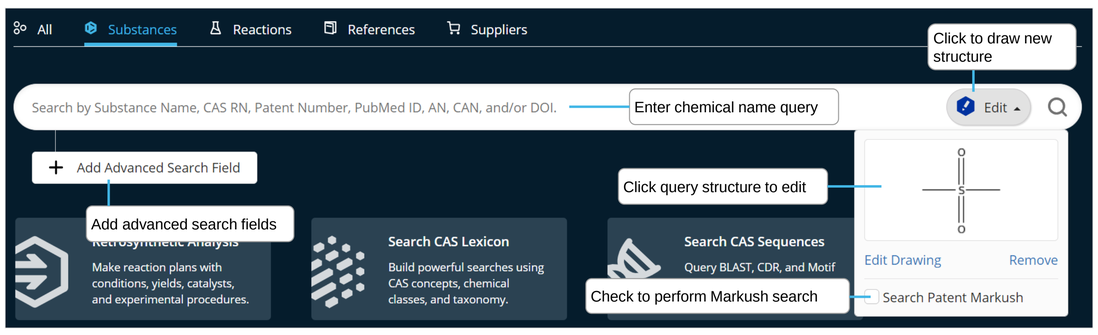
CAS SciFinder – Essential Features for Students

Substances Search

Substance name search

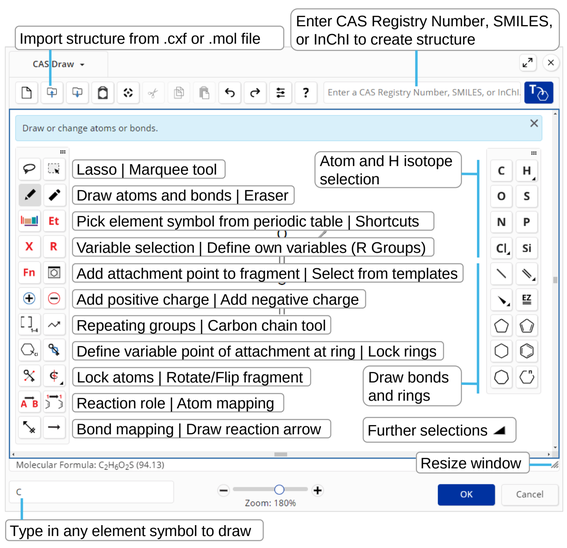
You can search substances by placing one or more substance names or identifiers into the query box. You can also draw or edit a structure. Below are name search option examples.

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



CAS Draw editor

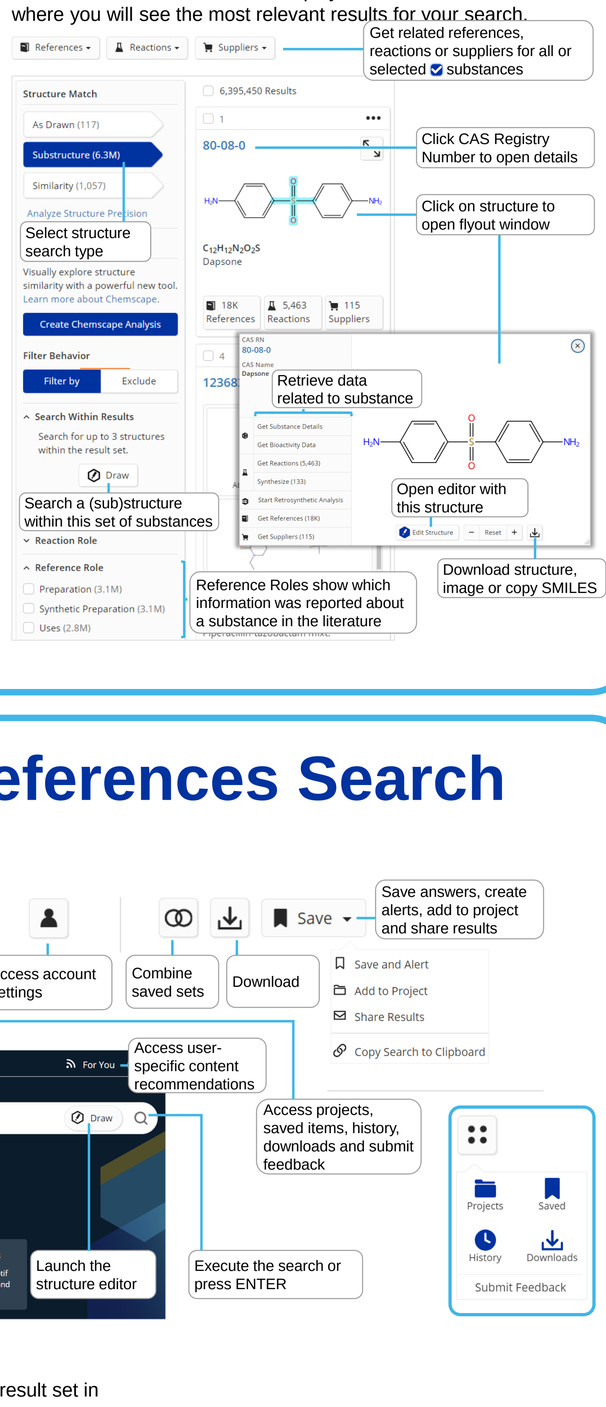
You can define structure and reaction queries using the CAS Draw structure editor.



