How to…Work with a Substance Answer Set

Easily identify and isolate substances of interest

Quickly retrieve relevant information from the world’s largest, publicly available source of substances and references. This guide provides an overview of some of the sort, refine and analyze tools for confidently evaluating and narrowing even a large answer set. From there, two clicks retrieve references or reactions associated with your substance of interest. For more detailed information and additional training resources, consult the online Help or visit www.cas.org/training/scifinder.

Substance Search Results

1. Exact and substructure answer sets are sorted by relevance. Click the drop-down arrow to select another sort option.

2. The blue arrow indicates that the results are sorted from most to least relevant. Click the arrow to reverse the sort order.

The number of retrieved substances and the number selected are displayed.

- To select an answer, click the box to the left of the answer number.
- Click the drop-down arrow for options related to selected answers.

Tip
Default sort options vary depending on the type of search conducted.
- Molecular formula, property and substance identification searches are sorted by CAS Registry Number®.
- Similarity search results are sorted by similarity score.
- Markush patent results are sorted from the newest to oldest reference.
Each answer includes:
- The CAS Registry Number; it is a link to the Substance Detail page
- Active icons indicate the availability of:
  - References for the substance
  - Reaction data
  - Chemical supplier information
- The chemical structure; the part that matches your query is red
- The molecular formula
- The CA Index Name (useful for government documents)
- Links to Regulatory information, Spectra and Experimental Properties, when available

Click Display Options to specify the number of answers displayed per page (15, 20, 25 or 50) and to select the number of columns to display.

Use the page controls to navigate through your answer set.

Mouse over a substance to access additional substance information and tools.
- Click the double blue arrow to access the additional search and export options shown here.
- Click the magnifying glass icon to launch the Quick View, a separate window that summarizes data about the substance (not shown)
- Close the Quick View window to return to the active session.
Click a CAS Registry Number on the answer page to open the **Substance Detail** page. It summarizes the available information for a substance.

1. The display at the top of the page includes the **CAS Registry Number**, molecular formula, CA Index Name, Molecular Weight and some common properties for this substance.

2. **Other Names** lists up to five chemical name synonyms.
   - When more names are available, a **Show More** link is at the bottom of the list.

3. To explore details about a substance, expand a menu by clicking the arrow next to a content area.
   - At the top of these menus are **Expand All** and **Collapse All** links.
You can expand the menus to see more information about a content area, as shown here. In many cases, tabs provide convenient access to additional information.

Tip

CAS Reference Roles indicate the function of a substance in the document. CAS Analysts have applied roles as part of the indexing process since 1967. The Preparation role goes back to 1907.
Evaluate Answers with Analysis Options

By default, the answer set is analyzed by Substance Role.

Click the drop-down arrow to see the available Analyze by: options.

Click Show More to see additional data, when available, or to select more than one analysis subset.
- Click the box to the left of a subset to select it.
- Sort by either Frequency (the default) or Natural Order (alphanumeric order).

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Narrow an Answer Set after Analysis

Click an Analyze bar to display that subset of answers. In this example, the answer set is analyzed by Bioactivity Indicators and Respiratory system agents (all).

- The analysis bar turns yellow.
- Other bars can also turn completely or partly yellow to indicate that substances from the selected bar are also present in other subsets.
- Click Substance Detail to see a summary of bioactivity and target indicator data, when available.

The yellow status bar indicates the answers that are currently displayed.

- Click Keep Analysis to make these answers your new answer set.
- Click Clear Analysis to return to your original answer set.

Tip
- **Bioactivity Indicators** are a predefined set of bioactivity terms for which relationships have been identified between substances and documents in the content.
- **Target Indicators** are a predefined set of protein, enzyme and other target terms for which relationships have been identified between substances and documents in the content.
Narrow an Answer Set with Refine Options

Click the **Refine** tab and click a radio button to select a **Refine by** option.

Specify additional criteria below the refine options.

Click **Refine**.

**Tip**

To **Refine** by **Chemical Structure**, click the thumbnail to re-open the **Structure Editor**.

Modify the structure and click **OK**. The modified structure is then displayed in the thumbnail on the **Refine** tab. Click **Refine** and the answer set is narrowed based on the new criteria.
Manage Your Searching


Click the Explore drop-down arrow to start a new references, substances or reactions search.

Click the Saved Searches drop-down arrow to access Saved Answer Sets, Keep Me Posted answer sets and your search History.

Click SciPlanner to open the SciPlanner workspace.
- It is an interactive window where you can store and organize reference, substance and reaction search results.

Click Save, Print or Export to open a dialog window and initiate each of these processes.
- See “How to… Print, Save and Export” for more information.

The breadcrumb trail shows each step in your current search history. Mouse over a step to see more information about it. Click a step to return to that part of the search.

Click Get References to retrieve references for part or all of your answer set.

Click Get Reactions to retrieve reactions for part or all of your answer set.

Click Get Commercial Sources to retrieve suppliers for part or all of your substances.

Click the Tools drop-down arrow to combine this answer set with a previously saved answer set (Combine Answer Sets).

Create Keep Me Posted Alert, when active, allows you to create an automated alert based on the current search strategy.

Click Send to SciPlanner to send selected answers to the SciPlanner workspace.
- Use it to gather information for a project, create a report or export research to share with colleagues.