

# How to...Create a Substance Answer Set

## Select among five search techniques to find substances

Substances can be described by multiple names or other characteristics, so SciFinder® gives you the flexibility to approach a substance search from different starting points, depending on your research needs. No matter how you begin, your results are from the CAS REGISTRY<sup>SM</sup>, the most trusted and comprehensive collection of publicly available chemical substances in the world. Refer to "How to ... Work with Substance Answer Sets" for ways to evaluate the results and find the most relevant answers. To learn more about using SciFinder, consult the online Help or visit [www.cas.org/training/scifinder](http://www.cas.org/training/scifinder).

## Types of Substance Searches

The screenshot shows the SciFinder interface with the following elements:

- Top navigation: CAS Solutions, Preferences, SciFinder Help, Sign Out.
- Sub navigation: Explore (selected), Saved Searches, SciPlanner.
- Left sidebar: REFERENCES (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), REACTIONS (Reaction Structure).
- Main content area: SUBSTANCES: CHEMICAL STRUCTURE. Includes a Structure Editor (Java/Non-Java), Search Type (Exact Structure, Substructure, Similarity), Show precision analysis checkbox, Import CXF button, and a Search button.
- Right sidebar: SAVED ANSWER SETS (reactant search example, PPak examples, derivatives of pyrimidine for immune disease, Hemiaminal polymers, Arylketone synthesis final answer set, Arylketone search, Reduce nitro to amino example, clopidogrel substructure rxn, Thiophene SSS RXN, great markush structure example, View All | Import).
- Bottom of search options: Advanced Search (with expand icon), Always Show (checked).

1 On the **Explore** tab, under **SUBSTANCES**, you can search by any of the five options.

2 Click **Advanced Search** to see criteria that you can add to a search to make it more specific.

The Advanced Search filter options are as follows:

- Advanced Search (expanded), Always Show (checked).
- Characteristics: Single component, Commercially available, Included in references.
- Classes: Alloys, Coordination compounds, Incompletely defined, Mixtures, Polymers, Organics, and others not listed.
- Studies: Analytical, Biological, Preparation, Reactant or reagent.

- These options are available in **Refine** and **Analyze**, so you can also apply them later in your search process.

### Tip

CXF is the file extension for saved structures and reactions in SciFinder.

# Search by Chemical Structure

**1** Select **Chemical Structure**.

**2** Click either the **Java** or **Non-Java** tab to select the type of **Structure Editor** that you want to use. Then click the picture of the structure drawing window to launch the **Structure Editor**.

**Tip**  
To learn about structure drawing, refer to the online Help or the "Introduction to the SciFinder Drawing Editor" tutorial on cas.org.

**3** Draw your structure.

**4** Specify the type of structure search.

**5** Click **OK** to transfer the structure and type of search to the search page.

*Continued*

SELECT...	IF YOU WANT TO RETRIEVE...
Exact Search	The specific structure as drawn in the query, including: <ul style="list-style-type: none"> <li>▪ Stereoisomers</li> <li>▪ Salts and mixtures</li> <li>▪ Polymers with one exactly matching monomer</li> <li>▪ Isotopes</li> <li>▪ Tautomers</li> </ul>
Substructure Search	The structure as drawn or as part of a larger molecule in which there is: <ul style="list-style-type: none"> <li>▪ Substitution at open positions</li> <li>▪ Additional ring fusion</li> </ul>
Similarity Search (Queries cannot include variable groups, repeating groups or variable attachment positions)	Similar chemical structures containing: <ul style="list-style-type: none"> <li>▪ Positional isomers</li> <li>▪ Different or fewer substituents</li> <li>▪ Different ring systems</li> </ul>

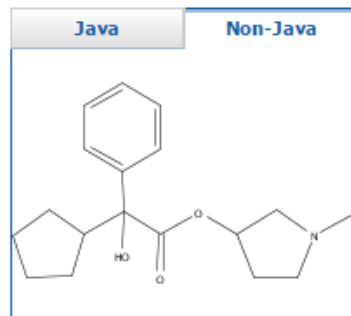
**3** Draw your structure.

