

# CAS SciFinder – Getting started

## Substances Search

### Substance name search

You can search substances by placing one or more substance names or identifiers into the query box. You can also draw or edit a structure. Below are name search option examples.

- Streptomycin** Finds Streptomycin record
- 57-92-1** Finds Streptomycin record, using CAS Registry Number® as identifier
- Sulfoximin** Finds all names that start with the stem Sulfoximin
- WO2019234160** Finds all indexed substances for this patent

Click to draw new structure

Enter chemical name query

Click query structure to edit

Add advanced search fields

Search CAS Lexicon

Search CAS Sequences

Check to perform Markush search

### CAS Draw editor

You can define structure and reaction queries using the CAS Draw structure editor.

Import structure from .cxf or .mol file

Enter CAS Registry Number, SMILES, or InChI to create structure

Draw or change atoms or bonds

Atom and H isotope selection

Draw atoms and bonds | Eraser

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Add attachment point to fragment | Select from templates

Add positive charge | Add negative charge

Repeating groups | Carbon chain tool

Define variable point of attachment at ring | Lock rings

Lock atoms | Rotate/Flip fragment

Draw bonds and rings

Reaction map | Atom mapping

Bond mapping | Draw reaction arrow

Further selections

Resize window

Type in any element symbol to draw

ChemDraw allows to search structures in SciFinder by using the SciFinder add-in from the menu or icon. The SciFinder history will show 'Searched from ChemDraw'.

### Substances search result

Substances search results are displayed in an intuitive interface where you will see the most relevant results for your search.

Get related references, reactions or suppliers for all or selected substances

Click CAS Registry Number to open details

Click on structure to open flyout window

Retrieve data related to substance

Open editor with this structure

Reference Roles show which information was reported about a substance in the literature

Download structure, image or copy SMILES

## Reactions Search and Substance Details

### Reaction Searching

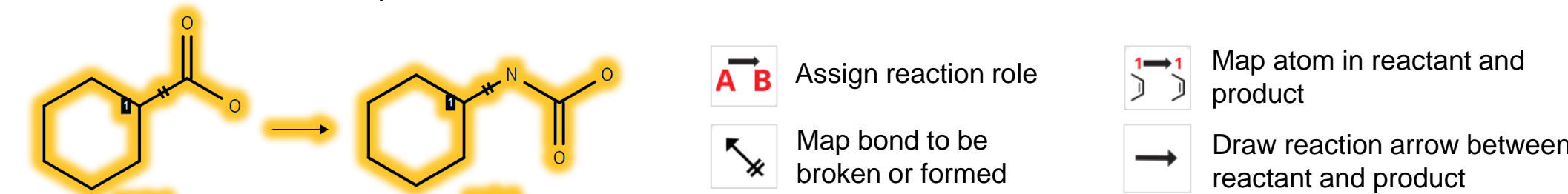
#### (1) Text search.

**Vanillin** → Refine with substance roles in the next step to limit to the correct context, e.g. product or reactant

**Synthesis of solatenol catalyzed by copper oxide**

**Suzuki** → Use Search Within in the next step to draw out specific reaction participants following the Suzuki coupling scheme

(2) Draw reaction diagram. Draw a reaction diagram in the drawing editor or from a reaction answer set using 'Search Within'. Draw a reaction arrow between reactant and product. If you draw reagents, please make sure to assign an appropriate role.



### Reaction search results

Change grouping to 'By Document' or 'By Transformation'

Save, alert and share options

Click on structure to view substance information

Yield for displayed reactions

View reaction details, incl. synthetic protocols

View reaction reference

Access annotated patent full-text

### Substance properties and details

Substance details and spectra can be searched utilizing advanced search and filters. By clicking on the CAS RN details are shown.

Download substance details

Overview of most important properties

Options to filter for substances with experimental spectra and properties

Published properties and spectra can be obtained via the experimental accorions and predict properties are generated utilizing ACD Labs

Hyperlink to spectra

Search by properties either combined with or without a structure

Property	Value	Condition	Source
Melting Point	7.969		(1) CAS
Glass Transition Temperature	(530)		(1) CAS
Optical Rotatory Power	(134)		(1) CAS
Elongation at Break	(123)		(1) CAS
Tensile Strength	(122)		(1) CAS
Proton NMR	(4,408)		(1) CAS
Carbon-13 NMR	(3,089)		(1) CAS
Mass	(6,603)		(1) CAS

## Interface and References Search

### Search interface

CAS SciFinder features a streamlined search interface.

