

# HOW TO

Explore by Substructure



SciFinder® substructure searching capabilities give you unparalleled substructure 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 editor.

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

Substructure-specific tools let you:

- Draw variables and/or R-groups
- Block atoms from additional substitution
- Block rings from additional fusion

Once you have finished drawing, select **Substructure 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 to further define your search.

Click **Search**.

Explore Substances

Chemical Structure Chemical Structure

Molecular Formula

Substance Identifier

Click image to change structure or view detail

Search type:  Exact Structure  
 Substructure  
 Similarity

Show precision analysis

**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

**Tips:**

- Change the search type to Substructure, if you forgot to do that 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. If your query structure includes stereochemistry, SciFinder automatically analyzes the results by stereo.

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

Stereo Candidates

3 Candidates 1 Selected

Select All Deselect All

Stereo Candidates	Substances
<input checked="" type="checkbox"/> Absolute stereo match	114
<input type="checkbox"/> Absolute stereo mirror image	6
<input type="checkbox"/> Relative stereo match	0
<input type="checkbox"/> Stereo that doesn't match query	0
<input type="checkbox"/> No stereo in answer structure	2

4. Review your answers.

The screenshot displays the CAS Substances interface with three substance detail panels. The interface includes a top navigation bar with 'Substances', 'Get References', 'Get Reactions', and 'Get Commercial Sources'. Below this is a toolbar with '114 Substances', '0 Selected', 'Keep Selected', 'Remove Selected', 'Save', 'Print', and 'Export'. A 'Sort by: CAS Registry Number' dropdown and 'Answers per Page [20]' are also visible. The three panels are:

- 1. Substance Detail 1054661-69-6**: Shows a complex chemical structure with a central nitrogen atom bonded to a benzimidazole ring system, a furfuryl group, and a chiral auxiliary. The auxiliary is a five-membered ring with a sulfur atom and two oxygen atoms, with a phenyl group and a hydroxyl group. The text below the structure reads: 'Absolute stereochemistry. C44 H34 N4 O10 INDEX NAME NOT YET ASSIGNED'. A reference icon and '~0 References' are at the bottom.
- 2. Substance Detail 1053698-12-6**: Shows a similar chemical structure to the first panel. The text below reads: 'Absolute stereochemistry. C34 H27 N3 O8 INDEX NAME NOT YET ASSIGNED'.
- 3. Substance Detail 1053640-90-6**: Shows a chemical structure with a benzimidazole ring system, a furfuryl group, and a chiral auxiliary with two hydroxyl groups. The text below reads: 'Absolute stereochemistry. Double bond geometry as shown. NMe 2'.

5. 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 exact structure and similarity searches. See the How To Guides for:

- Explore by Chemical Structure
- Explore by Structure Similarity