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 REGISTRYSM, 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.

Types of Substance Searches

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

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

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.
   - Non-Java is recommended.

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.

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SELECT... | IF YOU WANT TO RETRIEVE...
--- | ---
Exact Search | The specific structure as drawn in the query, including:
  - Stereoisomers
  - Salts and mixtures
  - Polymers with one exactly matching monomer
  - Isotopes
  - Tautomers

Substructure Search | The structure as drawn or as part of a larger molecule in which there is:
  - Substitution at open positions
  - Additional ring fusion

Similarity Search (Queries cannot include variable groups, repeating groups or variable attachment positions) | Similar chemical structures containing:
  - Positional isomers
  - Different or fewer substituents
  - Different ring systems

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

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

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**.

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

Precision Analysis Window (Unrelated Example)

**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

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.

<table>
<thead>
<tr>
<th>SELECT…</th>
<th>IF YOU WANT TO RETRIEVE…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variable only at the specified positions</td>
<td>Structures in which substitution is only allowed where it is specifically indicated by R-groups or other variable atom or bond features</td>
</tr>
<tr>
<td>Substructure of more complex structures</td>
<td>Structures in which substitution is allowed on all positions where it is not explicitly blocked</td>
</tr>
</tbody>
</table>

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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

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.”

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Search by Property

To begin, click Property.

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.

Enter the value or range.

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

To begin, click **Substance Identifier**.

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.

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.


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