CAS SCIFINDER^{n}

QUICK REFERENCE GUIDE

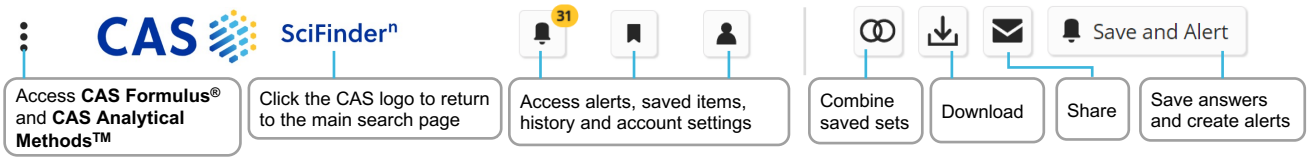
CAS
A division of the
American Chemical Society

Contents

Solution interface and References search

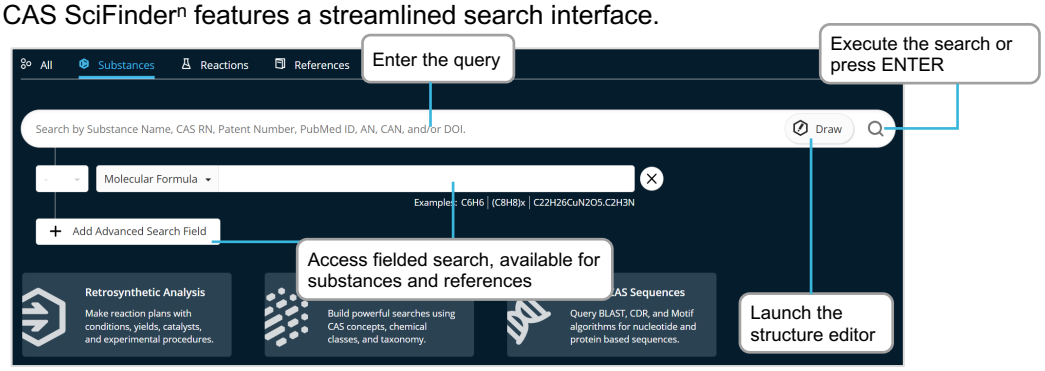
Main interface

The options below are found on the main interface in CAS SciFinder^n.



Search interface

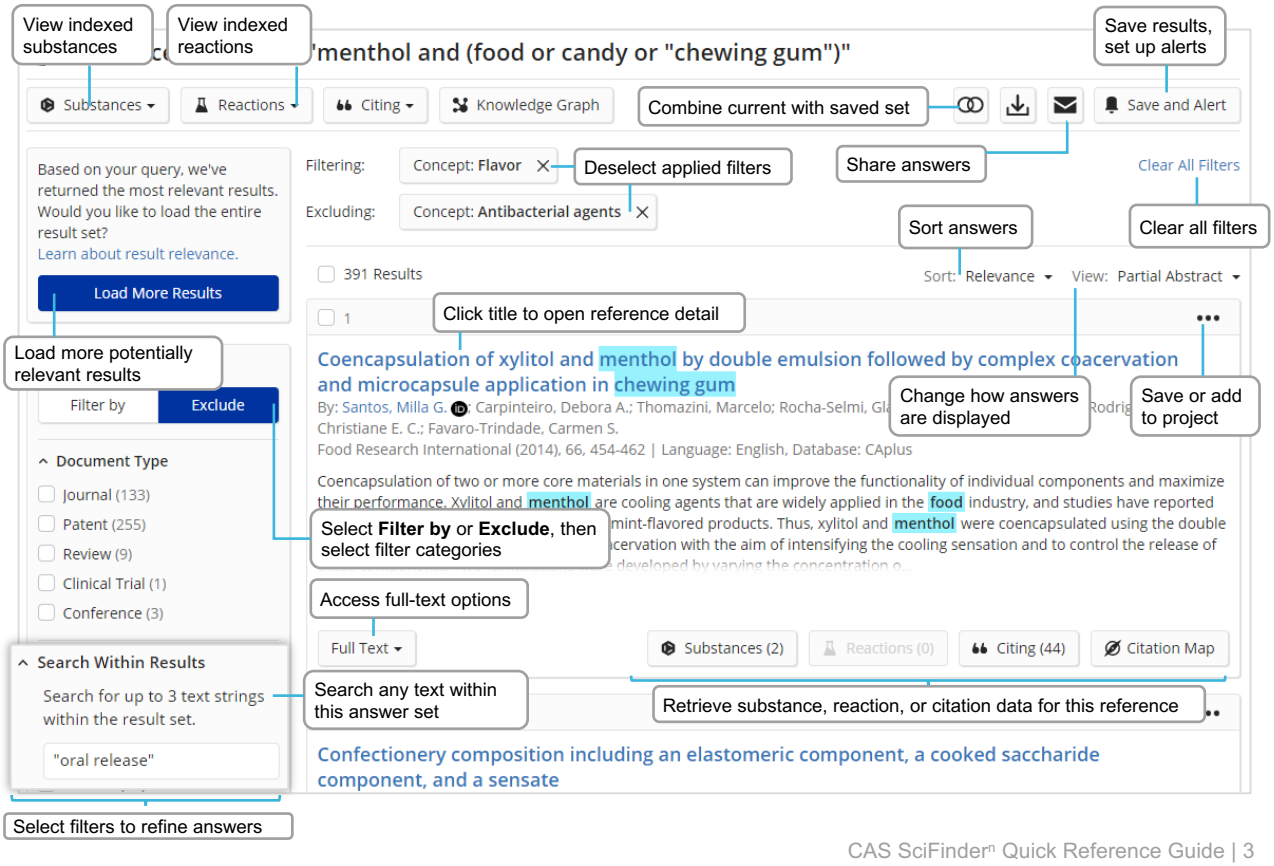
CAS SciFinder^n features a streamlined search interface.



References search result

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

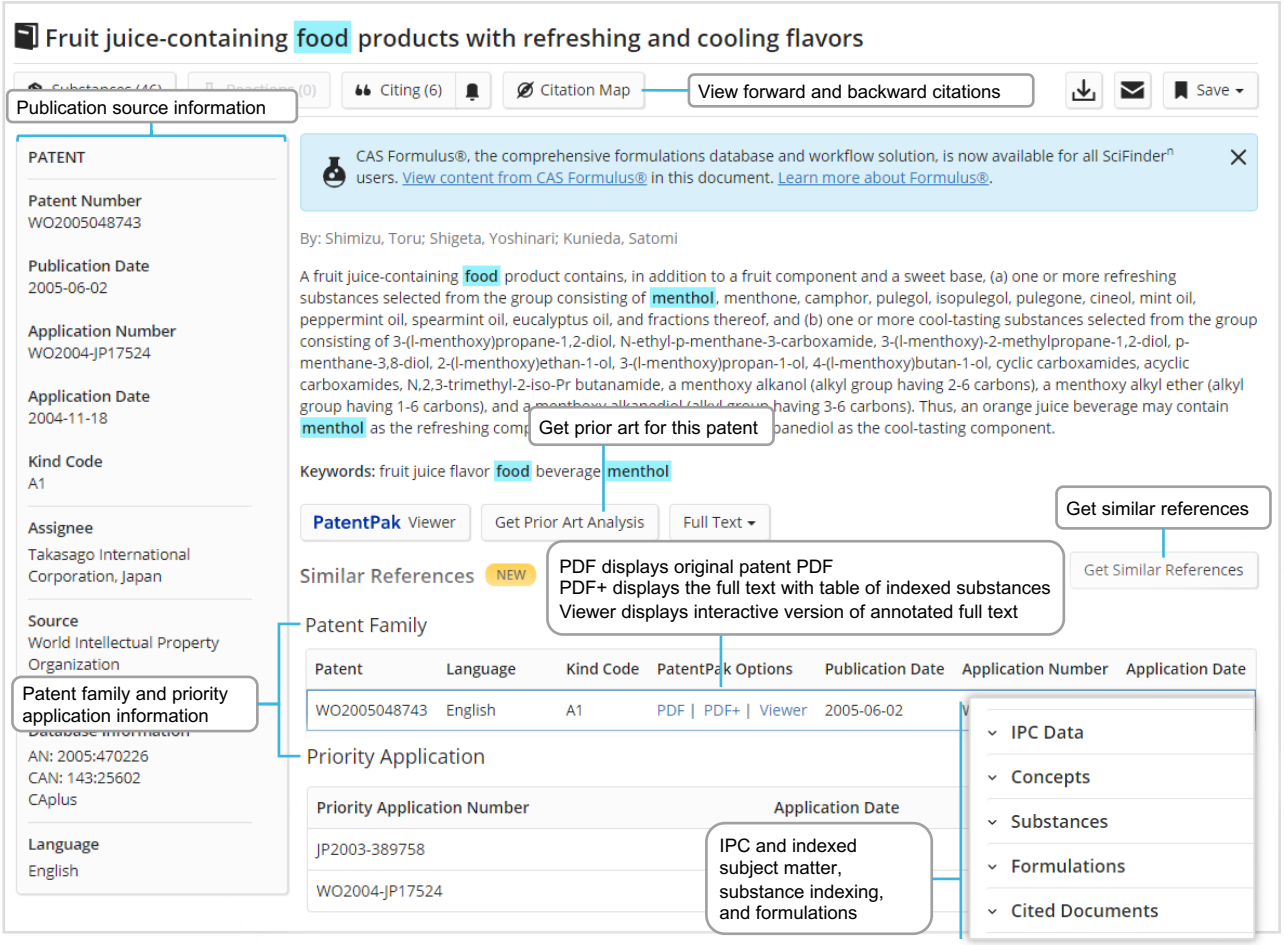
- References are default sorted by relevance with customizable sorting options.
- You can focus your answer set further using filters.
- You can save searches, send a link, set up alerts, or add results to a project list.
- You can quickly access full details for any of the references displayed.



