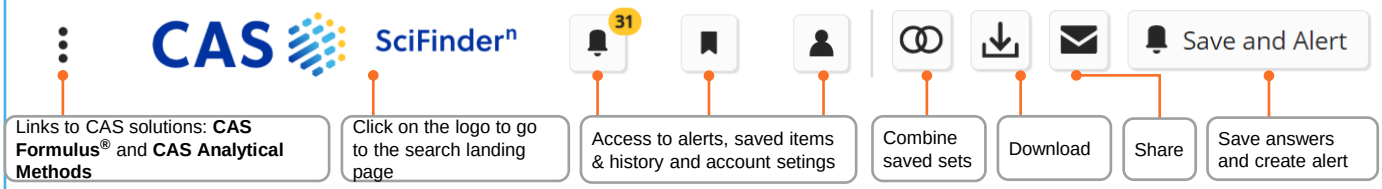
CAS SciFinder^{n} Quick Reference Guide

May 2nd, 2023

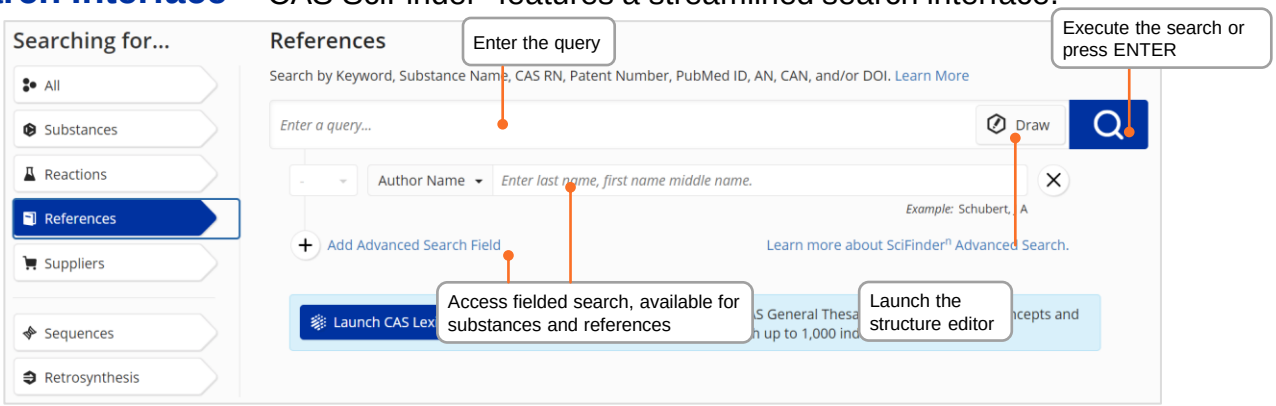
CAS
A division of the American Chemical Society

Interface and Reference Search



Search Interface

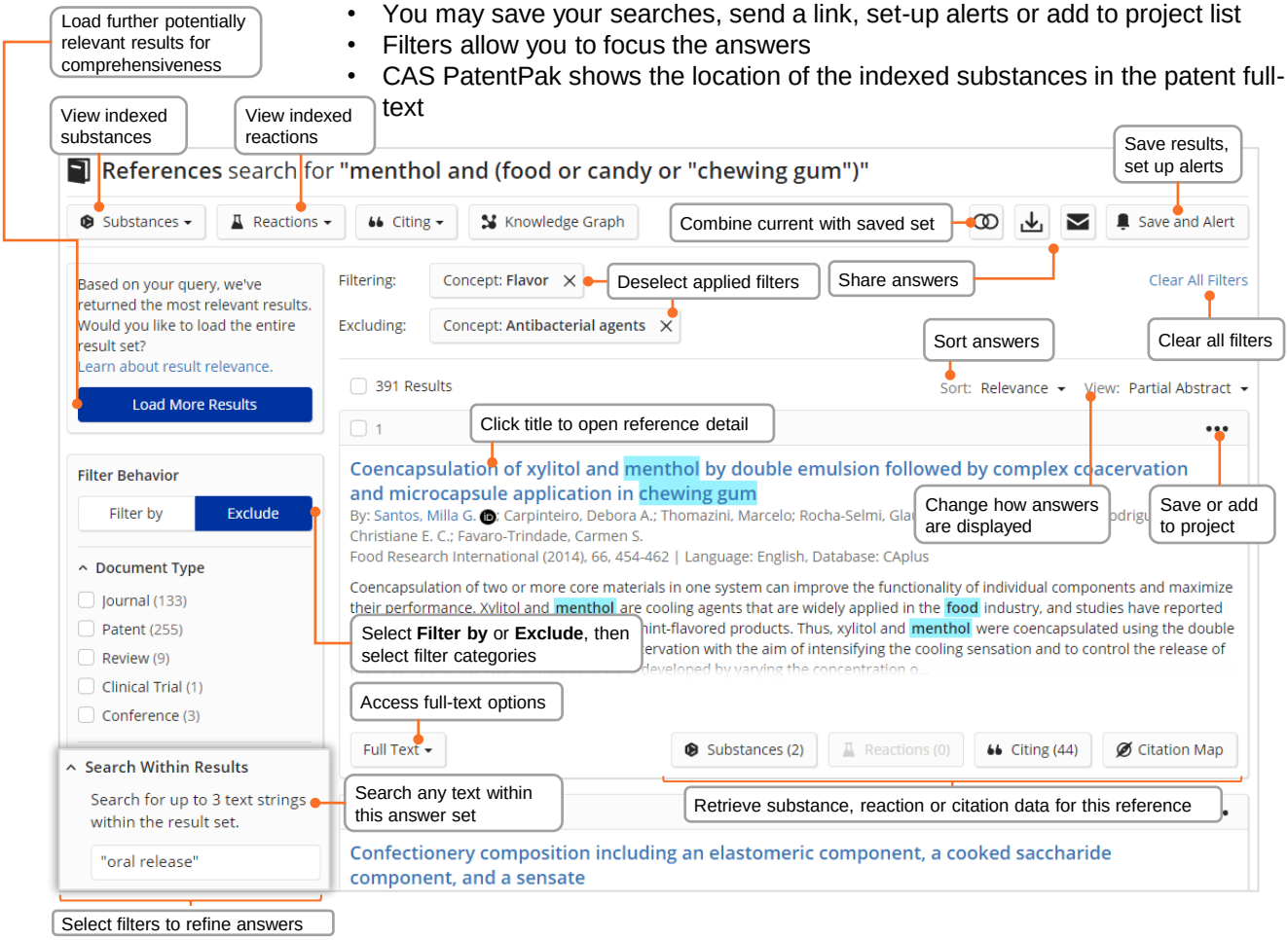
CAS SciFinder^n features a streamlined search interface.



