

HOW TO

Explore Structure Similarity



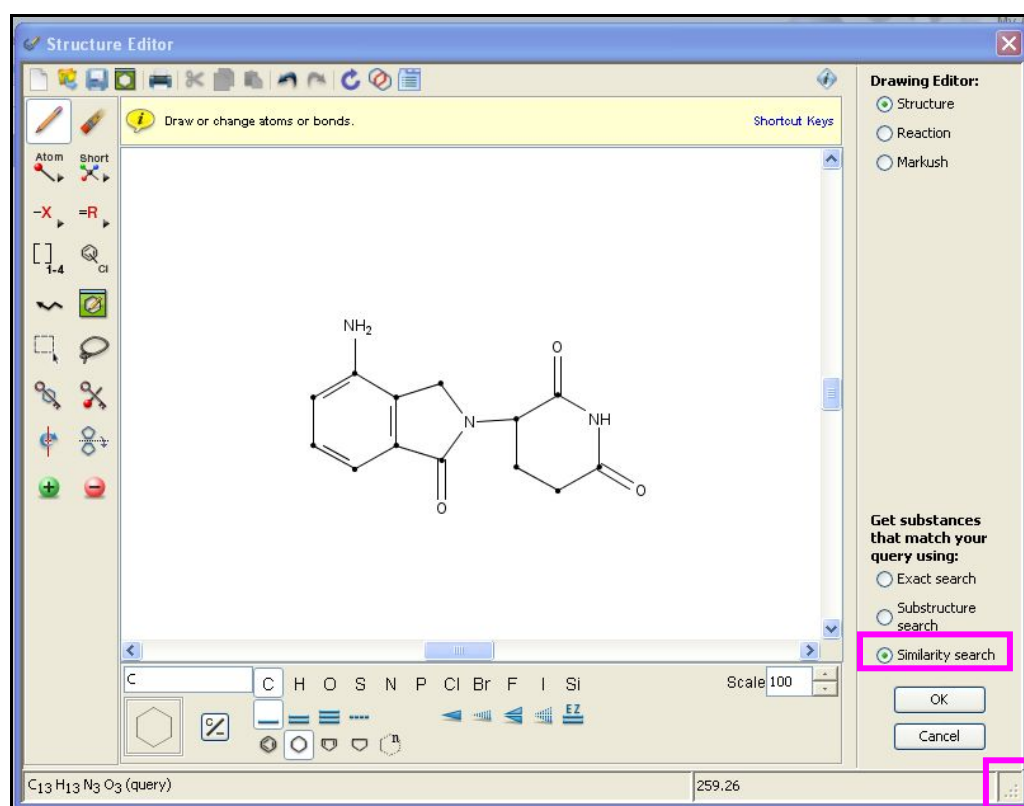
SciFinder® uses the Tanimoto algorithm to compare substances in the database with your structure query, and then determines which are the most similar.

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 editor.

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

Select **Similarity 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.

Note: Similarity searches cannot be done with structures that contain:

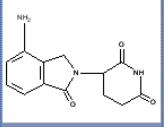
- R-groups, variables, repeating groups, or variable attachment positions
- Multiple fragments
- Stereo bonds

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

Studies

Analytical Preparation
 Biological Reactant or reagent

Tips:

- Change the search type to Similarity, if you forgot to do that within the drawing editor.
- Specify whether you want to see a precision analysis (but remember that precision candidates are not available for substance queries that include stereo information).
- Select specific Characteristics, Classes, or Studies that you want to apply to your search.

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

Note: SciFinder groups substance results by similarity score. Substances with the highest scores are most similar to your query structure.

Similarity Candidates

9 Candidates 1 Selected

Select All Deselect All

Similarity Candidates	Substances
<input checked="" type="checkbox"/> ≥ 99 (most similar)	22
<input type="checkbox"/> 95-98	3
<input type="checkbox"/> 90-94	127
<input type="checkbox"/> 85-89	82
<input type="checkbox"/> 80-84	143
<input type="checkbox"/> 75-79	180
<input type="checkbox"/> 70-74	413
<input type="checkbox"/> 65-69	1161
<input type="checkbox"/> 60-64 (least similar)	4307

4. Review your answers.

Notice that the similarity score is displayed to the right of the CAS Registry Number. Substances are sorted by Similarity Score in descending order. You can also sort by CAS Registry Number®, number of references, molecular formula, or molecular weight

22 Substances 0 Selected | Keep Selected | Remove Selected Save Print Export
Select All Deselect All Sort by: Similarity Score Answers per Page [15] 1 2 View: [Icons]

1. **Substance Detail** 191732-72-6 *Score: ≥ 99*
Nc1ccc2c(c1)nc(=O)[C@@H]3CCNC(=O)N3
C₁₃ H₁₃ N₃ O₃
2,6-Piperidinedione, 3-(4-amino-1,3-dihydro-1-oxo-2H-isoindol-2-yl)-
~724 References
Reactions
Commercial Sources

2. **Substance Detail** 202271-91-8 *Score: ≥ 99*
Nc1ccc2c(c1)nc(=O)[C@@H]3CCNC(=O)N3
C₁₃ H₁₃ N₃ O₃
2,6-Piperidinedione, 3-(4-amino-1,3-dihydro-1-oxo-2H-isoindol-2-yl)-, (3S)-
Absolute stereochemistry.
~10 References
Reactions

3. **Substance Detail** 847871-99-2 *Score: ≥ 99*
(Component: 191732-72-6)
Nc1ccc2c(c1)nc(=O)[C@@H]3CCNC(=O)N3
C₁₃ H₁₃ N₃ O₃ · 1/2 H₂O
2,6-Piperidinedione, 3-(4-amino-1,3-dihydro-1-oxo-2H-isoindol-2-yl)-, hydrate (2:1)

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:

- 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 substructure searches. See the How To Guides for:

- Explore by Chemical Structure
- Explore by Substructure