

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

The screenshot displays the SciFinder web interface. On the left, a navigation pane is open to the 'REACTIONS' section, where 'Reaction Structure' is highlighted. The main content area is titled 'REACTIONS: REACTION STRUCTURE'. It features a 'Structure Editor' with two tabs: 'Java' and 'Non-Java'. Below the tabs is a window labeled 'Click to Edit'. To the right of the editor, the 'Search Type' section has two radio buttons: 'Allow variability only as specified' (unselected) and 'Substructure' (selected). At the bottom of the main area is a blue 'Search' button. Below the search button are links for 'Advanced Search' and a checked 'Always Show' checkbox. A 'ChemDraw' advertisement is located at the bottom right of the interface.

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

Structure Editor - reaction ring cyclization example.cxf

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

1

reactant

product

2

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

3 OK Cancel

$C_{12}H_9NO_2 \cdot C_{12}H_9N$ 199.21 . 167.21

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

Explore | Saved Searches | SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REACTIONS: REACTION STRUCTURE

Structure Editor:

Java | Non-Java

Search Type:

- Allow variability only as specified
- Substructure

Click image to change structure or view detail.

Import CXF

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

Search

1 Advanced Search Always Show

Solvents [Select Solvents](#)

Non-participating Functional Groups [Select Groups](#)

Number of Steps

Examples: 1, 1-3, 1-, -3

Classifications

| | |
|--|--|
| <input type="checkbox"/> Biotransformation | <input type="checkbox"/> Non-catalyzed |
| <input type="checkbox"/> Catalyzed | <input type="checkbox"/> Photochemical |
| <input type="checkbox"/> Chemoselective | <input type="checkbox"/> Radiochemical |
| <input type="checkbox"/> Combinatorial | <input type="checkbox"/> Regioselective |
| <input type="checkbox"/> Electrochemical | <input type="checkbox"/> Stereoselective |
| <input type="checkbox"/> Gas-phase | |

Sources

- Any source
- Patents only
- Sources other than patents

Publication Years

Examples: 1995, 1995-1999, 1995-, -1995

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

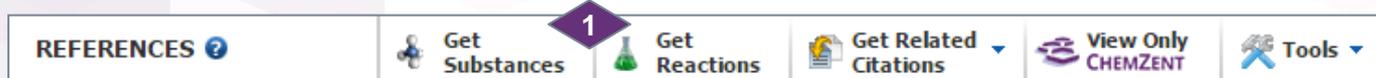
The limiters are available as part of the **Refine** and **Analyze** functions, so it is often advantageous to start with a broad search and narrow the answer set later.

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.

Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Sort by: Relevance Display Options

0 of 535 Substances Selected Page: 1 of 27

1. 13118-11-1 CAS Registry Number: 13118-11-1

2. 616866-21-8

3. 207856-83-5

4. 207856-85-7

2

View Substance Detail
Explore by Structure
Synthesize this...
Get Reactions where Substance is a
Get Commercial Sources
Get Regulatory Information
Get References
Export as Image
Export as molfile
Send to SciPlanner

Product
Reactant
Reagent
Reactant/Reagent
Catalyst
Solvent
Any Role

$C_{18}H_{25}NO_3$
Benzeneacetic acid, α -cyclopentyl- α -hydroxy-, 1-methyl-3-pyrrolidinyl ester

Key Physical Properties
Regulatory Information
Experimental Properties

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

The screenshot shows the SciFinder web interface. At the top left, there is a 'CAS Solutions' dropdown menu and the SciFinder logo with the tagline 'A CAS SOLUTION'. Below the logo are three main navigation buttons: 'Explore', 'Saved Searches', and 'SciPlanner'. On the right side of the top navigation bar, there are links for 'Preferences', 'SciFinder Help', and 'Sign Out'. Below the navigation bar, a breadcrumb trail reads 'Reaction Structure substructure > reactions (5370)'. At the bottom right of the interface, there are three buttons: 'Save', 'Print', and 'Export'. Seven purple diamond-shaped callouts with white numbers 1 through 7 are overlaid on the interface to highlight specific features.

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>