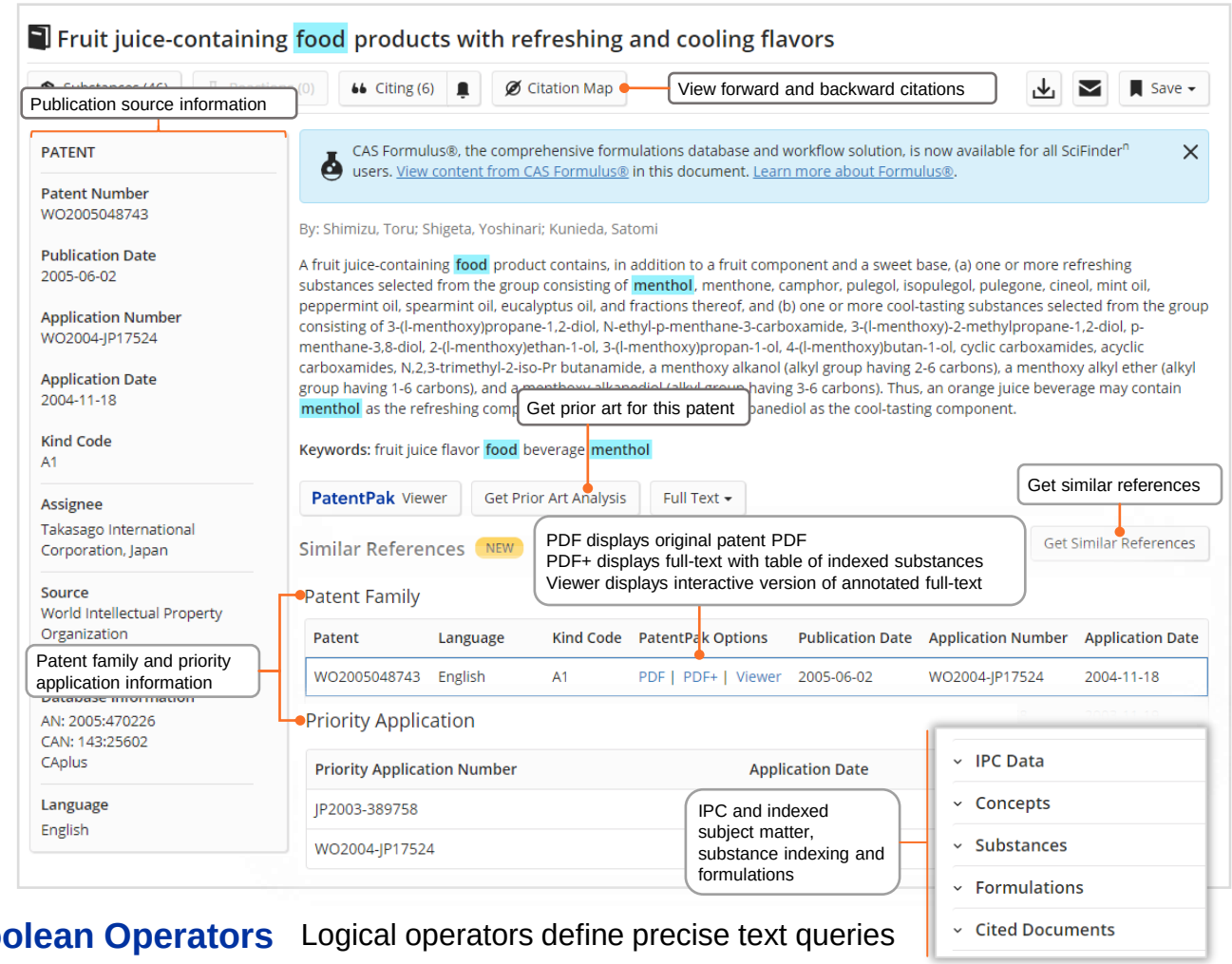
Reference Search

The References display features visualizations, dynamic facets and an easy-to-use interface layout

- References are ranked and sorted by relevance
- You may save your searches, send a link, set-up alerts or add to project list
- Filters allow you to focus the answers
- CAS PatentPak shows the location of the indexed substances in the patent full-text



Reference detail and search operators



Boolean Operators

Logical operators define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.:

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

Wildcards allow for more comprehensive retrieval
Use is allowed in reference, substance and filter searches
Internal and right-hand truncation is available

***** Replaces 0 to any number of characters E.g.: polymorph* | immunoglobulin*conjugate*

? Replaces 0 or 1 character E.g.: benzonorbornen?