Reference detail and search operators

Reference detail

Access full details for each reference found in CAS SciFinder^n.



Boolean operators

You can use logical operators to create precise text queries.

Use parentheses to group logical expressions, such as related terms usinng "OR", ex:

References (flavor **or** odor) **and** menthol **not** cigarette Draw

AND Requires both terms to be present within the document

OR Requires either one or both terms to be present (connect synonyms with OR)

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

Wildcards allow for more comprehensive results in reference, substance, and filter searches. Internal and right-hand truncation is possible.

***** Replaces 0 to any number of characters ex: polymorph* | immunoglobulin*conjugate*

? Replaces 0 or 1 character ex: benzonorbornen?

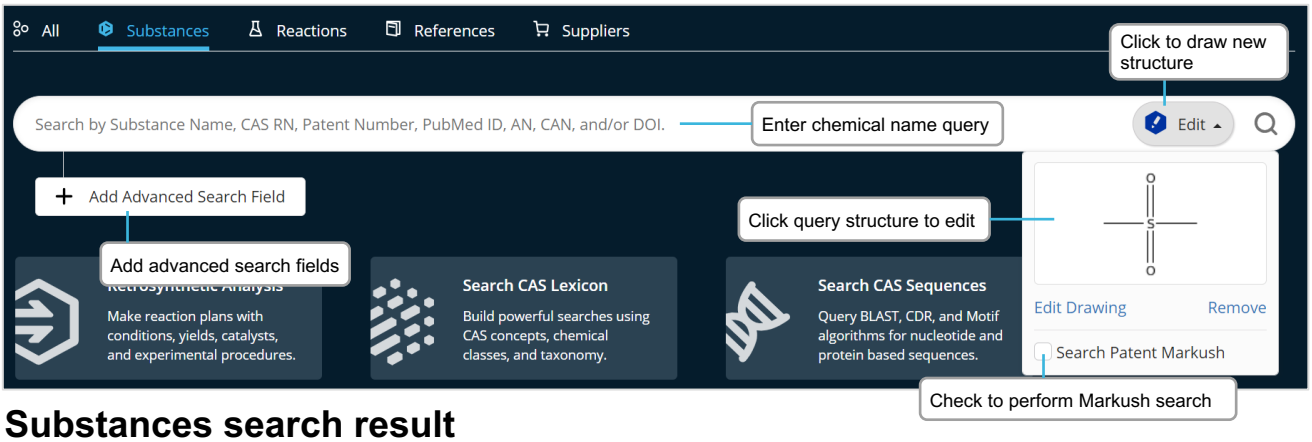
Phrases containing double quotes will be searched as a precise phrase.
Ex: a search for "Programmed cell death protein“ only finds results that exactly match: “Programmed cell death protein.”

Substance name and structure search

Substances search

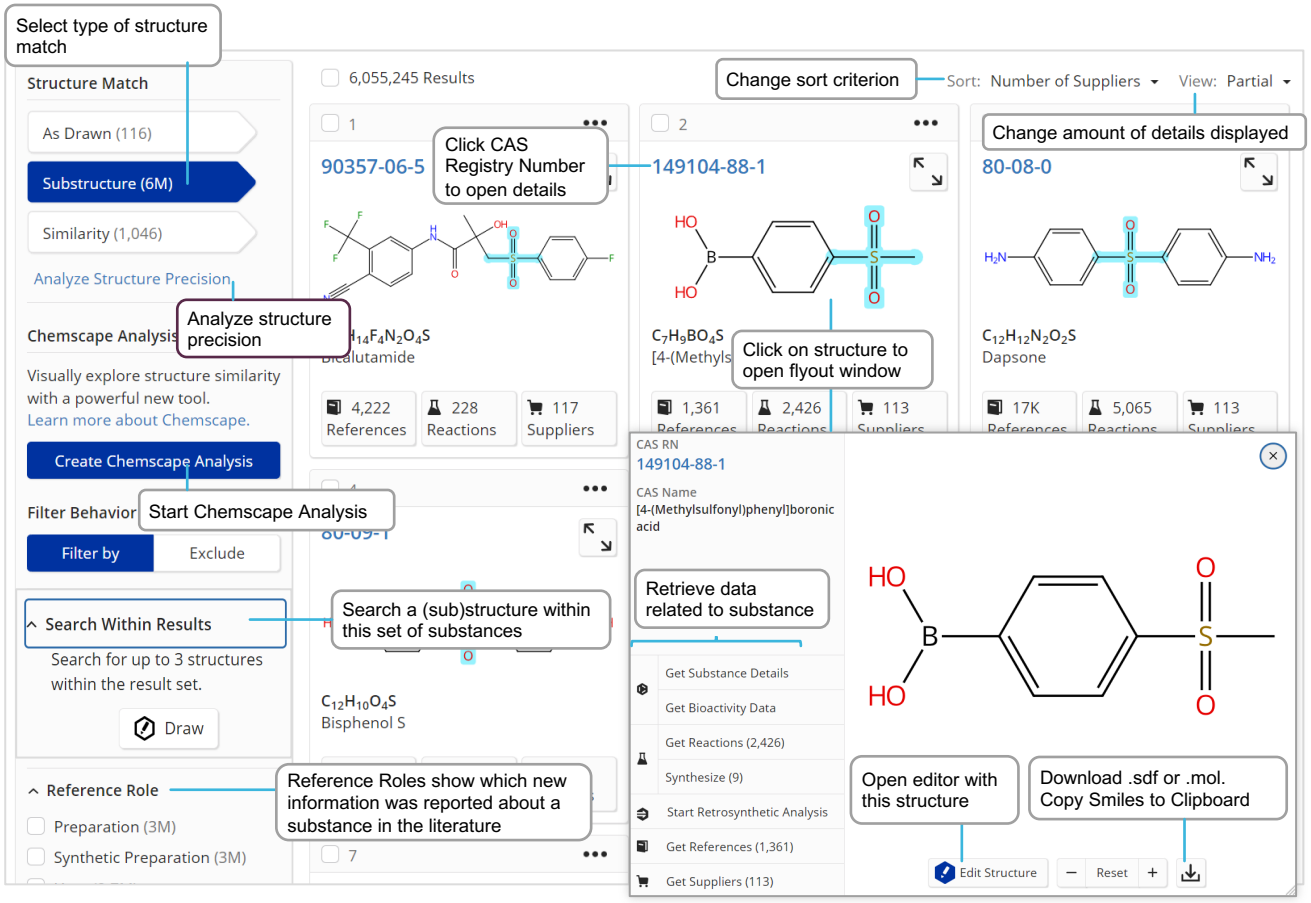
You can search substances by placing one or more substance names or identifiers into the query box. You can also draw or edit a structure. Below are name search option examples.

