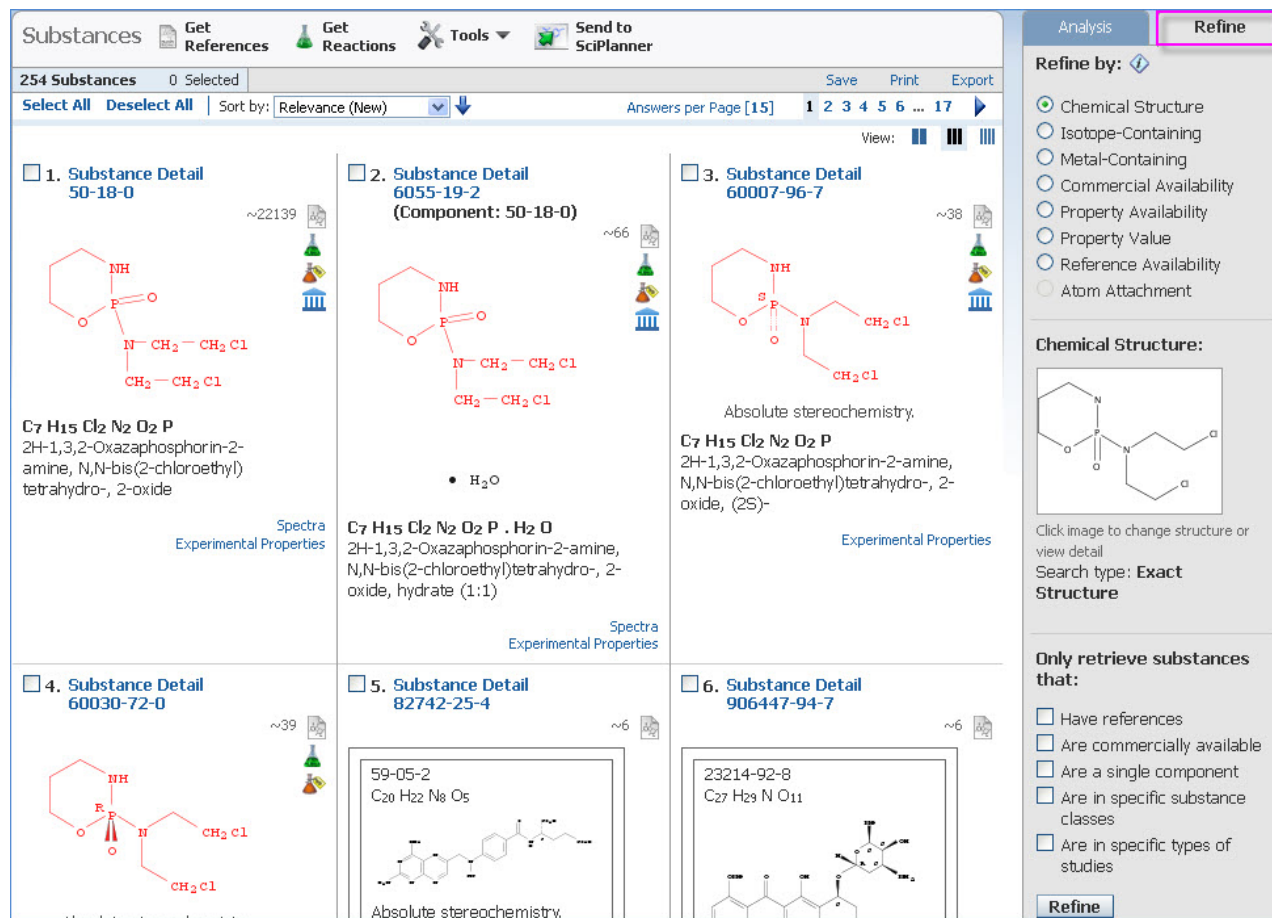


How To...

Refine Substance Answers

Use Refine to explore, evaluate, or review a substance answer set. Refining can help you extract the most relevant compounds from your substance answer set based on the criteria you specify.