Terms masked with double quotes will be searched as a precise phrase.
E.g.: "Programmed cell death protein" only finds Programmed cell death protein

Substance name and structure

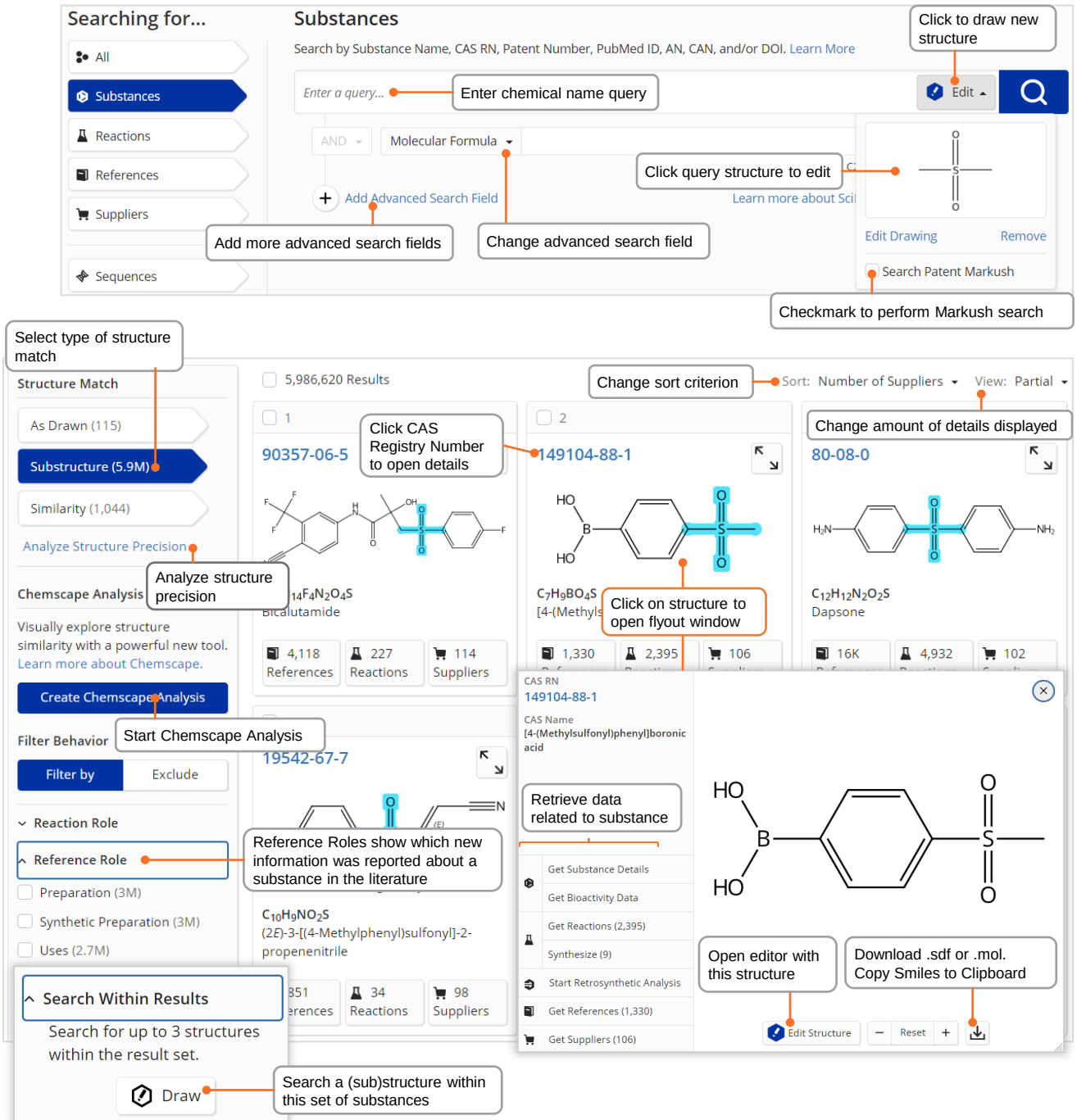
Name searches

Search with one or more substance names or identifiers

Streptomycin	Finds Streptomycin record
57-92-1	Finds Streptomycin record, uses CAS Registry Number® as identifier
Streptomycin sulfate	Finds 3 records: Streptomycin, Streptomycin sulfate and Sulfate
"Streptomycin sulfate" Streptomycin	Finds 2 records: Streptomycin sulfate and Streptomycin
Sulfoximin*	Finds all names that start with the stem Sulfoximin
WO2019234160	Finds all indexed substances for this patent