Streptomycin	Finds Streptomycin record
57-92-1	Finds Streptomycin record, uses CAS Registry Number® as identifier
Streptomycin sulfate	Finds three records: Streptomycin, Streptomycin sulfate, and Sulfate
"Streptomycin sulfate" Streptomycin	Finds two records: Streptomycin sulfate and Streptomycin
Sulfoximin*	Finds all names that start with the stem Sulfoximin
WO2019234160	Finds all indexed substances for this patent



Substances search result

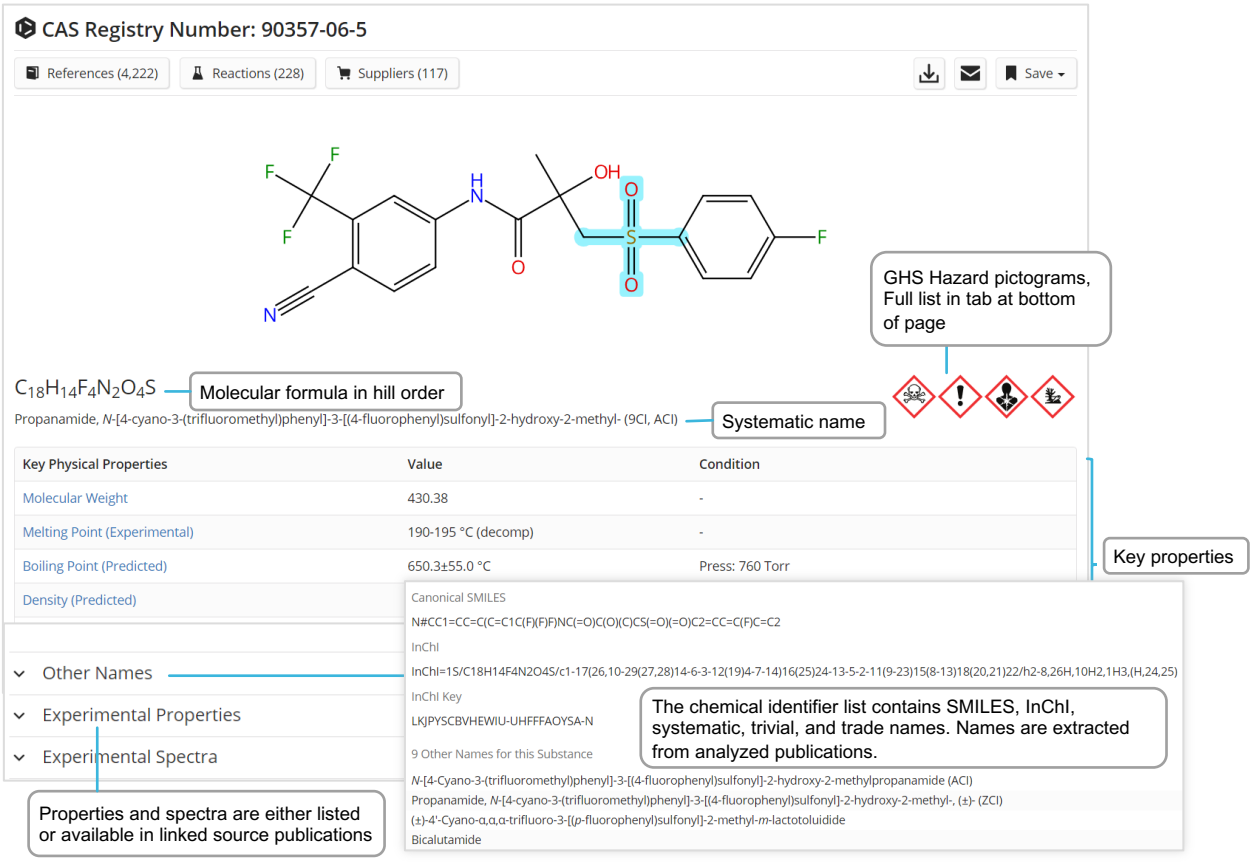
Substances search results are displayed in an intuitive interface where you will see the most relevant results for your search, including critical property information and high-resolution images.



Substance detail and structure editor

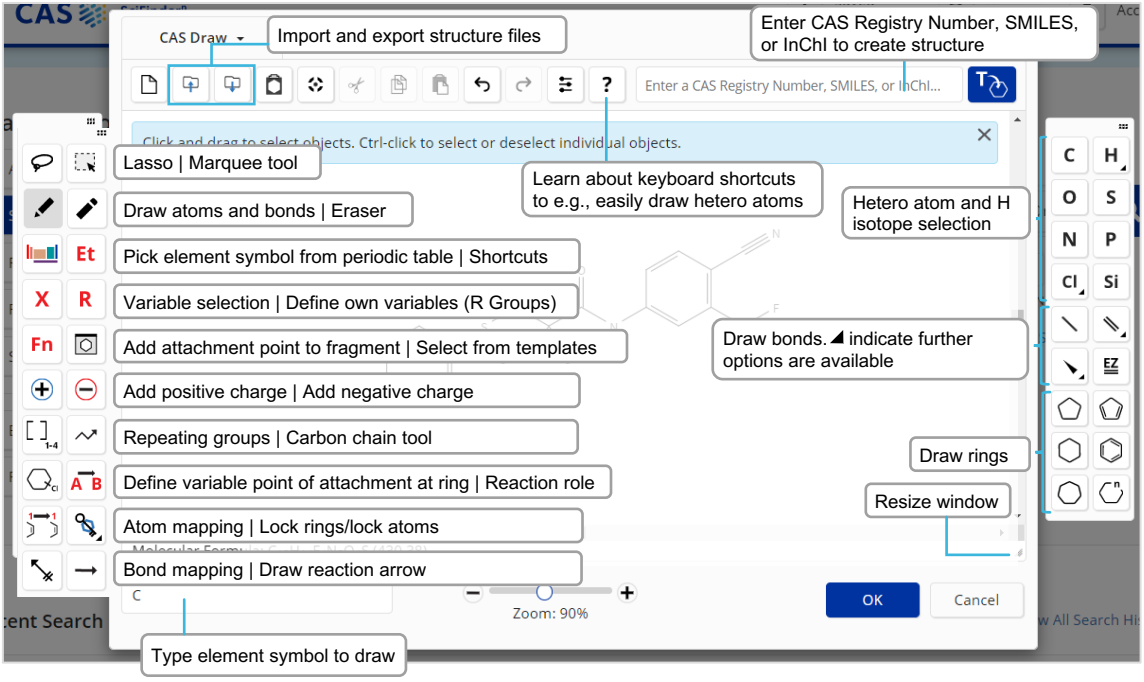
Substance detail

When you click a CAS Registry Number for one of your Substances search results, substance details including structure, molecular formula, properties, and further data are displayed.



CAS Draw editor

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

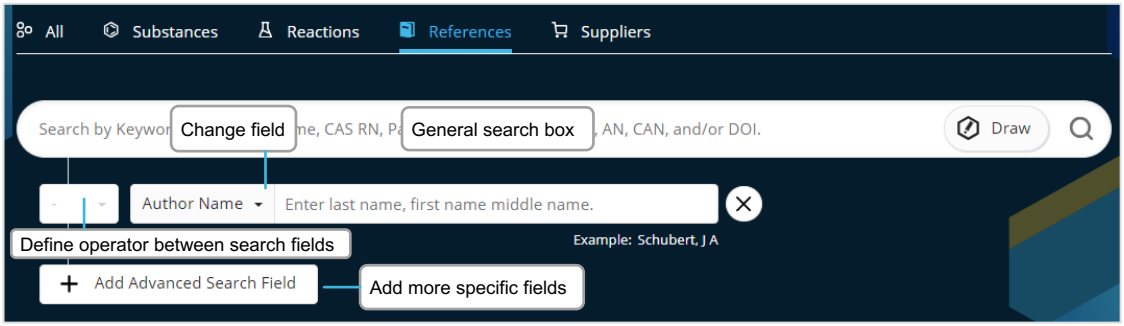


Advanced Search

Performing an Advanced Search

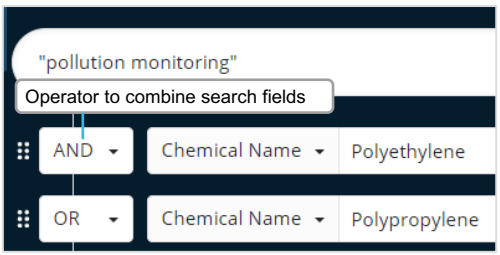
You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinder^n.

