol. and distribution of the particles were preserved.

~0 Citings

The PDF document

Export Substances Example



Export answers for use with other software applications or to collaborate with a colleague. When you export, the file is stored on your computer.

1. Click **Export** in the upper right.
2. Specify the answers to **Export**.
3. Specify the file format.
   - See the table for descriptions of commonly used formats.
   - The file formats and options vary, based on the type of answer set you have.
   - Consult the online **SciFinder Help** for additional information about exporting data.
4. Under **Details**, specify a **File Name**, and, optionally, **Annotation**.
   - The options in this section vary depending on the file format you select.
5. Click **Export**. The file is placed into your download folder. You are returned to your active session.

To store the file on the SciFinder server, use **Save**.

FILE FORMAT	PURPOSE
.ris	To export references for use with citation management software (check your application to confirm which file format to use)
.akx	To export data for collaboration with other SciFinder users
.sdf	To export structures and substance identifiers to a file format readable by some molecule database programs; structures are represented in molfile format

Tip
The file types and details that can be saved vary, depending on whether you are exporting references, substances or reactions. Refer to the online Help for more details.