Structure searches

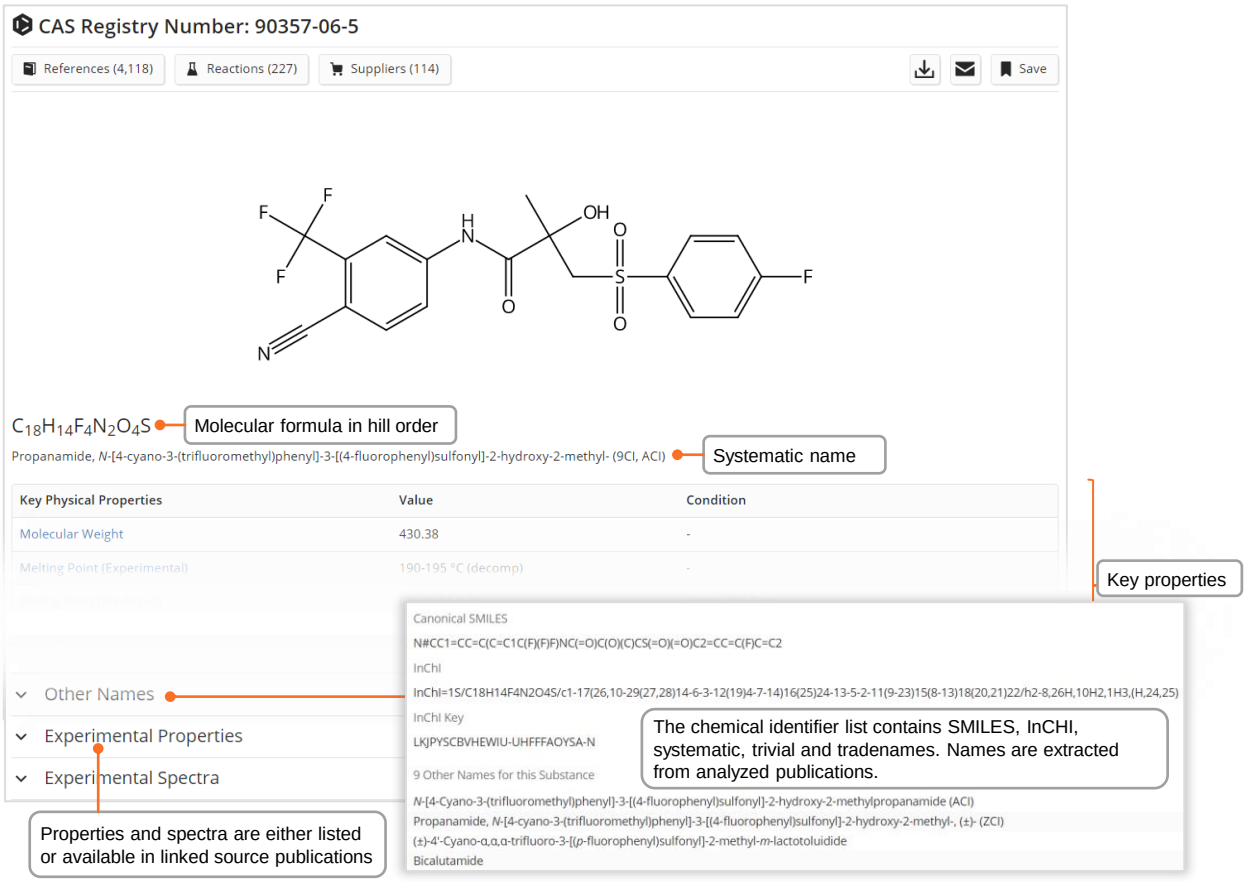
Substance searches return results in an intuitive interface. The display highlights most relevant hits, critical property information and high-resolution images



Substance detail and structure editor

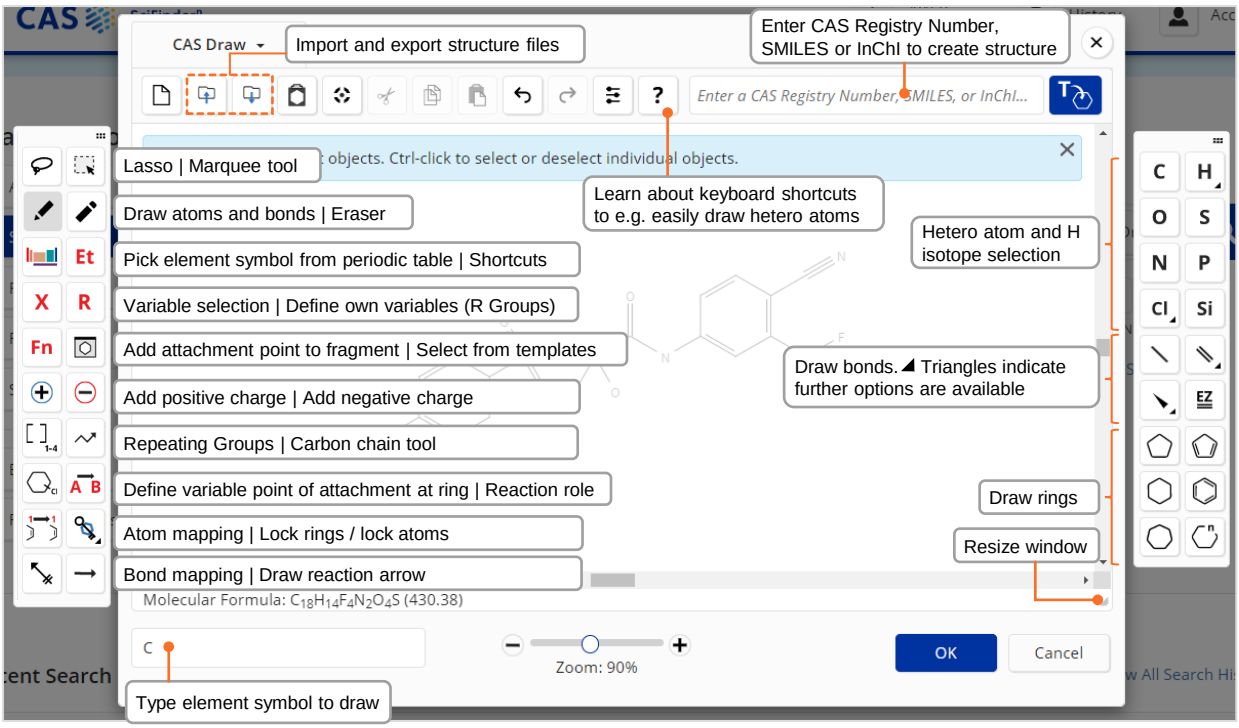
Substance detail

Click on the CAS Registry Number to show substance details with structure, molecular formula, properties and further data