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

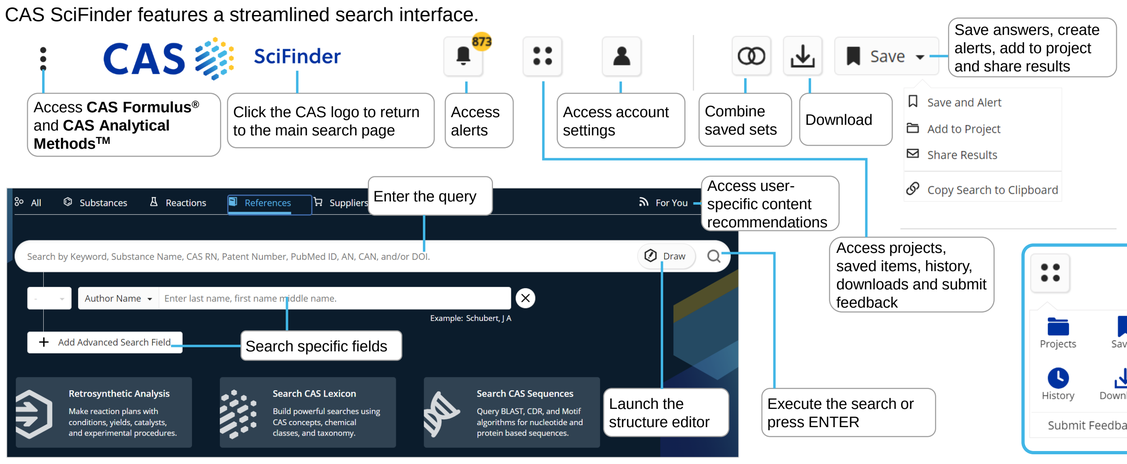
Substances search results are displayed in an intuitive interface where you will see the most relevant results for your search.



Interface and References Search

Search interface

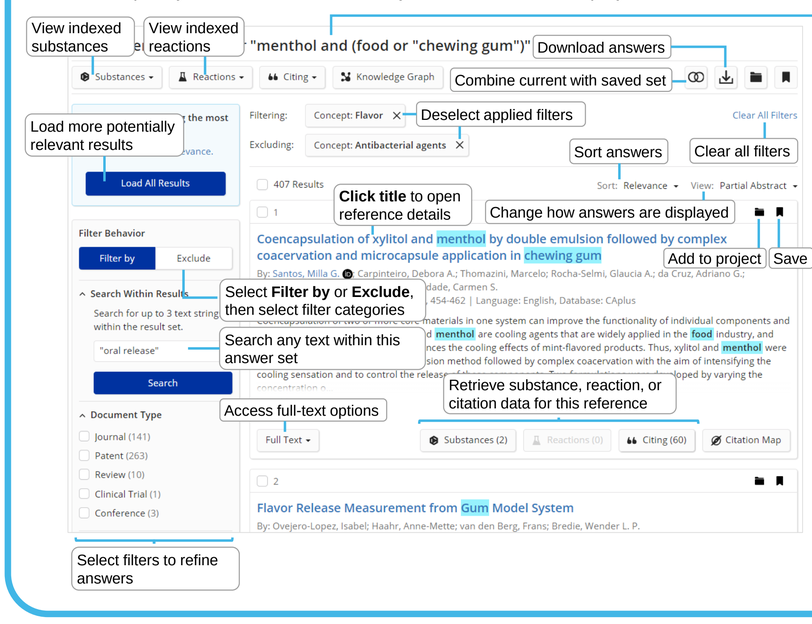
CAS SciFinder features a streamlined search interface.