1. Click the **Refine** tab at the right of the displayed substances to select criteria for narrowing your answer set.



The screenshot displays the SciFinder interface with a list of six substances. The 'Refine' sidebar on the right is active, with 'Chemical Structure' selected under 'Refine by:'. The main area shows substance cards with chemical structures and details. The first card is for 2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl) tetrahydro-, 2-oxide. The second card is for the same compound as a hydrate. The third card is for the same compound with absolute stereochemistry. The fourth card is for the same compound with absolute stereochemistry. The fifth card is for 59-05-2, C₂₀H₂₂N₈O₅. The sixth card is for 23214-92-8, C₂₇H₂₉N O₁₁.

You may refine multiple times with any combination of the options.

SELECT THIS OPTION...	TO IDENTIFY SUBSTANCES...
Chemical Structure	That contain an additional or particular structural component.
Isotope-Containing	That include/exclude isotopic labels.
Metal-Containing	That include one or more metals.
Commercial Availability	For which commercial supplier information is available.
Property Availability	For which experimental or predicted properties are available or for which a specific P. property is available.
Property Value	For which experimental or predicted properties with specified values are available.
Reference Availability	For which journal or patent references are available.
Atom Attachment	With one or more attachments at a particular node in the query structure.

2. Select an option for refining your answer set. Then specify the required information.

For example, if you choose **Property Value**, click **Select Properties**. Then, select the specific property or properties of interest, and specify their respective values.

3. Click **Refine**. The new answer set includes only those substances that meet the criteria selected.

Analysis | **Refine**

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value**
- Reference Availability
- Atom Attachment

Select Properties

Refine by Property Value ⓘ

Select a property on the left, and specify values or limits on the right. Repeat for multiple properties.

Properties - 1 selected	Values - Predicted H Acceptor/Donor Sum
Experimental	Specify range: 0 to 5.0 Min: 0 Max:
<input type="checkbox"/> Boiling Point	
<input type="checkbox"/> Melting Point	
Predicted	
<input type="checkbox"/> H Acceptors	
<input type="checkbox"/> H Donors	
<input type="checkbox"/> Molecular Weight	
<input type="checkbox"/> logP	
<input type="checkbox"/> Freely Rotatable Bonds	
<input type="checkbox"/> Bioconcentration Factor	
<input type="checkbox"/> Boiling Point	
<input type="checkbox"/> Density	
<input type="checkbox"/> Enthalpy of Vaporization	
<input type="checkbox"/> Flash Point	
<input checked="" type="checkbox"/> H Acceptor/Donor Sum	
<input type="checkbox"/> Koc	
<input type="checkbox"/> logD	
<input type="checkbox"/> Mass Intrinsic Solubility	
<input type="checkbox"/> Mass Solubility	
<input type="checkbox"/> Molar Intrinsic Solubility	
<input type="checkbox"/> Molar Solubility	

Include substances with no values for selected properties.

Reset **Refine** **Cancel**

Tip:

- To see substances for which the specified property is either not present at all or present but without a value reported, select Include substances with no values for selected properties.
- Review your answers.
 - (optional) To return to the answer set prior to refining, use the breadcrumb trail.

The screenshot shows the CAS SciFinder interface with the following details:

- Search path: Chemical Structure exact > substances (254) > refine "property value" (3)
- Navigation: Substances, Get References, Get Reactions, Tools, Send to SciPlanner
- Results: 3 Substances, 0 Selected. Sort by: Relevance (New). Answers per Page: 15.
- View: Three columns of substance detail cards.

1. Substance Detail 50-18-0
~22139
ClCCN(CCCl)P(=O)(O1CCOCC1)N
C₇ H₁₅ Cl₂ N₂ O₂ P
2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide
Spectra Experimental Properties

2. Substance Detail 60007-96-7
~38
ClCCN(CCCl)P(=O)(O1CCOCC1)N
Absolute stereochemistry.
C₇ H₁₅ Cl₂ N₂ O₂ P
2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide, (2S)-
Experimental Properties

3. Substance Detail 60030-72-0
~39
ClCCN(CCCl)P(=O)(O1CCOCC1)N
Absolute stereochemistry.
C₇ H₁₅ Cl₂ N₂ O₂ P
2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide, (2R)-
Experimental Properties

Additional resources

To learn more about working with substance answer sets, refer to

- SciFinder online help files
- How To Guides for:
 - Analyze Substance Answers
 - Find Commercial Sources
 - Combine Answer Sets
 - Keep Me Posted Alerts
 - Print, Save, and Export
- Self-directed learning options in the [Learning Solutions](#) resource center



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