CAS Draw editor

Define structure and reaction queries with the structure editor

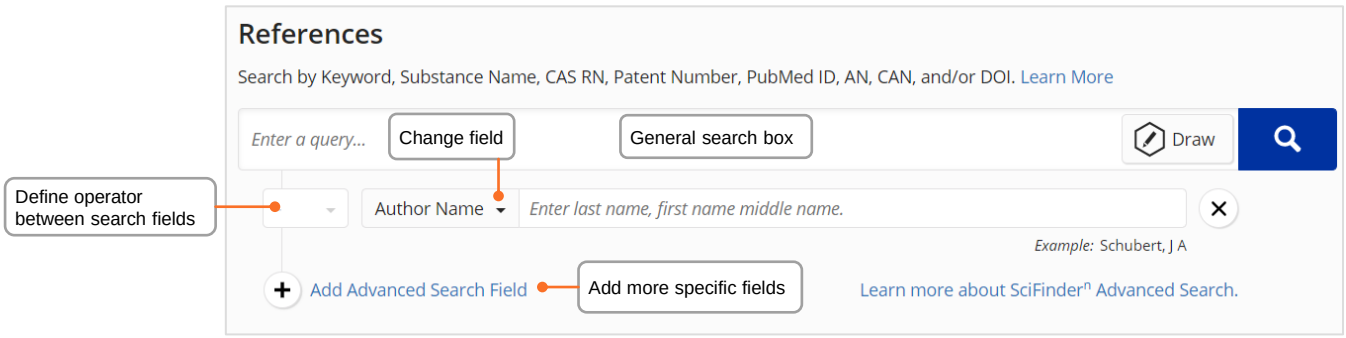


Advanced search query builder

Advanced Search Query Builder

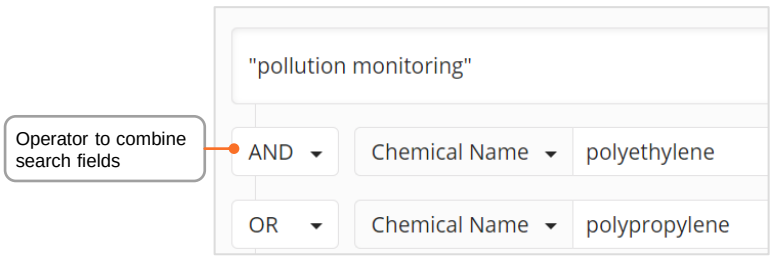
Provides specific reference and substance search fields from CAS SciFinderⁿ's landing page

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



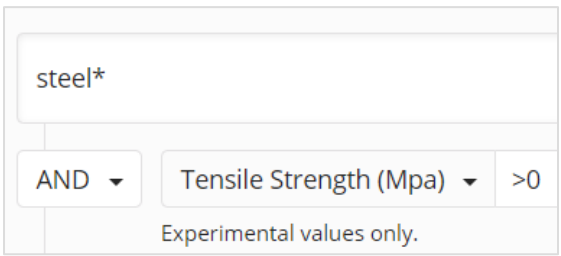
Examples

Advanced Reference Search



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

Advanced Substance Search



Query interpretation:
Steel with tensile strength property information

Advanced Search Fields

The below advanced search fields and categories are available

Reference

- Author Name
- Publication Name
- Organization Name
- Title
- Abstract/Keywords
- Concept
- Substances
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Substance

- Molecular Formula
- CAS Registry Number / Component Registry Number
- Chemical Name
- Document Identifier
- Patent Identifier

- Experimental Spectra
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

CAS Roles

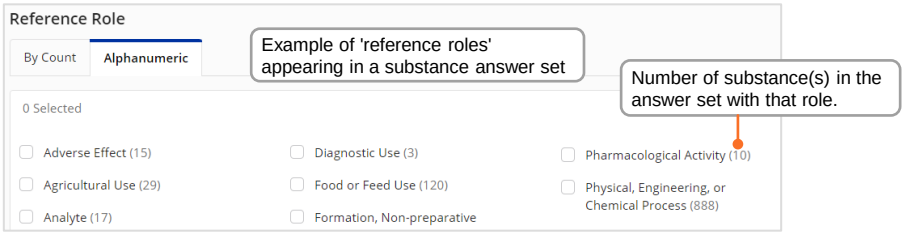
CAS Roles

Roles are linked to the substances and allow you to find focused publications connecting the 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 a 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 type of roles that are connected to the substance(s) in the publications.