- Operators are processed in this order: **OR**, **AND**, **NOT**
- Operators are not available for a search using a single advanced search field
- Wildcards are allowed, e.g., peek*
- Use up to 50 Advanced Search Fields (49 if also using the main search field)



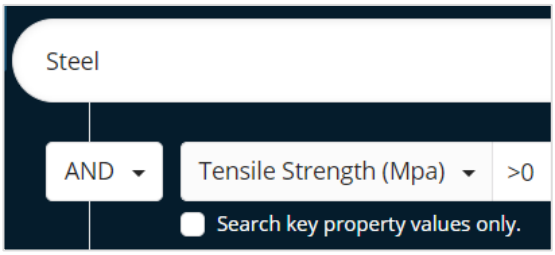
Advanced Search examples

Advanced References Search

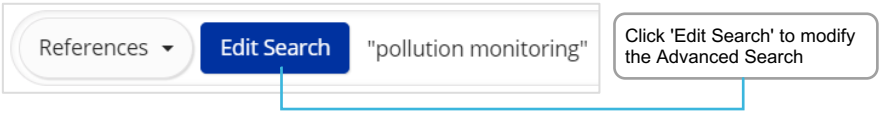


Query interpretation:
"pollution monitoring" and (polyethylene or polypropylene)

Advanced Substances Search



Query interpretation:
Steel with tensile strength property information



Available Advanced Search fields

You can utilize many search fields and categories as part of an Advanced Search query, including:

References Search

- Authors
- Publication Name
- Organization
- Title
- Abstract/Keywords
- Concept
- Substances
- Bioactivity Data
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Substances Search

- Molecular Formula
- CAS Registry Number
- Chemical Identifier
- Document Identifier
- Patent Identifier
- Experimental Spectra
- Bioactivity Data
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

CAS Roles

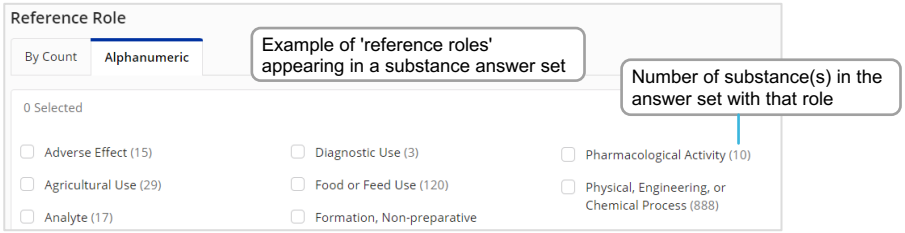
CAS Roles overview

Roles are linked to substances, allowing you to find focused publications connecting a substance of interest to its specific role within the scope of the publication.

- Super roles are broad categories and comprise all related specific roles. Examples are Analytical Study, Preparation, or Occurrence.
- Specific roles are more precise. They relate to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in a plant (Natural Product Occurrence).

Roles in substance results

From a search on substance(s), the roles filter will indicate the types of roles that are connected to the substance(s) in the publications.

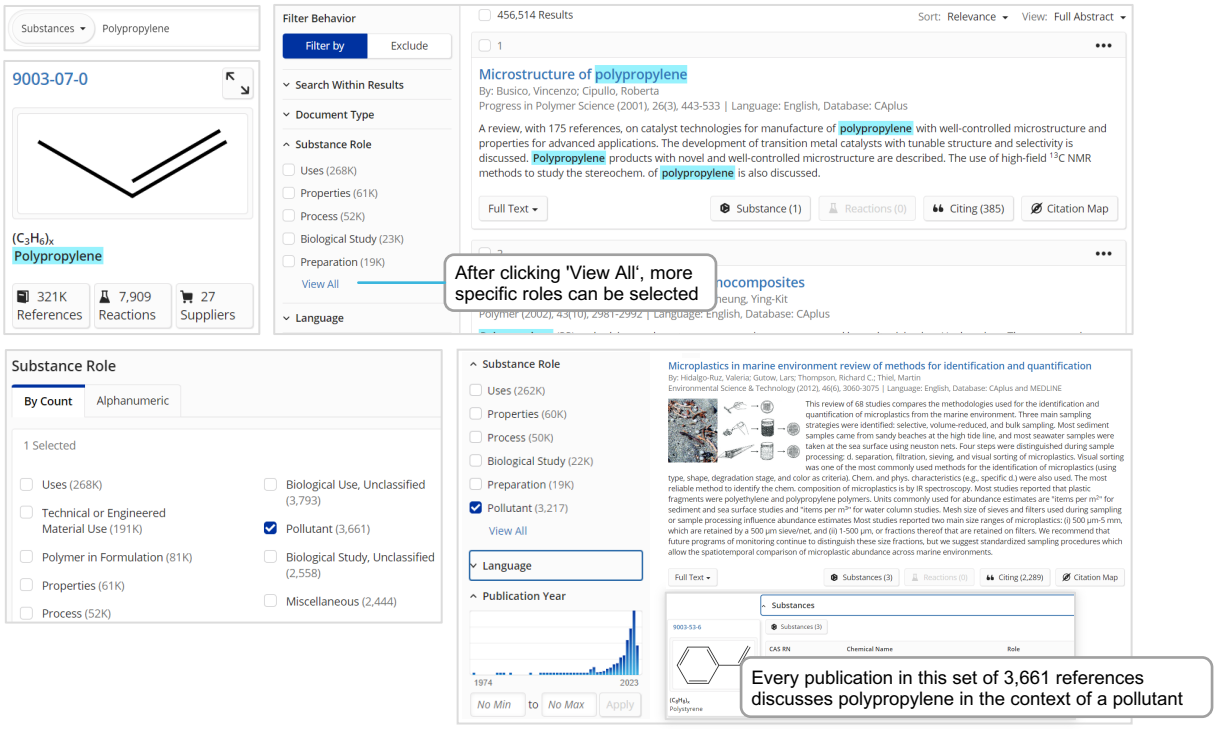


Roles in reference results

Roles will appear as a filter in reference result sets whenever you have retrieved hits in the substance indexing segment of the records, i.e., by retrieving substance names or performing a crossover after substance-based searches.

Example: I am interested in the subject of (marine) pollution, how can I find publications where polypropylene is specifically described as a pollutant?

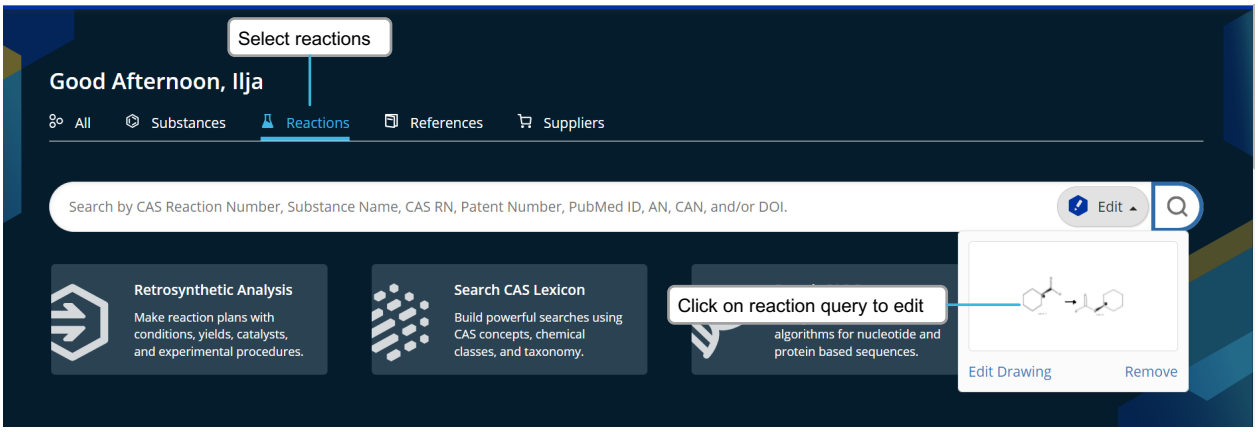
The search for polypropylene retrieves many references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3,661 publications that describe polypropylene as a pollutant. The Search Within function or concepts can be used to restrict results to marine pollution.



