

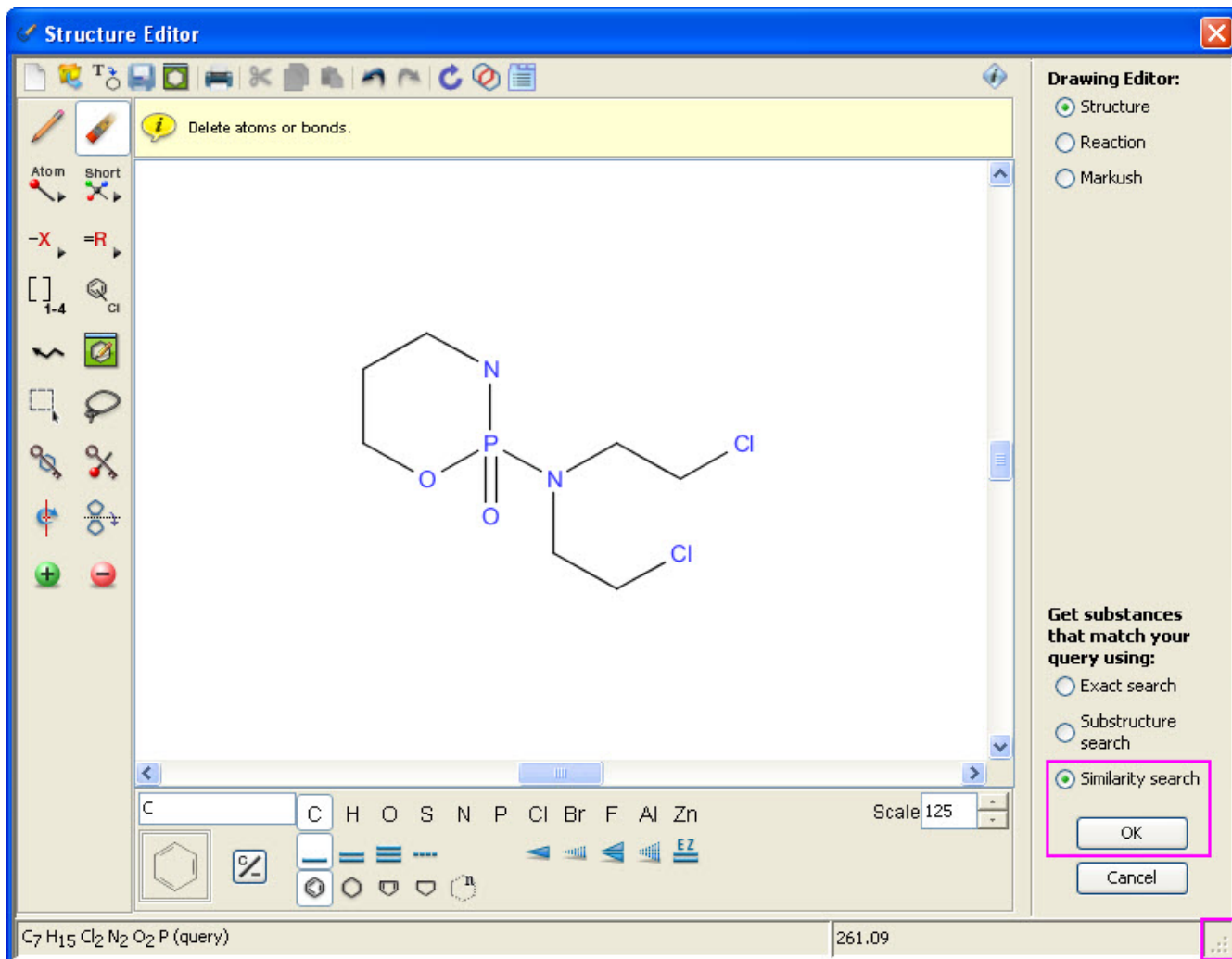
# How To...

## Explore by Structure Similarity


SciFinder® uses the Tanimoto algorithm to compare substances in the database with your structure query, and then determines which are the most similar.

Similarity searching is complementary to the other structure search options since it can return answers that are neither exact nor substructure answers.

1. Click the structure drawing thumbnail to open the drawing editor.
2. Use the tools along the left side and across the bottom to draw your structure. Keyboard shortcuts are also available.
3. After completing the structure, specify the type of search you wish to conduct, in this case **Similarity search** and click **OK**.



### 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.

Similarity searches cannot be done with structures that contain:

- R-groups, variables, repeating groups, or variable attachment positions
- Multiple fragments
- Stereo bonds

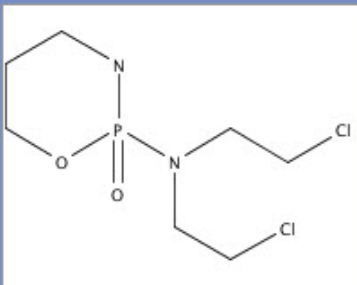
Your structure is displayed in the Chemical Structure search window.