**4** Specify the type of structure search.

**5** Click **OK** to transfer the structure and type of search to the search page.

## SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:



Import CXF

6

Search

Advanced Search

Search Type:

- Exact Structure  
 Substructure  
 Similarity

7

Show precision analysis

### Tip

Optional: Select Show precision analysis to include additional structure criteria in your search, as shown below:

SUBSTANCES	
Select All	Deselect All
3 of 3 Precision Candidates Selected	
<input type="checkbox"/>	Conventional Substructure 84370
<input checked="" type="checkbox"/>	Closely Associated Tautomers and Zwitterions 31
<input checked="" type="checkbox"/>	Loosely Associated Tautomers and Zwitterions 3
<input type="checkbox"/>	Other 0
<input type="button" value="Get Substances"/>	

Precision Analysis Window (Unrelated Example)

6

Click **Search** to retrieve the answers that meet your query requirements.

7

For **Similarity** searches, after you click **Search**, you will see a **Similarity Candidates** window. To select the degree(s) of similarity for your answers, check the box(es) of interest. Then, click **Get Substances**.

SUBSTANCES	
Select All	Deselect All
3 of 9 Similarity Candidates Selected	
<input checked="" type="checkbox"/>	≥ 99 (most similar) 18
<input checked="" type="checkbox"/>	95-98 168
<input checked="" type="checkbox"/>	90-94 74
<input type="checkbox"/>	85-89 213
<input type="checkbox"/>	80-84 686
<input type="checkbox"/>	75-79 1436
<input type="checkbox"/>	70-74 3324
<input type="checkbox"/>	65-69 5915
<input type="checkbox"/>	0-64 (least similar) 19313
<input type="button" value="Get Substances"/>	

### Now what?

After you click Search, SciFinder will retrieve the answers that meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

# Search by Markush Structure

Explore Saved Searches SciPlanner

Chemical Structure substructure > substances (535)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: MARKUSH

Structure Editor:

Java Non-Java

Click to Edit

Search by **Markush** to find patents that contain Markush structures which meet your structure query requirements.

- 1 To begin, click **Markush**.
- 2 Click the picture of the structure drawing window to launch the **Structure Editor**.
- 3 Draw your structure.
- 4 Specify the type of structure search and then click **OK** to transfer the structure and type of search to the search page.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Drawing Editor:

- Structure
- Reaction
- Markush

Get Markush patents where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK Cancel

SELECT...	IF YOU WANT TO RETRIEVE...
Variable only at the specified positions	Structures in which substitution is only allowed where it is specifically indicated by R-groups or other variable atom or bond features
Substructure of more complex structures	Structures in which substitution is allowed on all positions where it is not explicitly blocked

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure substructure > substances (535)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

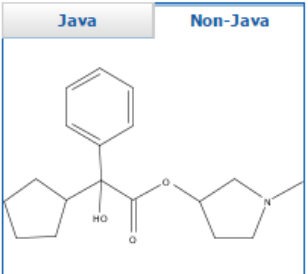
REACTIONS

- Reaction Structure

SUBSTANCES: MARKUSH ?

Structure Editor:

Java Non-Java



Search Type:

- Allow variability only as specified
- Substructure

Click image to change structure or view detail.

Import CXF

5 Search

5 Click **Search** to find the answers that meet your query requirements.

SciFinder is useful for a preliminary patentability or freedom to operate search. For a thorough patentability search, consult a patent attorney, information professional or Science IP at CAS.

**Tip**

A Markush search is a great way to extend a structure search, especially if you did not find any substances with a structure search and are interested in patentability.

**Now what?**

After you click Search, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Reference Answer Set."

# Search by Molecular Formula


The screenshot shows the SciFinder interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar menu is open to the 'SUBSTANCES' section, with 'Molecular Formula' selected. The main area is titled 'SUBSTANCES: MOLECULAR FORMULA'. A search input box contains the text 'C18 H25 N O3'. Below the input box, there are examples: 'H4SiO4' and '(C3H6O.C2H4O)x'. A blue 'Search' button is located below the examples. Three numbered callouts are present: 1 points to the 'Molecular Formula' option in the sidebar; 2 points to the search input box; 3 points to the 'Search' button.