Access CAS Formulas® and CAS Analytical Methods™

Click the CAS logo to return to the main search page

Access alerts

Access account settings

Combine saved sets

Download

Save and Alert

Add to Project

Share Results

Copy Search to Clipboard

Enter the query

Access user-specific content recommendations

Access projects, saved items, history, downloads and submit feedback

Execute the search or press ENTER

Submit Feedback

### References search result

Performing a references search provides you with access to a full result set in an easy-to-use interface where:

- References are default sorted by relevance with customizable sorting options.
- You can focus your answer set further using filters.
- You can save searches, send a link of the results, set up alerts, or add results to a project list.
- You can quickly access full details for any of the references displayed.

Boolean operators

You can use logical operators to create precise text queries.

Ex: **menthol and (food or "chewing gum")**

AND Both terms are present within the document

OR Either one or both terms are present (connect synonyms with OR)

NOT Excludes documents from the set containing the word(s) after NOT

Ex: **menthol not cigarette**

Wildcards allow for more comprehensive results Internal and right-hand truncation is possible.

\* Replaces 0 to any number of characters

Ex: **crosslink| | alk\*ne**

Phrases enclosed with double quotes ("...") will be searched as a precise phrase.

A search for **cell death protein** only finds results that exactly match: cell death protein.

View indexed substances

View indexed reactions

Download answers

Combine current with saved set

Filtering: Concept: Flavor X Deselect applied filters

Excluding: Concept: Antibacterial agents X

Sort answers

Clear all filters

Load more potentially relevant results

Click title to open reference details

Change how answers are displayed

Search within Results

Select Filter by or Exclude, then select filter categories

Search any text within this answer set

Retrieve substance, reaction, or citation data for this reference

Access full-text options

Select filters to refine answers

## Save, Alerts, Download, Share, Projects

**Save** allows to save the search and related filter settings or up to 20,000 answers. Tags can be added and used for later filtering.

Name: Suzuki coupling

Search Options: Query Only | Selected Answers | All Answers (Up to 20,000)

Add Existing Tags (Optional): green\_chem, ammonia cracking, analytical study, anticancer, axitin transport alerts

New Tag (Optional): name reactions

Tag Color: Dark Blue

**Share** has two options:

- Share Results** allows to share with a SciFinder user identified by the email address. A message can be added.

Share Results

- Copy Search to Clipboard** stores the URL of the search in the clipboard. This URL can be shared with any SciFinder user.

Copy Search to Clipboard

**Add to Project** will add selected reference or substance information to a project folder. The folder content can be edited collaboratively, making projects an ideal collaboration tool when collecting research- or project-specific reference or substance data.

Project Name: green chemistry project

Project Color: Lime

Existing Projects: PHS, bicyclic pesticides, herbicides - nicotinic acid derivatives, Arabidopsis - endophyt

**Alerts** will re-run the underlying search and filters in a frequency you choose. Results will be available in SciFinder and an email will be sent to the recipients, including links to SciFinder results.

Alerts: Frequency: Weekly

Add Email(s): email@abc.com

**Download** will transfer results to your local storage device. Available options depend on the File Type.

File Type: Citation (.ris)

Display: Result Summary | Result Details

File Name: Reference\_20240724\_1607

2 references selected to download.

Include: Task History, Abstract, Concepts, Substances, Formulations, Analytical Methods, Citations

A description can be added, and the project can be shared with SciFinder users. Its content can be downloaded.

Project Description: Chitosan as a reusable solid base catalyst for Knoevenagel condensation reaction

Collaborators: Jan H Baur (You), kfaerber@acs-lorg (Pending)

Project collaborators and their roles can be defined.

Project Collaborators: Jan H Baur (You) - Administrator, kfaerber@acs-lorg (Pending) - Editor

## Request training

Please send an email to Dr. Karin Färber at [kfaerber@acs-lorg](mailto:kfaerber@acs-lorg).

## Advanced search Sequence search

Annotated patents  
Markush structures  
Formulations

Suppliers  
CAS Roles  
Spectra  
CAS Lexicon  
Citations  
Bioactivity data



Get the full guide

Regulatory data  
Detailed protocols

## Analytical Methods