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  
Property **NEW**  
Substance Identifier



Click image to change structure or view detail

Search type: ⓘ  Exact Structure  
 Substructure  
 Similarity

Show precision analysis

**Search**

**Characteristic(s)**

- Single component
- Commercially available
- Included in reference(s)

**Class(es)** ⓘ

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

**Studies** ⓘ

- Analytical
- Biological
- Preparation
- Reactant or reagent

6. Select the candidate(s) of interest, and click **Get Substances**. SciFinder groups substance results by similarity score. Substances with the highest scores are most similar to your query structure.

**Similarity Candidates**

9 Candidates 4 Selected

Select All Deselect All

Similarity Candidates	Substances
<input type="checkbox"/> ≥ 99 (most similar)	254
<input checked="" type="checkbox"/> 95-98	5
<input checked="" type="checkbox"/> 90-94	14
<input checked="" type="checkbox"/> 85-89	30
<input checked="" type="checkbox"/> 80-84	39
<input type="checkbox"/> 75-79	108
<input type="checkbox"/> 70-74	112
<input type="checkbox"/> 65-69	198
<input type="checkbox"/> 0-64 (least similar)	320

**Get Substances**

7. Review your answers.

The similarity scores are displayed to the right of the CAS Registry Numbers®.

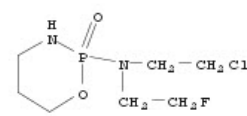
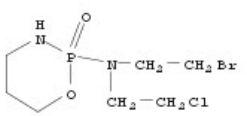
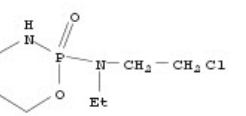
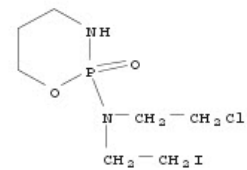
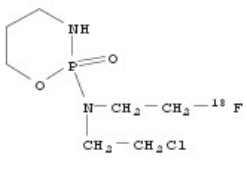
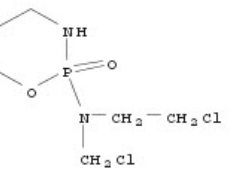
Substances are sorted by Similarity Score in descending order. To change the order, select an option from the Sort by drop-down list.

88 Substances 0 Selected

Select All Deselect All Sort by: Similarity Score

Answers per Page [15] 1 2 3 4 5 6

View: [Icons]

<input type="checkbox"/> 1. <b>Substance Detail</b> 5001-29-6  C <sub>7</sub> H <sub>15</sub> Cl F N <sub>2</sub> O <sub>2</sub> P 2H-1,3,2-Oxazaphosphorin-2-amine, N-(2-chloroethyl)-N-(2-fluoroethyl) tetrahydro-, 2-oxide <b>Score: 95</b>	<input type="checkbox"/> 2. <b>Substance Detail</b> 13036-62-9  C <sub>7</sub> H <sub>15</sub> Br Cl N <sub>2</sub> O <sub>2</sub> P 2H-1,3,2-Oxazaphosphorin-2-amine, N-(2-bromoethyl)-N-(2-chloroethyl) tetrahydro-, 2-oxide Score: 95	<input type="checkbox"/> 3. <b>Substance Detail</b> 50650-73-2  C <sub>7</sub> H <sub>16</sub> Cl N <sub>2</sub> O <sub>2</sub> P 2H-1,3,2-Oxazaphosphorin-2-amine, N-(2-chloroethyl)-N-ethyl tetrahydro-, 2-oxide Score: 95
<input type="checkbox"/> 4. <b>Substance Detail</b> 863331-87-7  C <sub>7</sub> H <sub>15</sub> Cl I N <sub>2</sub> O <sub>2</sub> P 2H-1,3,2-Oxazaphosphorin-2-amine, N-(2-chloroethyl) tetrahydro-N-(2- iodoethyl)-, 2-oxide Score: 95	<input type="checkbox"/> 5. <b>Substance Detail</b> 891203-08-0  C <sub>7</sub> H <sub>15</sub> Cl F N <sub>2</sub> O <sub>2</sub> P 2H-1,3,2-Oxazaphosphorin-2-amine, N-(2-chloroethyl)-N-[2-(fluoro-18F) ethyl] tetrahydro-, 2-oxide Score: 95	<input type="checkbox"/> 6. <b>Substance Detail</b> 1348384-36-0  C <sub>6</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> P 2H-1,3,2-Oxazaphosphorin-2-amine, N-(2-chloroethyl)-N-(chloromethyl) tetrahydro-, 2-oxide <b>Score: 94</b>

## 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 Chemical Structure
  - Explore by Substructure
- Self-directed learning options in the [Learning Solutions](#) resource center



A division of the American Chemical Society

CAS Customer Center  
Phone: 800-753-4227 (North America)  
614-447-3700 (worldwide)  
Fax: 614-447-3751  
E-mail: [help@cas.org](mailto:help@cas.org)  
Internet: [www.cas.org](http://www.cas.org)