Reactions search

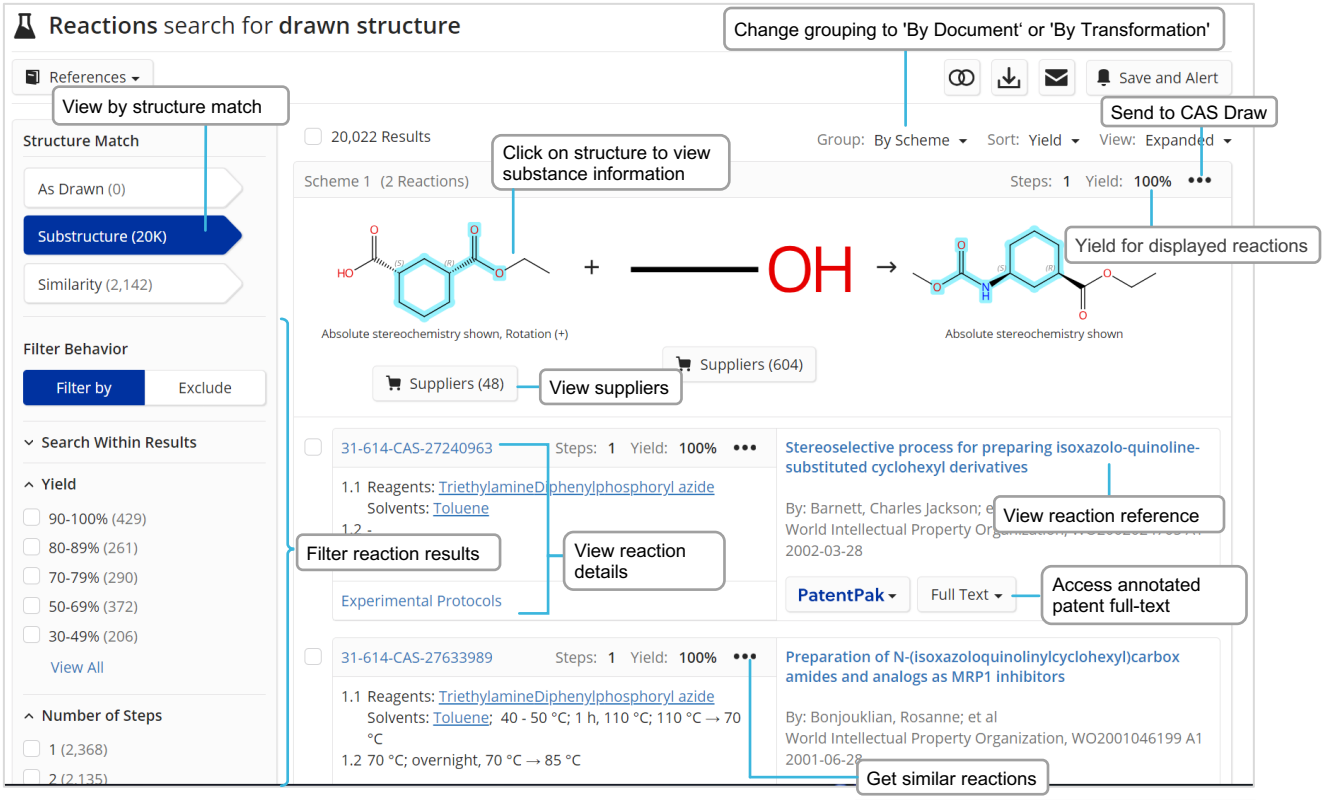
Performing a Reactions search

Reactions queries can be performed using CAS Reaction Numbers, substance names, CAS Registry Numbers, document identifiers, or a chemical structure.



Reactions search results

Reactions search results are grouped into schemes with identical reactants and products or into transformations. A robust panel of filters, including yield and steps, enables further refinement.

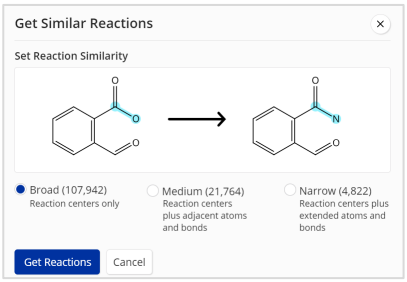


For single-step, single-stem reactions, you may view similar reactions based the similarity to of adjacent atoms to the specific reaction center.

•**Broad:** Retrieve reactions that share a reaction center with the selected reaction.

•**Medium:** Retrieve reactions that share a reaction center as well as adjacent atoms.

•**Narrow:** Retrieve reactions with a shared reaction center and extended atoms and bonds.



Reaction details

Reviewing Reaction details

The details of a reaction provide you with access to information including solvents, catalysts, reagents, conditions, and experimental protocols extracted from the publication and its supplement.

Get Similar Reactions — Search for similar reactions

Reaction Overview

Steps: 1 Yield: 85%

Reaction reference

JOURNAL

Development of a Scalable Synthesis of an Azaindolyl-Pyrimidine Inhibitor of Influenza Virus Replication

By: Liang, Jiangliu et al.

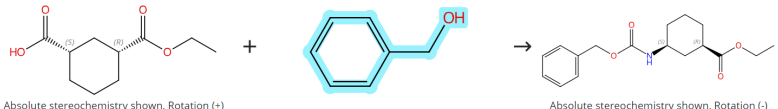
View All — View all authors

Organic Process Research & Development (2016), 20(5), 965-969

View Source | Full Text

Company/Organization

Vertex Pharmaceuticals Incorporated
Boston, Massachusetts 02210
United States



Suppliers (48) | Suppliers (149) | Suppliers (2)

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Triethylamine Diphenylphosphoryl azide	-	Toluene	2 h, reflux; reflux → 60 °C
2	-	-	-	overnight, 60 °C → 80 °C

View alternatives — Alternative Steps (5)

Experimental Protocols

Synthetic Methods — View detailed procedures

Products	Ethyl (1*R*,3*S*)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate, Yield: 85%
Reactants	1-Ethyl (1*R*,3*S*)-1,3-cyclohexanedicarboxylate Benzyl alcohol
Reagents	Triethylamine Diphenylphosphoryl azide
Solvents	Toluene
Procedure	1. Add diphenylphosphoryazide (DPPA) (166 mL, 769 mmol) and triethylamine (107 mL, 769 mmol) to (1S, 3R) -3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).

Characterization Data — View characterization data

Ethyl (1*R*,3*S*)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate

Proton NMR Spectrum	(300 MHz, $CDCl_3$) δ7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q,J= 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t,J= 11.8 Hz, 1H), 2.28 (d,J = 12.6 Hz, 1H), 2.10-1.79 (m, 3H), 1.50-1.19 (m, 6H), 1.19-1.00 (m, 1H).
Optical Rotatory Power	=-33.3° (c = 1 in DCM).
HRMS	(ESI) $[M + H]^+$ calculated for $C_{17}H_{24}NO_4$ 306.1700, found 306.1700
State	sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations — Overview of transformations
1. Schmidt Reaction

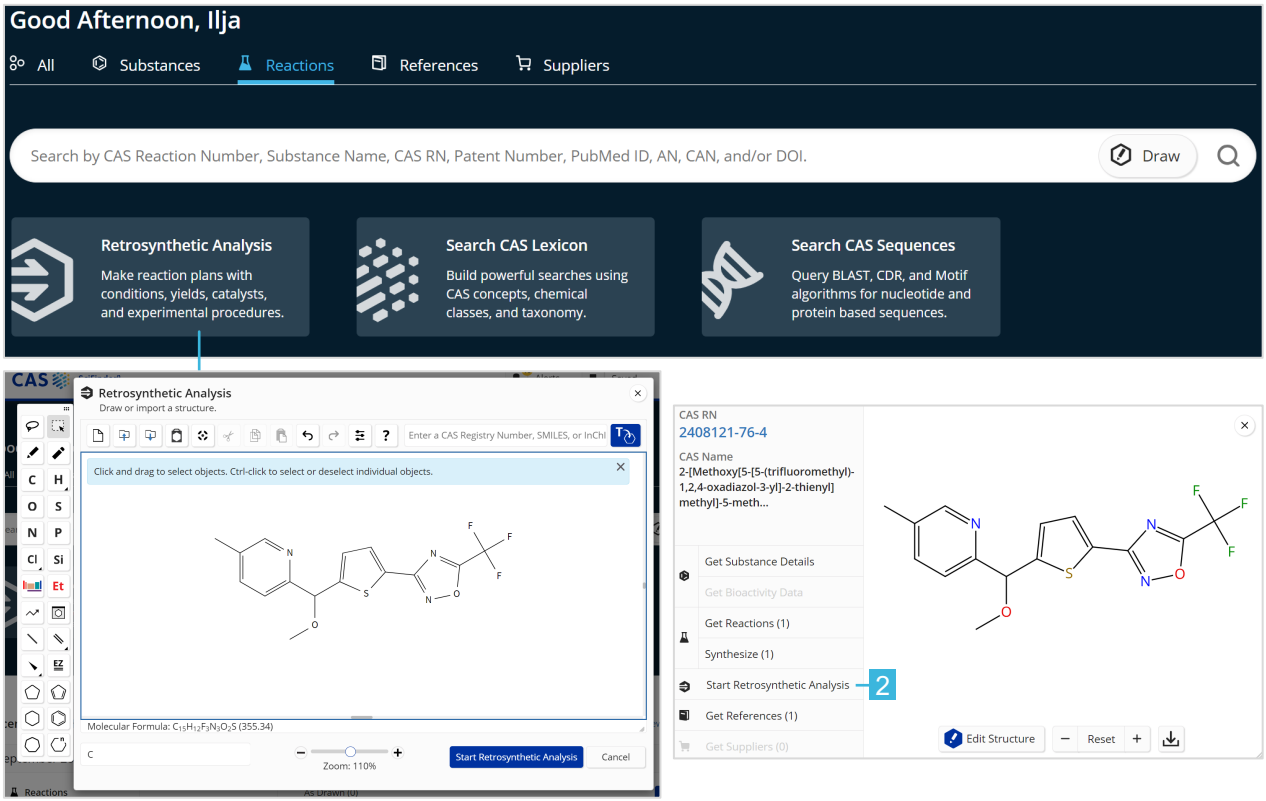
Reaction Notes — Further important notes
scalable

Retrosynthesis planner

Launching the tool

There are two primary ways to launch the retrosynthesis tool within CAS SciFinder^n:

1. Draw or import a structure into the Retrosynthesis window accessed by selecting the Retrosynthesis option on the main page. The substance can be novel.
2. Choose the Start Retrosynthetic Analysis option found on the substance flyout window.



