

How To...

Explore by Substructure

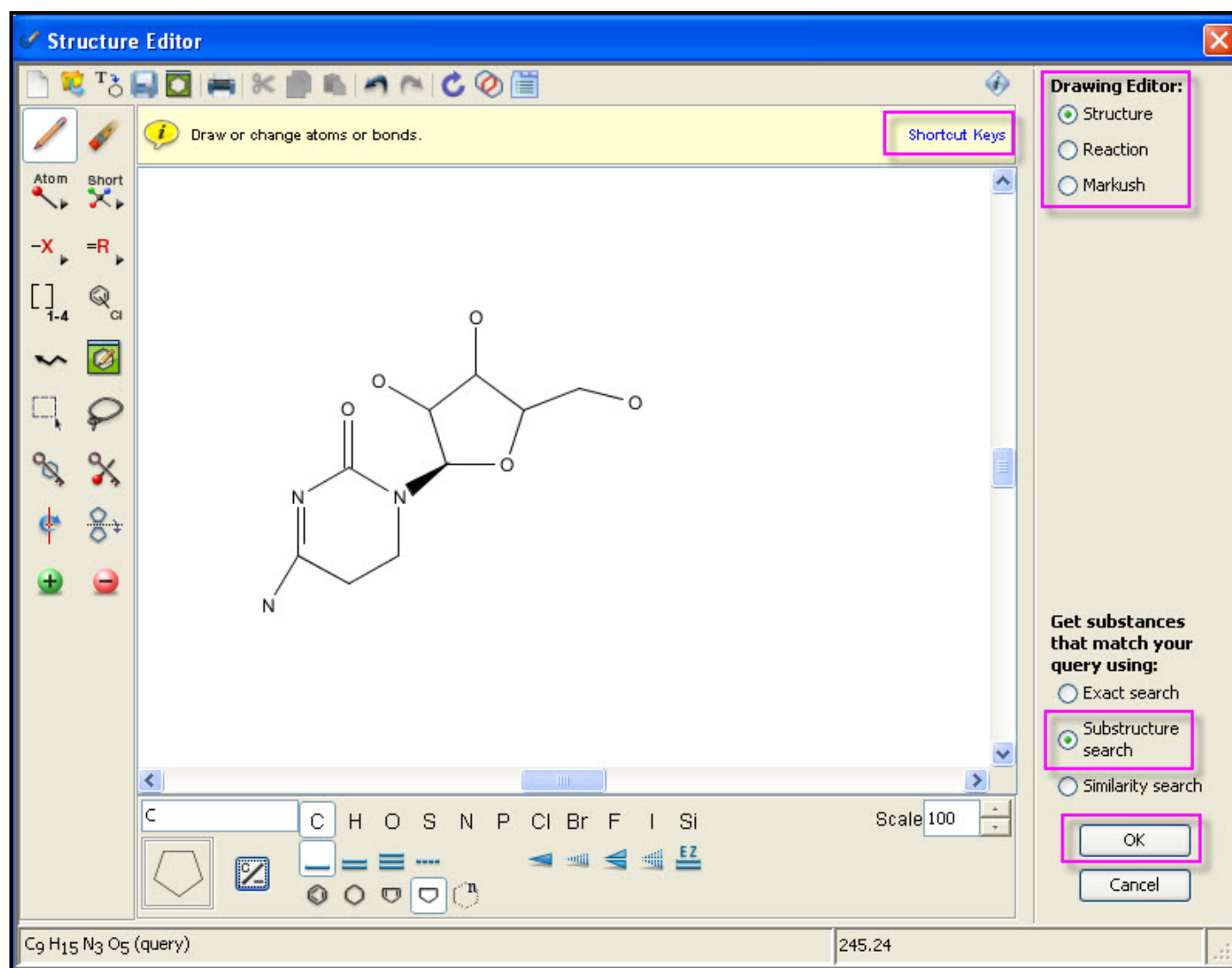
Use SciFinder® substructure searching capabilities to give access to the world's largest and most current chemical substance database.

Additional tools – for example, tools to include variable groups and R-groups in your structure – let you broaden or narrow your structure query. By default, substructure searches retrieve exact results, plus substances with additional substitution and/or ring fusion.

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

Use the tools along the left side and across the bottom to draw your structure. Keyboard shortcuts are also available. Substructure-specific tools let you draw variables and/or R-groups, block atoms from additional substitution, and block rings from additional fusion.

Once you have finished drawing, select **Substructure search** (default) and click **OK**.



Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4

Scale 100

C H O S N P Cl Br F I Si

Drawing Editor:

- Structure
- Reaction
- Markush


Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK
Cancel


C₉ H₁₅ N₃ O₅ (query) 245.24

Tips:

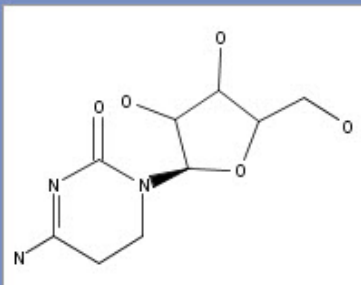
- You can resize the window by dragging its lower-right corner .
- Mouse over tool buttons to see names or descriptions for the tools.
- Information about a selected tool is displayed above the drawing area (tool tips).
- You can toggle between the Structure, Reaction, and Markush Drawing Editors.
-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

2. (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
3. Click **Search**.

Explore Substances


Chemical Structure Chemical Structure 

Markush
Molecular Formula
Substance Identifier



Click image to change structure or view detail


Search

Search type:  Exact Structure
 Substructure
 Similarity


Show precision analysis

Characteristic(s)

Single component
 Commercially available
 Included in reference(s)

Class(es) 

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

Studies 

Analytical Preparation
 Biological Reactant or reagent

4. Your candidate answers are displayed.

If your query structure includes stereochemistry, SciFinder automatically analyzes the results by stereo.

5. Select the candidate(s) of interest, and click **Get Substances**.

Stereo Candidates

4 Candidates 1 Selected

Select All Deselect All

Stereo Candidates	Substances
<input checked="" type="checkbox"/> Absolute stereo match	450
<input type="checkbox"/> Absolute stereo mirror image	13
<input type="checkbox"/> Relative stereo match	0
<input type="checkbox"/> Stereo that doesn't match query	1
<input type="checkbox"/> No stereo in answer structure	30

Get Substances

6. Review your answers.

Substances are sorted by Relevance in descending order. You can select a different sort order by selecting an option from the **Sort by:** drop-down list.

Substances Get References Get Reactions Tools Send to SciPlanner

449 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 ... 30 View: [Icons]

1. Substance Detail 51860-53-8 Absolute stereochemistry. C₉ H₁₅ N₃ O₅ Cytidine, 5,6-dihydro- (6CI,9CI)

3. Substance Detail 107672-20-8 Absolute stereochemistry. C₉ H₁₄ N₃ O₅ 4-Pyrimidinyl, 6-amino-2,3,4,5-tetrahydro-2-oxo-3-β-D-ribofuranosyl- (9CI)

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 Structure Similarity
- Instructor-led and self-directed learning options in the [Learning Solutions](#) resource center



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