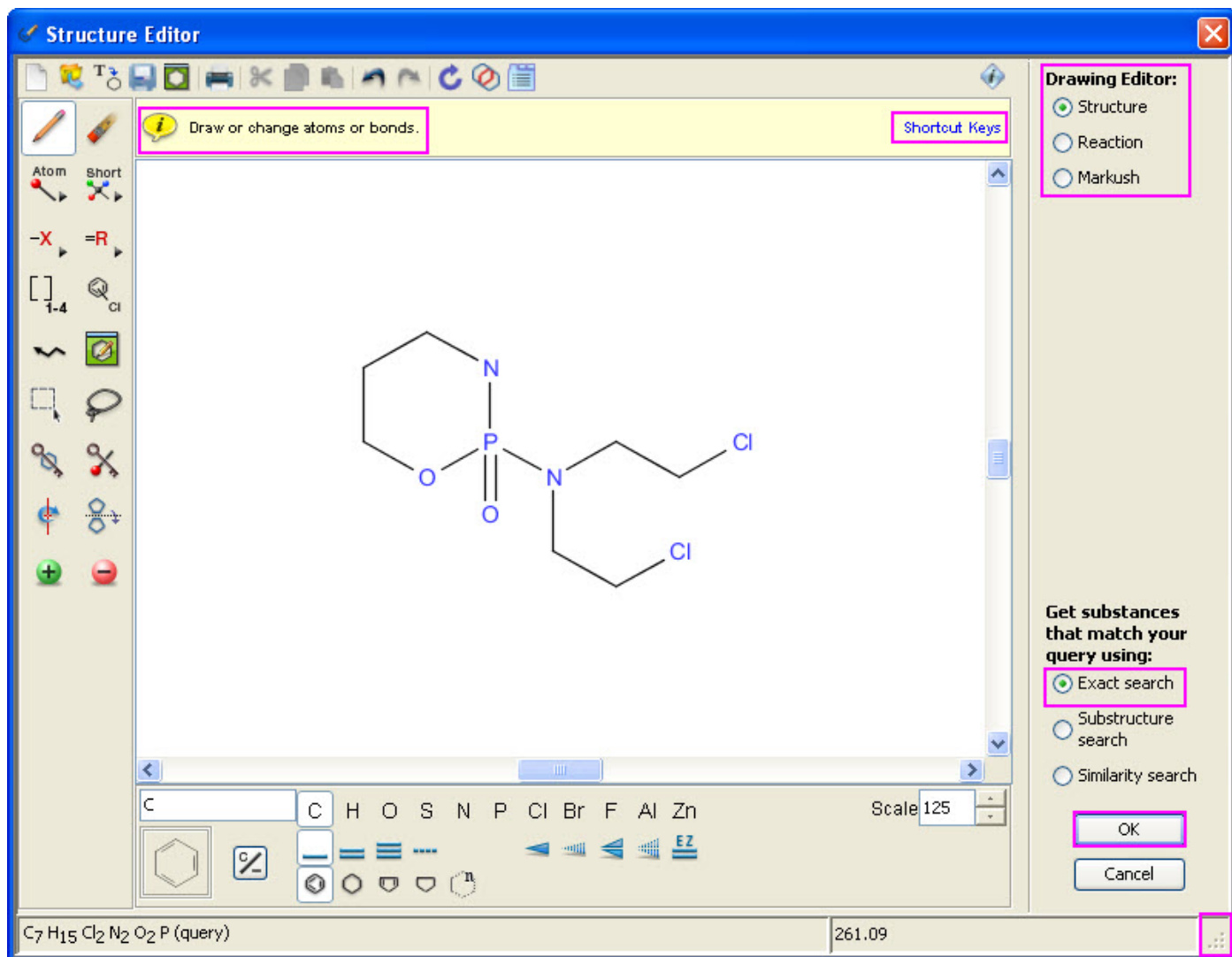


# How To...

## Explore by Chemical Structure

Use SciFinder® to draw a chemical structure and find a particular substance or group of substances that match the structure.

1. Click the structure drawing thumbnail to open the drawing editor. You can toggle between the Structure, Reaction, and Markush Drawing Editors.
2. Use the tools along the left side and across the bottom to draw your structure. Keyboard shortcut keys are also available.
3. After completing the structure, specify the type of search you wish to conduct, in this case **Exact search**, and click **OK**.



Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:


- Exact search
- Substructure search
- Similarity search

OK

Cancel

C7 H15 Cl2 N2 O2 P (query) 261.09

### Tips:

- You can resize the window by dragging its lower-right corner .
- Mouse over tool buttons to see names or descriptions for the tools.
- Information about a selected tool is displayed above the drawing area (tool tips).
- For details about drawing structures and using each of the tools, see the SciFinder help files or the Drawing curriculum in CAS Learning Solutions.

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

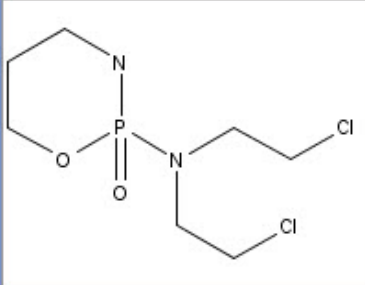
Your structure is displayed in the Chemical Structure search window.

4. (Optional) Before executing the search, you can modify or further refine your search. You may choose to
- Change the search type (Exact Structure, Substructure, or Similarity)
  - Choose to see a precision analysis (not available with stereo feature or similarity search)
  - Specify additional criteria (Characteristics, Classes, or Studies) to further define your search
5. Click **Search**.

### Explore Substances

Chemical Structure Chemical Structure ⓘ

Markush  
Molecular Formula  
Substance Identifier



Click image to change structure or view detail

Search type: ⓘ  Exact Structure  
 Substructure  
 Similarity

Show precision analysis

**Search**

**Characteristic(s)** ⓘ

**Class(es)** ⓘ

**Studies** ⓘ

Single component  
 Commercially available  
 Included in reference(s)

Alloys  
 Coordination compounds  
 Incompletely defined

Analytical  
 Biological

Mixtures  
 Polymers  
 Organics, and others not listed

Preparation  
 Reactant or reagent

## 6. Review your answers.

Answers from an Exact Structure search can include stereoisomers, isotopic variants, and multicomponent substances where the exact structure is one of the components.

Substances Get References Get Reactions Tools Send to SciPlanner

254 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) Relevance (New) CAS Registry Number Number of References Molecular Weight Molecular Formula

Answers per Page [15] 1 2 3 4 5 6 ... 17 View: [1] [2] [3] [4]

1. Substance Detail 50-18-0  
~22139  
ClCCN(CCCl)P(=O)(O)O  
C<sub>7</sub> H<sub>15</sub> Cl<sub>2</sub> N<sub>2</sub> O<sub>2</sub> P  
2H-1,3,2-Oxazaphosphorin-2-amine, N,  
N-bis(2-chloroethyl)tetrahydro-, 2-oxide  
Spectra  
Experimental Properties

2. Substance Detail 55-19-2  
(Component: 50-18-0)  
~66  
ClCCN(CCCl)P(=O)(O)O.O  
C<sub>7</sub> H<sub>15</sub> Cl<sub>2</sub> N<sub>2</sub> O<sub>2</sub> P · H<sub>2</sub>O  
2H-1,3,2-Oxazaphosphorin-2-amine, N,  
N-bis(2-chloroethyl)tetrahydro-, 2-oxide,  
hydrate (1:1)  
Spectra  
Experimental Properties

3. Substance Detail 60007-96-7  
~38  
ClCCN(CCCl)P(=O)(O)O  
C<sub>7</sub> H<sub>15</sub> Cl<sub>2</sub> N<sub>2</sub> O<sub>2</sub> P  
2H-1,3,2-Oxazaphosphorin-2-amine, N,  
N-bis(2-chloroethyl)tetrahydro-, 2-oxide,  
(2S)-  
Absolute stereochemistry.  
Spectra  
Experimental Properties

### Tips:

- Use the **Sort by** options to specify the order in which your results are displayed
- Use the **View** icons to display results in two, three, or four columns. If structures are large, fewer columns may be preferable.

## Additional resources

To learn more about working with substances, refer to

- SciFinder online help files
- How To Guides for:
  - Analyze Substance Answers
  - Refine Substance Answers
  - Find Commercial Sources
  - Combine Answer Sets
  - Keep Me Posted Alerts
  - Print, Save, and Export
  - Select Structure Options
  - Explore by Substructure
  - Explore by Structure Similarity
- Instructor-led and self-directed learning options in the [Learning Solutions](#) resource center