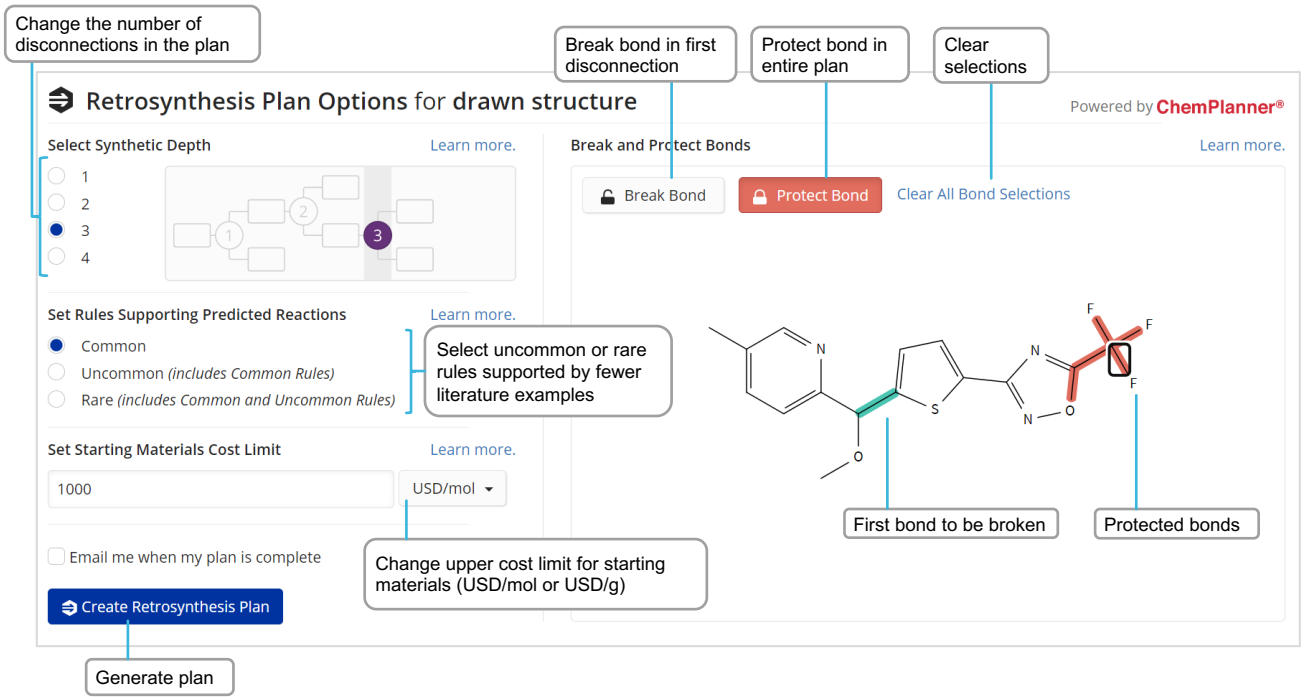
Retrosynthesis planner

Selecting plan options

You can edit plan options to:

- Increase the synthetic depth.
- Protect bonds through the entire synthetic route.
- Define bonds to be broken in the first disconnection.
- Change the starting material cost limit.
- Create a predictive plan with more meaningful alternatives, (such as poly- or heterocyclic molecules).

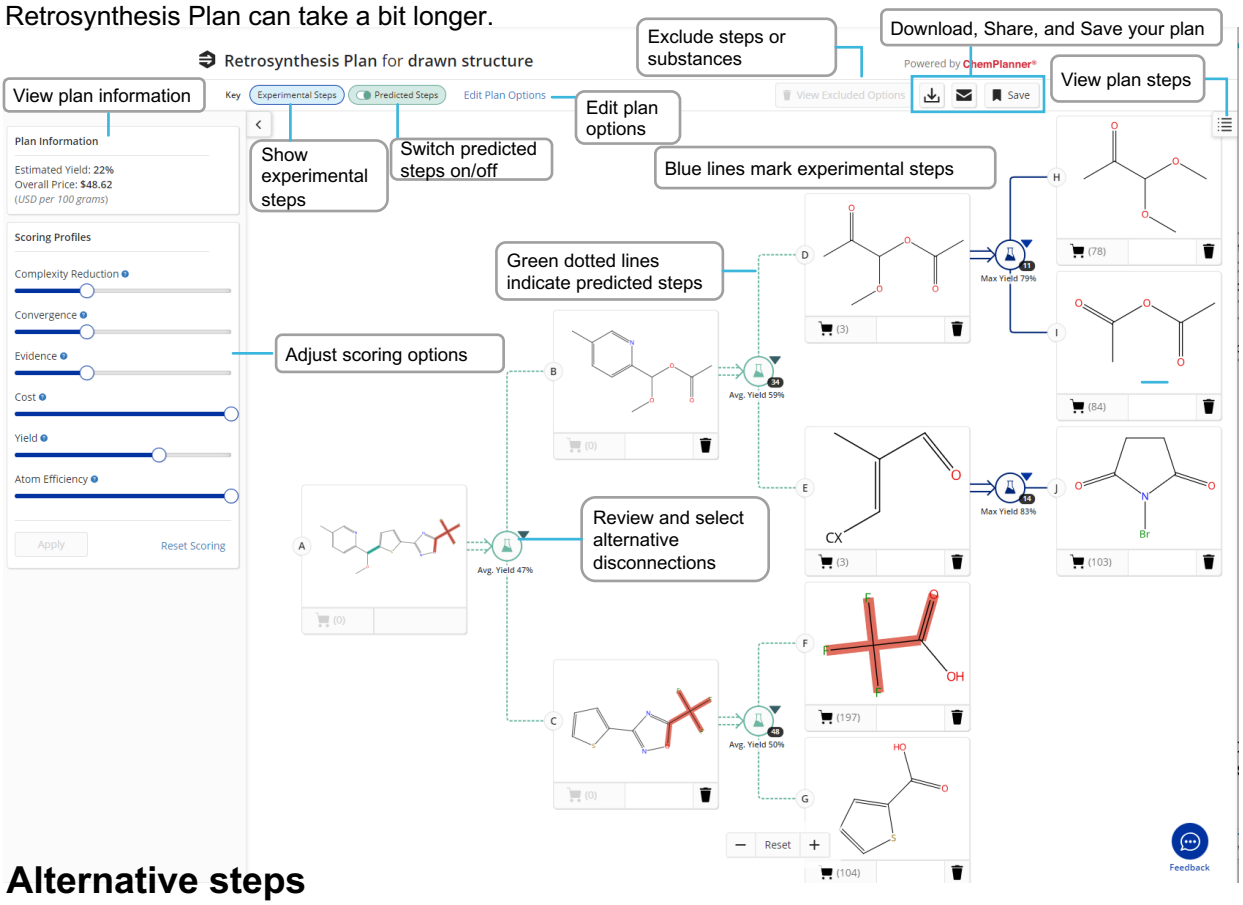
Once you have completed your option selections, choose the Create Retrosynthesis Plan button.



Retrosynthesis plan and alternative steps

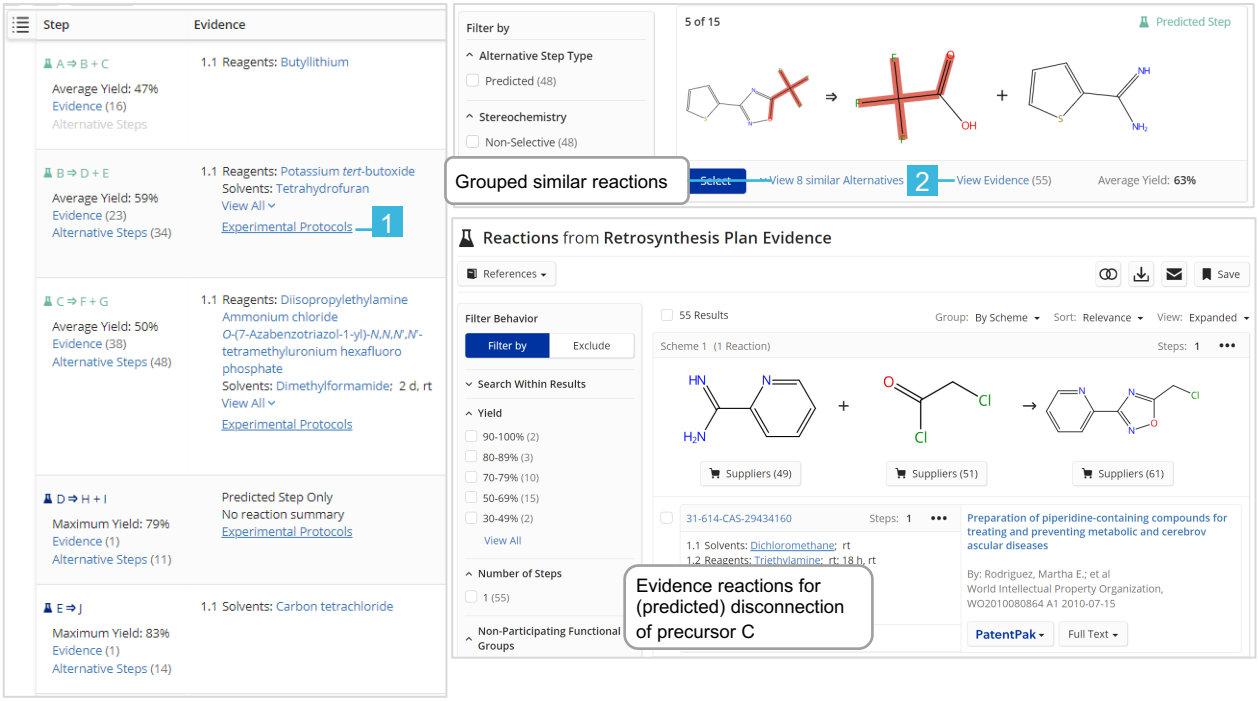
Open the plan

An Experimental plan is typically available within a few seconds. The calculation of a Predictive Retrosynthesis Plan can take a bit longer.