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.

Request training

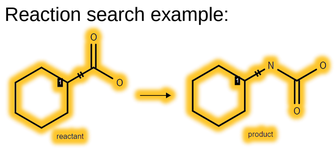
Please send an email to Dr. Karin Färber at **kfaerber@acs-i.org.**

Reactions Search and Retrosynthesis Planner

Reaction Searching

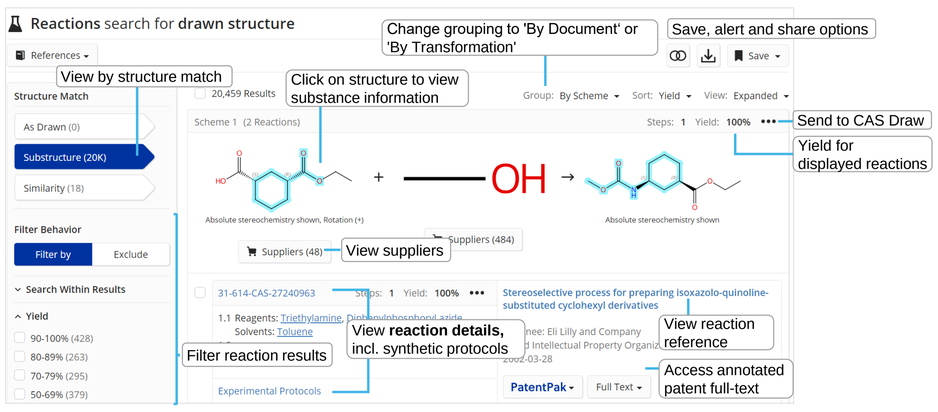
(1) Text search.
Vanillin → Refine with substance roles in the next step to limit to the correct context, e.g. product or reactant
Synthesis of solatenol catalyzed by copper oxide
Suzuki → Use **Search Within** in the next step to draw out specific reaction participants following the Suzuki coupling 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 A B .
Reaction search example:



Assign reaction role
Map atom in reactant and product
Map bond to be broken or formed
Draw reaction arrow between reactant and product

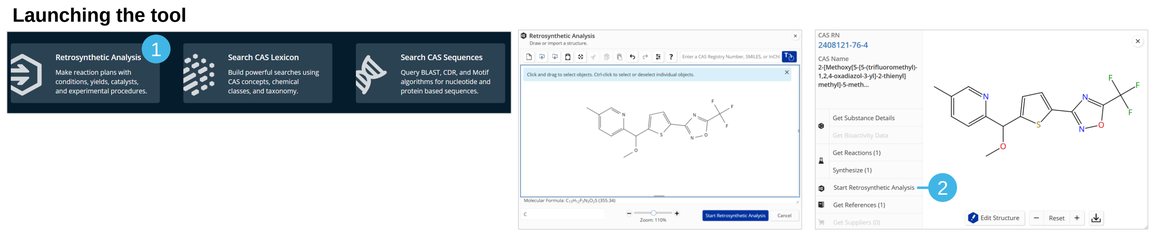
Reaction search results



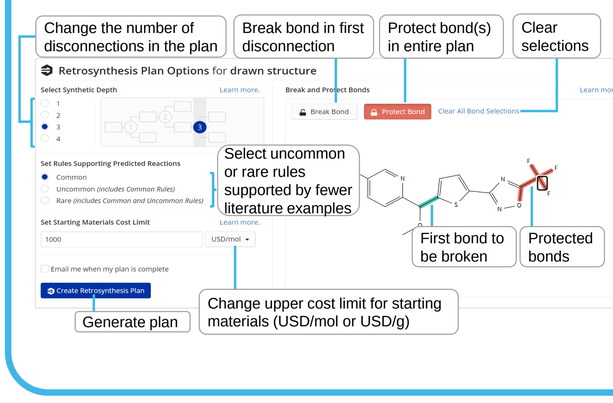
Retrosynthesis Planner

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.

