

HOW TO

Explore by Chemical Structure



With SciFinder[®], you can draw a chemical structure and then find a particular substance or group of substances that match the structure.

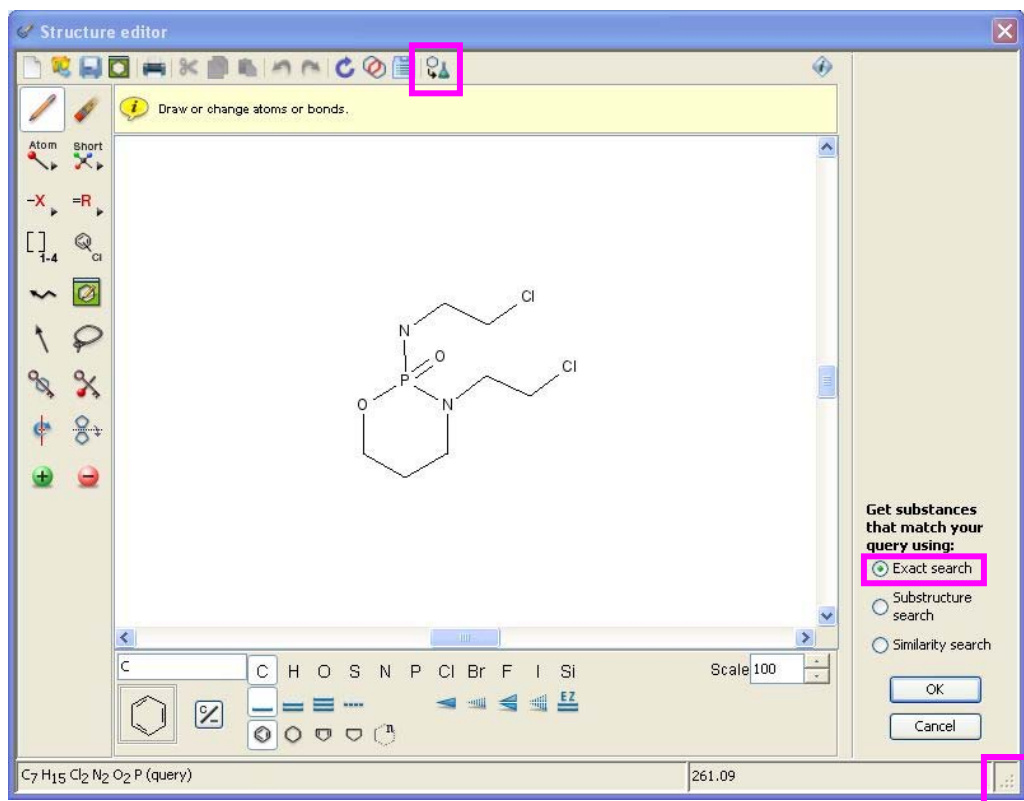
Exact search results may include:

- The structure exactly as you have drawn it
- Stereoisomers
- Tautomers (including keto-enol)
- Coordination compounds
- Charged compounds
- Radicals or radical ions
- Isotopes
- Polymers, mixtures, and salts



1. Click the structure drawing thumbnail to open the editor.

Use the tools down the left side and across the bottom to draw your structure.

Select **Exact search**, and click **OK**.



Tips:

- It may be helpful to set your browser to full screen when using the Structure Editor. You can also resize the window by dragging its lower-right corner .
- Mouse over the tool buttons to see names or descriptions for the tools.
- Once you select a tool, information also displays above the drawing area.
- For details about drawing structures and using each of the tools, see the SciFinder Help files.
- If you want to switch to the Reaction Editor, click .

2. SciFinder provides you with options for presenting your results and further defining your search.

Click **Search**.

Tips:

- Change the search type (exact, substructure, or similarity) from what you already specified within the drawing editor.
- Specify whether you want to see a precision analysis (not available with stereo feature or similarity search).
- Select specific Characteristics, Classes, or Studies that you want to apply to your search.

3. Review your answers.

Tips:

- Use the **Sort by** list to sort your answers in a variety of ways.
- Use the **View** icons to view substance answers in 1–4 columns.

4. Work with substances....

SciFinder allows you to work with substance answer sets in a variety of ways. For hints and tips, see the How To Guides for:

- Working with Substance Answer Sets: Overview
- Analyze Substance Answer Sets
- Refine Substance Answer Sets
- Obtain Commercial Sources
- View Properties
- Combine Answer Sets
- Print, Save, and Export Results

SciFinder also offers substructure and similarity searches. See the How To Guides for:

- Explore by Substructure
 - Explore by Structure Similarity
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