Alternative steps

Get an overview of all experimental and predicted disconnections along with the evidence reactions displayed as a reaction answer set. You can access these evidence reactions from either the (1) link in the steps overview or (2) alternative reaction scheme.



Retrosynthesis scoring options

Scoring options

For plans with predicted steps, you may increase or decrease the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

- Each scoring profile may be set to Off (extreme left), Low, Medium, or High (extreme right).
- The default setting for each profile is "Medium" as shown below.
- Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor in step selection or alternative ranking.

Scoring profiles

For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

Each scoring profile may be set to **Off** (extreme left), **Low, Medium**, or **High** (extreme right); the default setting for each profile is "Medium," as shown below. Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor step selection or alternative ranking.

Complexity Reduction

Reduces the complexity of a step's reactants compared to its product.

In retrosynthesis plans, you typically want high complexity reduction.

Convergence

Determines how "branched" the plan is; **you typically want the plan to be as branched as possible (high convergence)**, rather than linear.

For a given step, the more precursors there are, and the closer their relative sizes are, the more it's considered convergent.

Increasing Convergence displays steps/alternatives with more reactants.

Evidence

Ranks plan steps/alternatives based on the number of evidence examples supporting the particular reaction type.

More evidence examples for a step **means that the reaction type has more applications and is more versatile in terms of conditions and substrates**, and hence predictions made based on it are probably more reliable.

Increasing Evidence displays steps/alternatives with more supporting examples.

Cost

Weighs the expenses of the reactions by ranking starting materials based on the lowest price found amongst catalogs.

Yield

Applies to the yield of each step in the plan, which contributes to the yield of the target molecule.

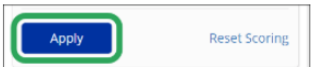
Increasing the Yield displays a higher yield target molecule and steps/alternatives.

Atom Efficiency

Reduces reactant parts not included in a plan step's product.

Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.

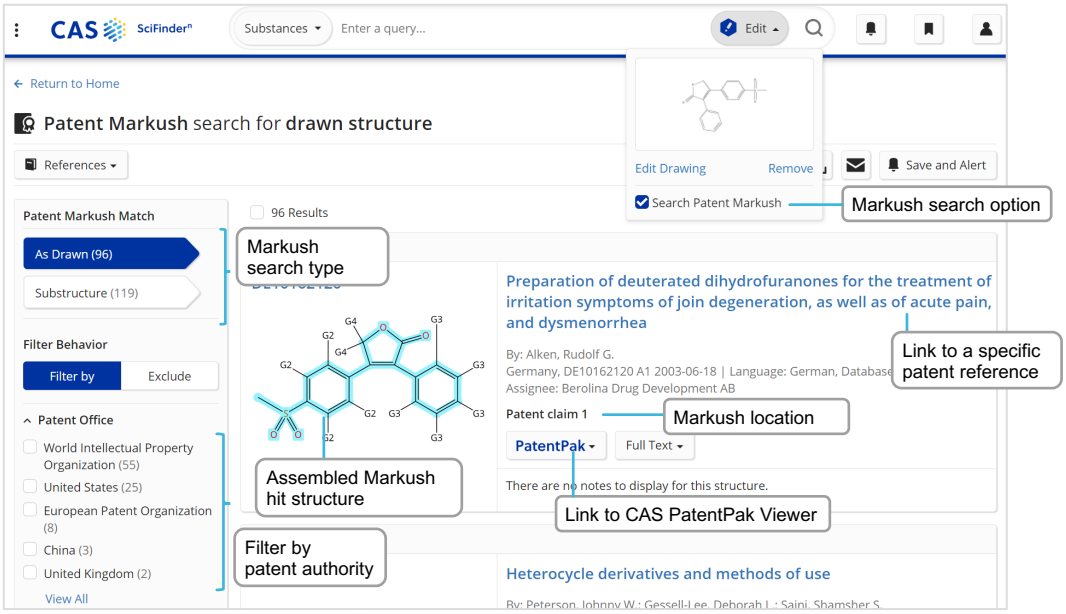
Clicking the **Apply** button redraws the retrosynthesis plan with the revised scoring profiles; clicking **Reset Scoring** restores the "Medium" default.



Markush search and CAS PatentPak

Markush search

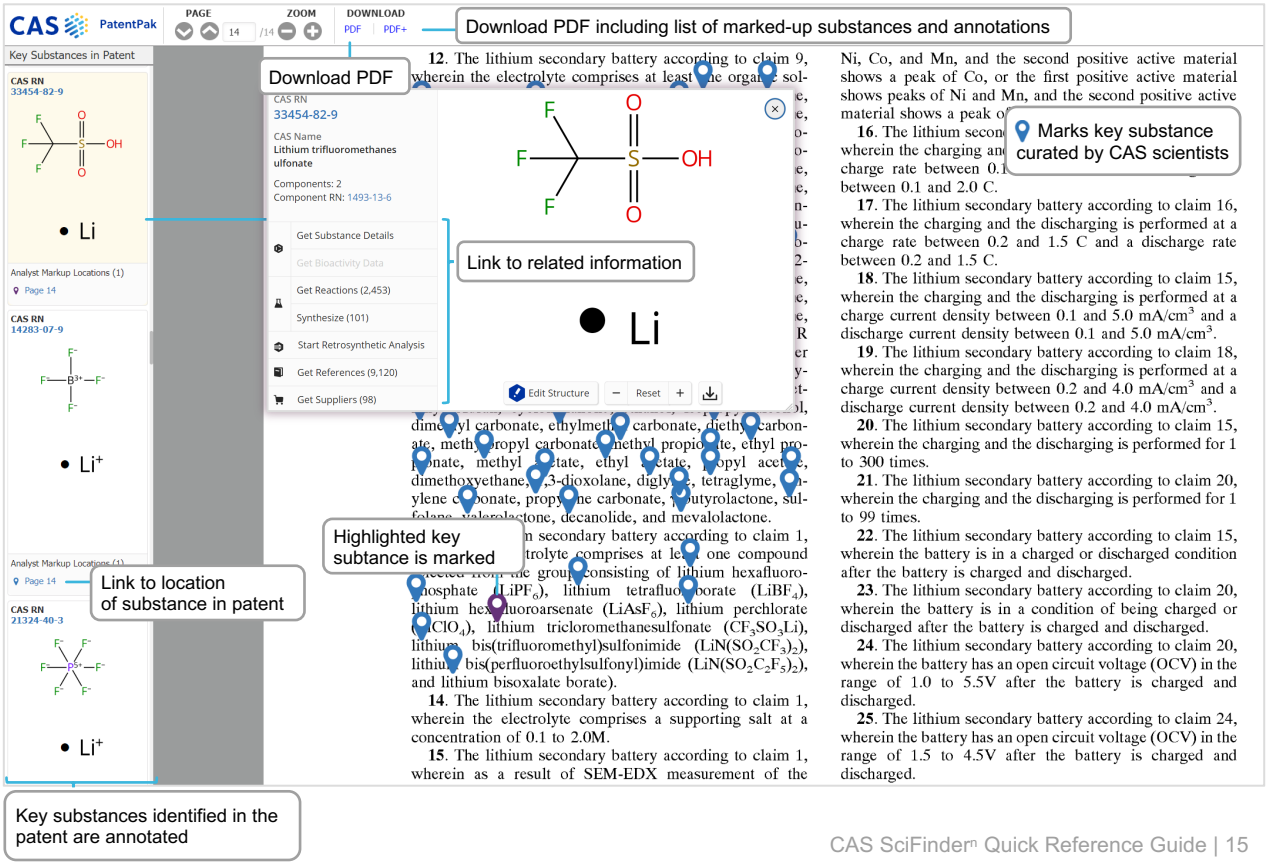
Markush structure searches can be performed using the Search Patent Markush option while in Substances search mode.