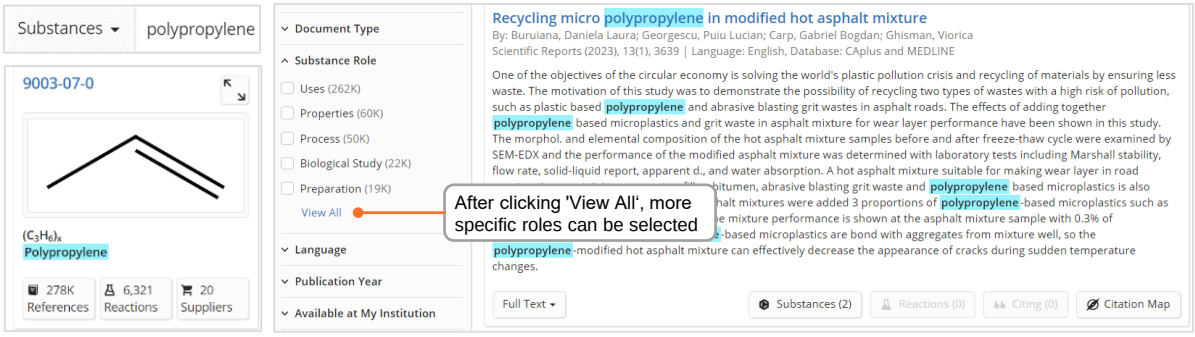


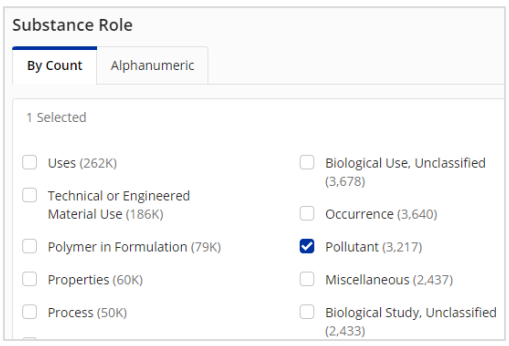
Roles in reference results

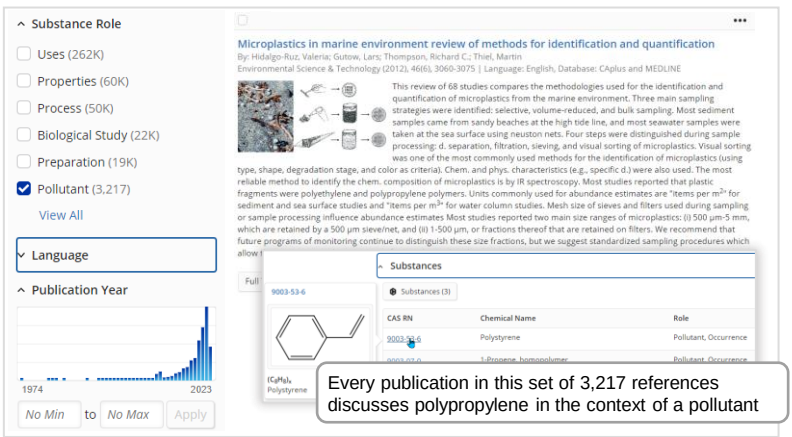
Roles will appear as a filter in reference result sets whenever you have retrieved hits in the substance indexing segment of the records, i.e. by retrieving substance names or performing a crossover after structure-based searches.

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 a large number of references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3217 publications that describe polypropylene as a pollutant. Search within or concepts can be used to restrict result to marine pollution.







Sequence searching

Search Options

Three different search modalities exist

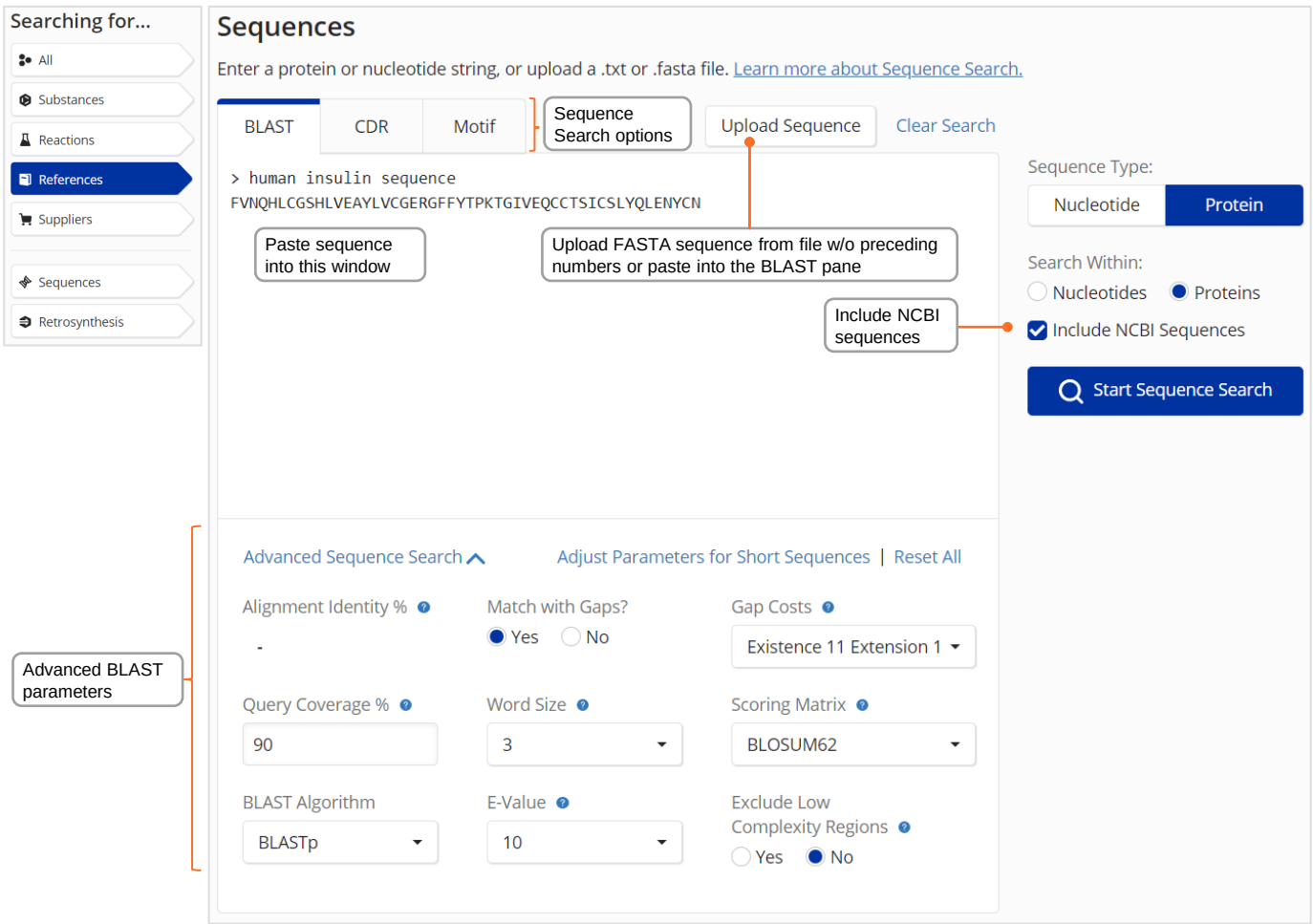
- BLAST: Search similar sequences
- CDR: Search antibodies and t-cell receptors via CDRs
- Motif: Search using variability symbols

