How to…Create a Reaction Answer Set

Find all relevant reactions based on criteria you specify

Search the world's largest, publicly available source of reactions 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.

Begin a Reaction Search

1 To begin, go to the left navigation pane and click **Reaction Structure**.

2 Click either the **Java** or **Non-Java** tab to select the type of **Reaction Editor** that you want to use. Then 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 how to draw in the **Reaction Editor** with the following tutorials, available in the online **SciFinder Help**:
- "Draw Structures"
- "Draw Reactions"

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 report structure data as it appears 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 a Reaction Answer Set."

Other Ways to Create a Reaction Answer Set

You can also create a reaction answer set after you get either reference or substance answers.
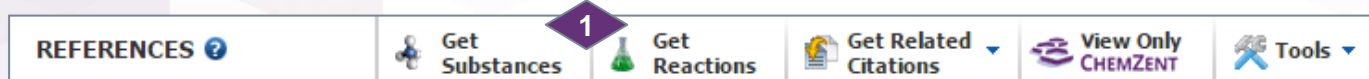
1 After you get a reference or substance answer set, click **Get Reactions** on the toolbar.

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 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 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 a Reaction Answer Set."

CAS Customer Center
E-mail: help@cas.org
Phone numbers: http://www.cas.org/contact-us/cas-customer-center