CAS PatentPak

There are three CAS PatentPak options for viewing a patent PDF:

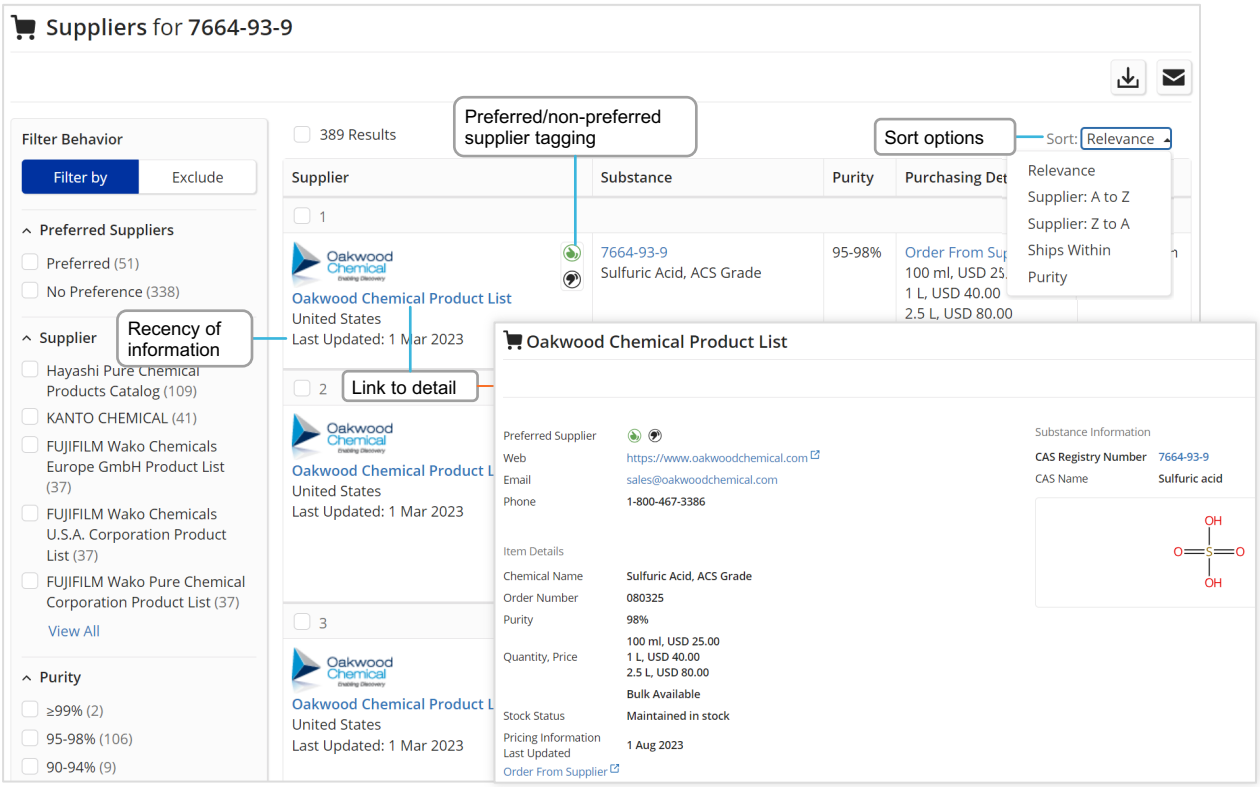
- **PDF**: Full-text patent PDF only; text-searchable PDF
- **PDF+**: Full-text patent PDF with marked-up Key Substances; text-searchable PDF
- **Viewer**: Patent PDF with linked markups of Key Substances (see below)



Supplier search and ChemDoodle®

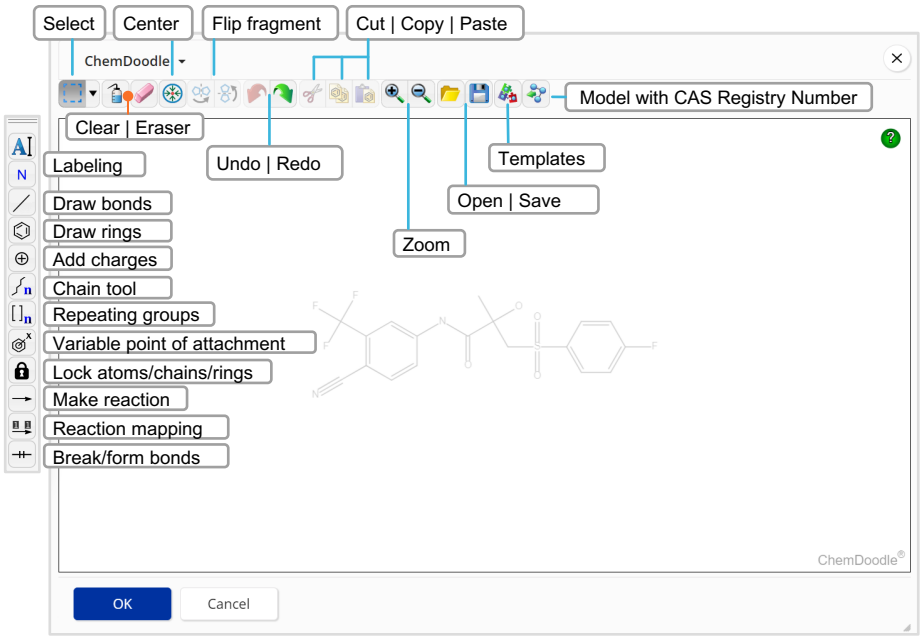
Suppliers search

Using Suppliers search allows you to directly access chemical catalog information based on chemical structure, names, or other identifiers.



ChemDoodle

The ChemDoodle structure editor is available in addition to the standard CAS Draw editor. ChemDoodle is useful for tablets and mobile devices.

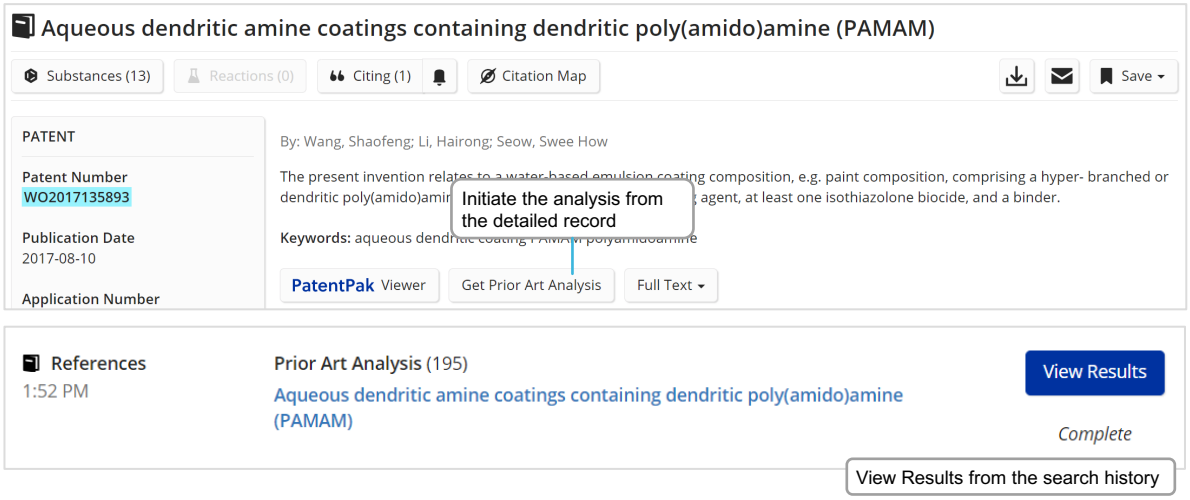


Prior Art Analysis

Reviewing Prior Art

When viewing a patent Reference Detail page, an option to "Get Prior Art Analysis" is available. Results will also appear in the search history. This functionality:

- Provides an AI-based relevance prediction.
- Is based on a single patent document as the starting point.
- Includes analysis of CAS concepts, indexed substances, IPC codes, and additional full-text.
- Generates a list of relevance-ranked previously known documents, comprising patent and non-patent literature.



Login, training, and support

Login details

Log in at scifinder-n.cas.org

Use your existing CAS SciFinder^n username and password.

Feedback button

Provide direct feedback to CAS from within the CAS SciFinder^n solution.

Training

Upcoming events and webinars:
www.cas.org/cas-webinars

Recorded events and webinars:
www.cas.org/cas-past-webinars

CAS SciFinder^n training topics: www.cas.org/support/training/scifinder-n

Support contact

Email help@cas.org to reach a CAS Customer Center representative in North America.

If you are outside of North America, see this website for regional contacts: https://www.cas.org/contact

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SCIGENENGREF101245231017– A4