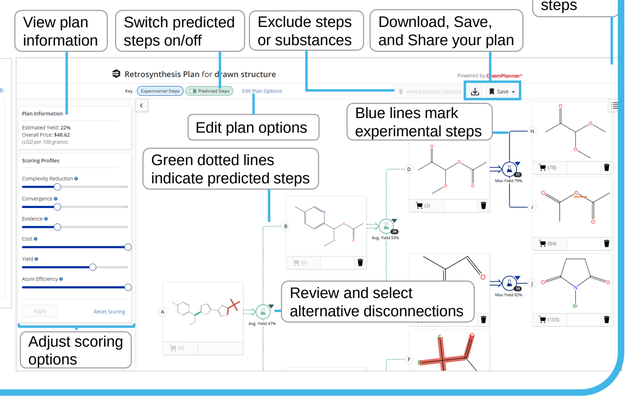
Launching the tool



Selecting plan options

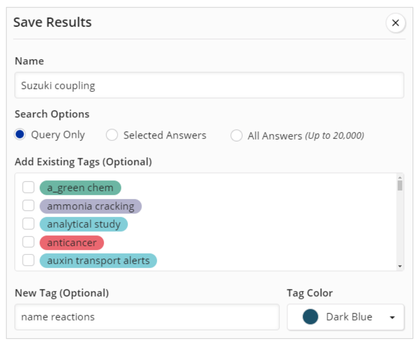


Opening the plan

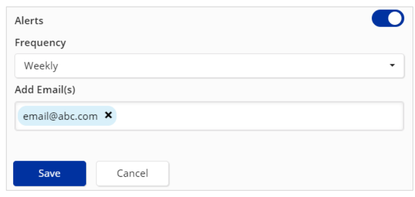


Save, Alerts, Download, Share, Projects

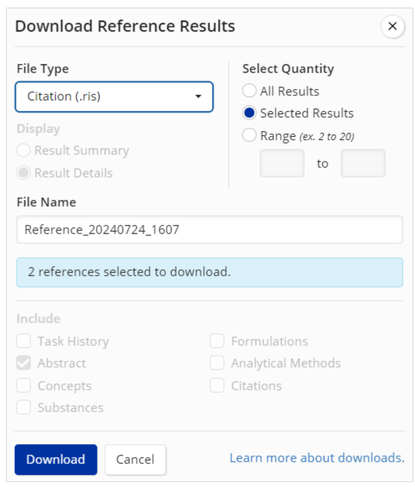
Save allows to save the search and related filter settings or up to 20,000 answers. Tags can be added and used for later filtering.



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.

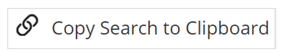


Download will transfer results to your local storage device.
Available options depend on the File Type.

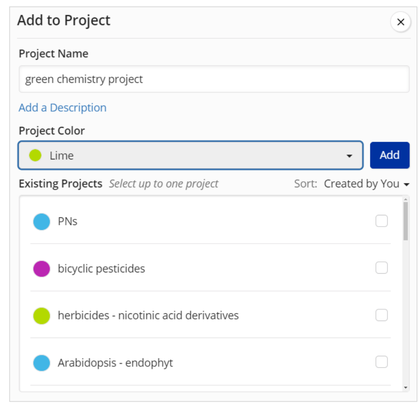


Share has two options:
(1) Share Results allows to share with a SciFinder user identified by the email address. A message can be added.

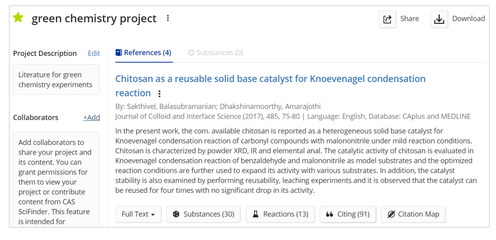
(2) Copy Search to Clipboard stores the URL of the search in the clipboard. This URL can be shared with any SciFinder user.



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.



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



Project collaborators and their roles can be defined.