

CAS SciFinder – Essential Features for Students

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 role | 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 Retrosynthesis Planner

Reaction Searching

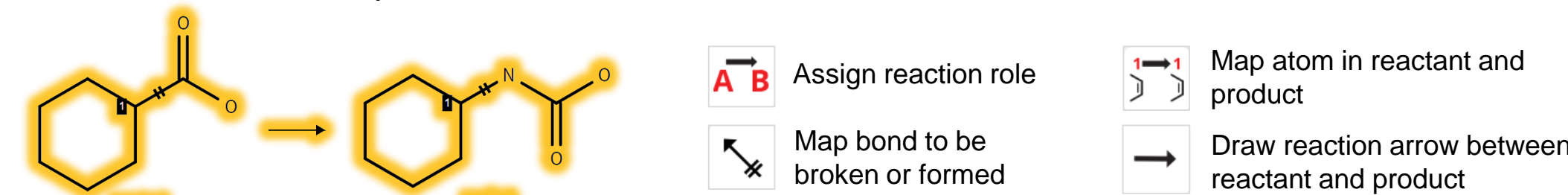
(1) Text search.

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 example:



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

Retrosynthesis Planner

There are two primary ways to launch the 'Retrosynthetic Analysis' in CAS SciFinder:

- (1) Draw or import a structure into the retrosynthesis draw window accessed by clicking on the 'Retrosynthetic Analysis' option on the landing page. The drawn substance can be novel.
- (2) Click on the 'Start Retrosynthetic Analysis' option found on the substance flyout window.

Launching the tool

Retrosynthetic Analysis

Search CAS Lexicon

Search CAS Sequences

Selecting plan options

Change the number of disconnections in the plan

Break bond in first disconnection

Protect bond(s) in entire plan

Clear selections

View plan information

Switch predicted steps on/off

Exclude steps or substances

Download, Save, and Share your plan

View plan steps

Select uncommon or rare rules supported by fewer literature examples

First bond to be broken

Protected bonds

Change upper cost limit for starting materials (USD/mol or USD/g)

Generate plan

Edit plan options

Blue lines mark experimental steps

Green dotted lines indicate predicted steps

Review and select alternative disconnections

Adjust scoring options

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

Save answers, create alerts, add to project and share results

Enter the query

Search specific fields

Access user-specific content recommendations

Access projects, 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.

View indexed substances

View indexed reactions

Download answers

Combine current with saved set

Sort answers

Clear all filters

Filtering: Concept: Flavor

Excluding: Concept: Antibacterial agents

Click title to open reference details

Change how answers are displayed

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

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.

Boolean operators

Access full-text options

Retrieve substance, reaction, or citation data for this reference

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

Add Existing Tags (Optional): green-chem, ammonia cracking, analytical study, anticancer, auxin transport alerts

New Tag (Optional): name reactions, Tag Color: Dark Blue

Share has two options:

- (1) **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

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.

Add to Project

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.

Download Reference Results

File Type: Citation (.ris)

Display: Result Summary

Select Quantity: Selected Results

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

Project collaborators and their roles can be defined.

Project Collaborators

Add project collaborators using an email address...

People with access (2): Jan H Baur (You) - Administrator, kfaerber@acs-l.org (Pending) - Editor

Request training

Please send an email to Dr. Karin Färber at kfaerber@acs-l.org.

Advanced search Sequence search

Suppliers

CAS Roles

Spectra

CAS Lexicon

Citations

Bioactivity data

Annotated patents

Markush structures

Formulations

Prior Art Analysis

Analytical Methods

Regulatory data

Detailed protocols

Get the full guide