BLAST similarity search

BLAST allows to search for similar nucleotide and amino acid sequences. Alignment results are shown in an intuitive graphical layout with easy-to-use precision filtering for identity and coverage percentages. Reference results are linked to the sequence hits.

Perform a BLAST search

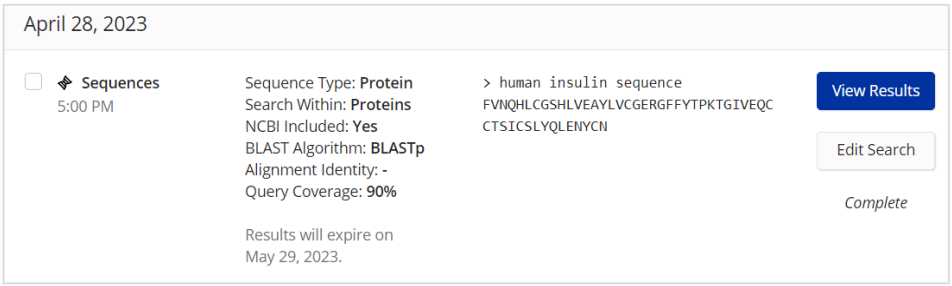
- Open the Sequences module from the main CAS SciFinder^{n} search page
- Load sequence from file or paste sequence
- Supported formats: Sequences containing residues represented by single-letter codes, e.g. in the FASTA format. Leading numbers are not allowed.
- Sequence input may contain header line (starting with **>**). Sequences can be separated by (multiple) headers, thus allowing for batch processing
- Adjust BLAST parameters as desired and start the biosequence search



BLAST result analysis

Access Results

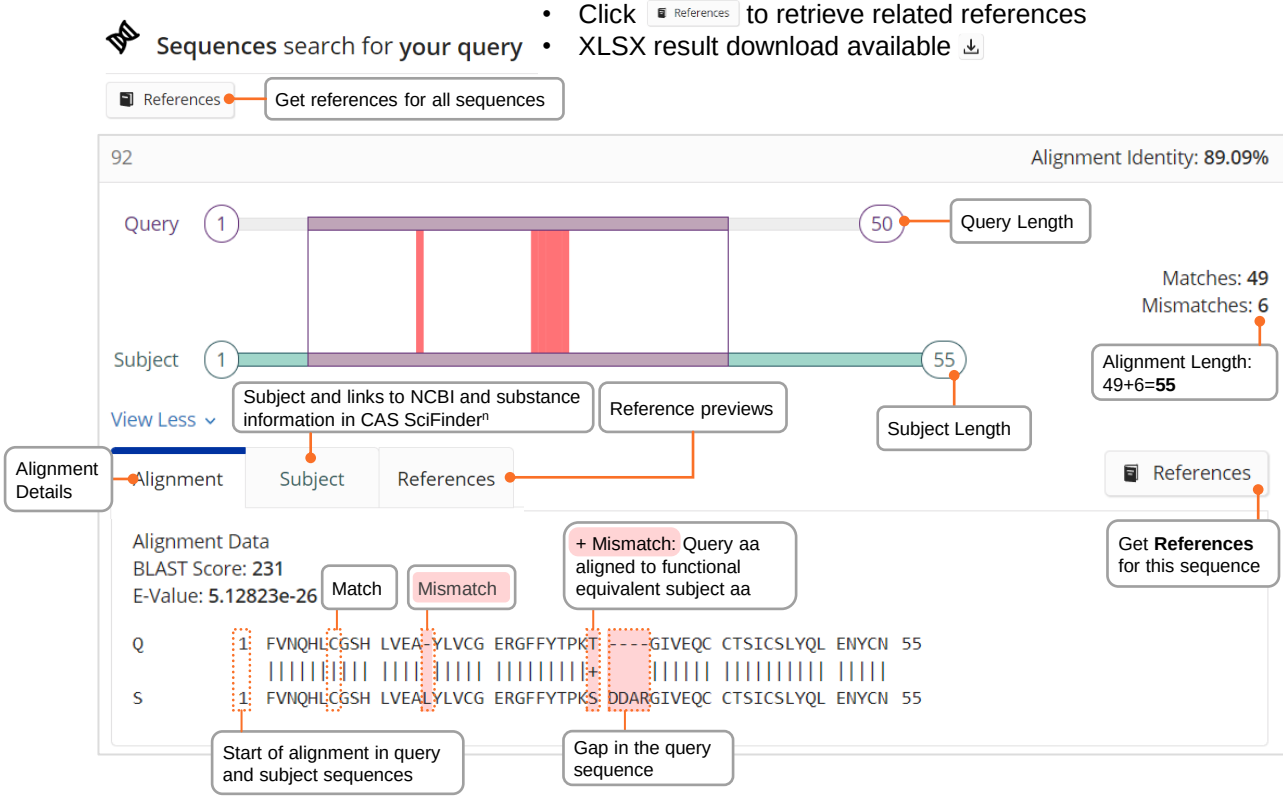
Sequence search results appear in the Recent Search History and general Search History (History). Click 'View Results' to view sequence answers.