1 To begin, click **Molecular Formula**.

2 Enter the molecular formula into the query box.

3 Click **Search**.

## Tip

Click a  to access context-specific online help. Click it next to Molecular Formula to see the help messages that provide many examples about how to search Molecular Formulas for polymers, salts and structure repeating units.

## Molecular Formula Query Guidelines

- Specify the full molecular formula; include the total number of hydrogens (Hill Order not required).
- For best results, it is useful to separate each element symbol and its count with a space.
- Capitalize the first character for multi-character symbols, and use lower case for the second letter (i.e., Si, Cl, Fe).
- You can search two isotopes: D = deuterium and T= tritium.

## Now what?

**Molecular Formula** searches often retrieve many isomeric substances and it is necessary to narrow answers. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

# Search by Property

Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

SUBSTANCES: PROPERTY ?

Experimental

Density (g/cm<sup>3</sup>) >10  
Examples: 44, 25-35, >125

Predicted

Select Property...  
Examples: 44, 25-35, >125

Search

- 1 To begin, click **Property**.
- 2 Click the appropriate radio button to select either **Experimental** or **Predicted** property. Next, click the drop-down menu and select the specific type of property you want to search.
- 3 Enter the value or range.
- 4 Click **Search** to retrieve the answers that meet your query requirements.

## Tip

If your property search results in a large answer set, you can narrow it by specifying additional criteria using **Refine** or **Analyze**.

## Now what?

After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

# Search by Substance Identifier

Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

SUBSTANCES: SUBSTANCE IDENTIFIER ?

103-90-2  
Endoxane  
PVC

Enter one per line.  
Examples:  
50-00-0  
999815  
Acetaminophen

Search

- 1 To begin, click **Substance Identifier**.
- 2 Enter up to 25 substance identifiers, one per line, in the query box.
  - A substance identifier can be a CAS Registry Number® or a chemical name.
  - Simple chemical names, trade names, abbreviations and common names often result in relevant answers.
- 3 Click **Search** to retrieve the answers which meet your query requirements.

## Tip

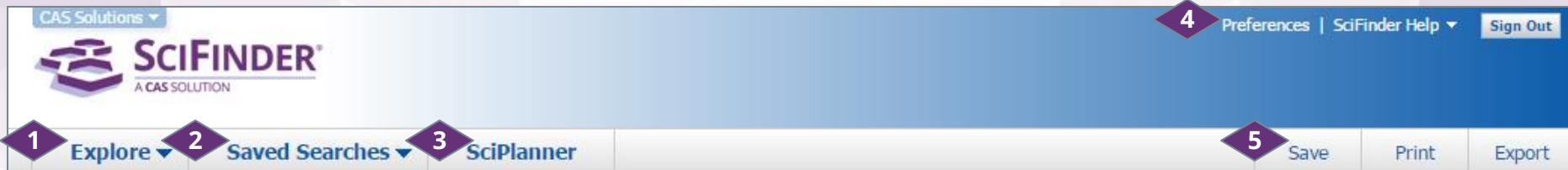
For complex, systematic names such as some IUPAC names, consider searching by the chemical structure. It is often easier to match a structure rather than it is to match all of the chemical symbols and punctuation exactly as it is entered into the database.

## Now what?

After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."



# Manage Your Search



1 Start a new **References**, **Substances** or **Reactions** search.

2 Access **Saved Answer Sets**, **Keep Me Posted** automated alert results and your search **History**.

3 Open the **SciPlanner** interactive workspace where you can organize your reference, substance and reaction search results.

4 Access **Preferences** and **SciFinder Help** options: **Help**, **Training**, **What's New** and **Contact Us**.

5 Click **Save**, **Print** or **Export** to open a dialog window and initiate these procedures. See "How to... Save, Print and Export Answers" for more information.

## Tip: Other Ways to Create a Substance Answer Set

You can also start with a reference answer set and then create a substance answer set. Just click the "Get Substances" icon at the top of the page.



## CAS Customer Care Center

E-mail: [help@cas.org](mailto:help@cas.org)

Phone numbers: <http://www.cas.org/contact-us/cas-customer-center>