View Results

View BLAST sequence similarity results.

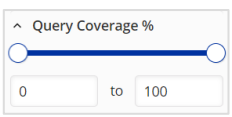
- Alignments are sorted by Sequence Identity
- Simplified graphical overview shows alignment quality
- Mismatches are indicated by red lines
- Detailed alignments can be viewed in 'Alignment' tab
- Subject details and patent previews are available in separate tabs
- Click References to retrieve related references
- XLSX result download available



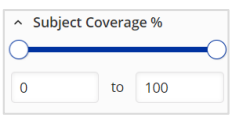
Filter Results

Filtering dynamically changes the result set

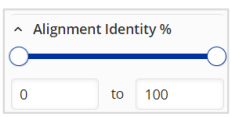
Expectation Value



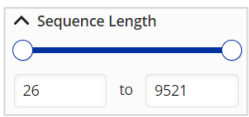
$$\frac{\text{Alignment Length}}{\text{Query Length}}$$

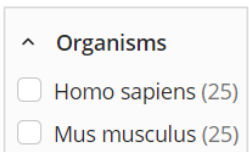


$$\frac{\text{Alignment Length}}{\text{Subject Length}}$$



$$\frac{\text{Number of Matches}}{\text{Alignment Length}}$$



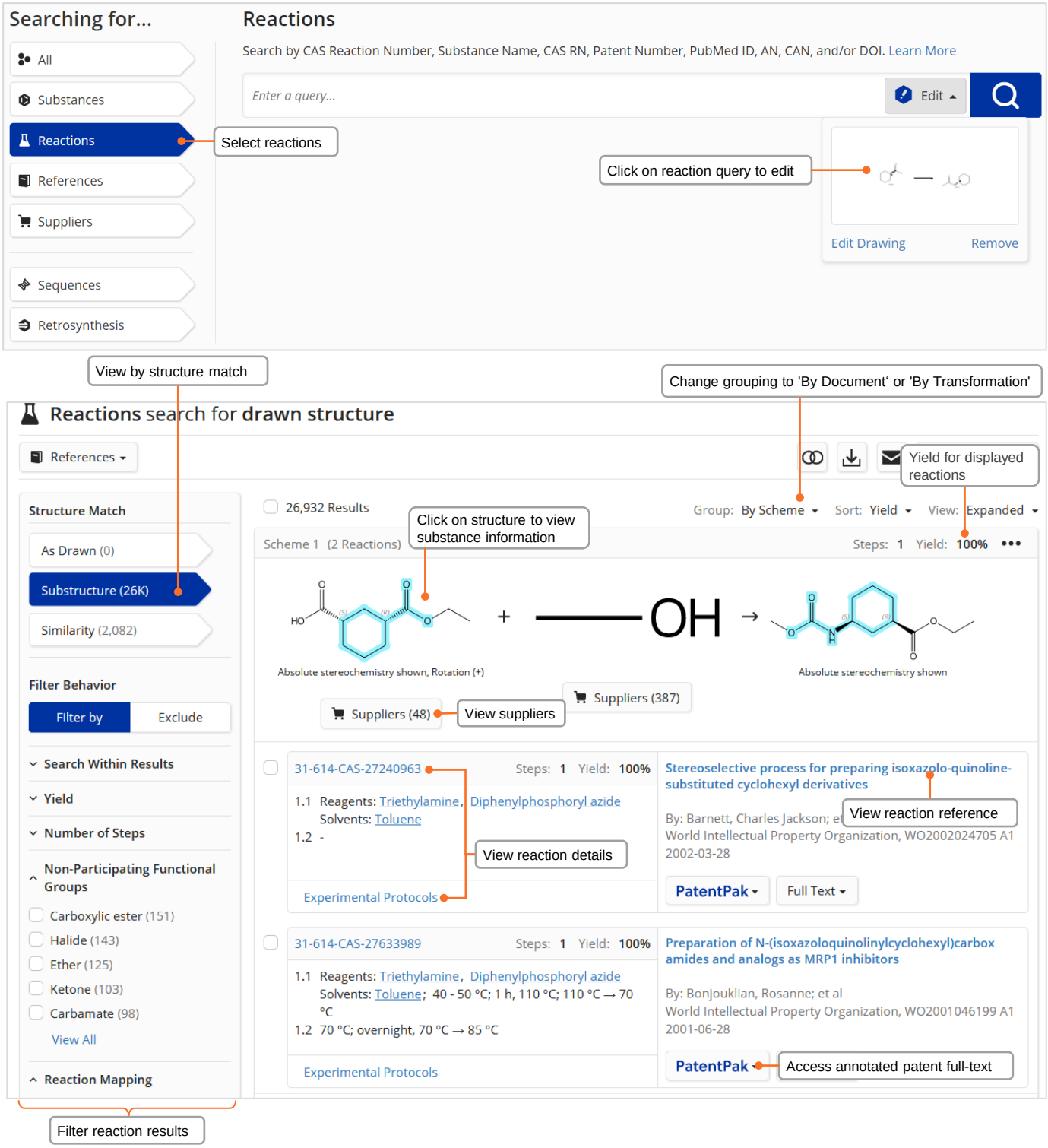


Reaction searching

Reaction searches

Reactions queries can be CAS Reaction Numbers, Substance Names, CAS Registry Numbers, document identifiers, or a chemical structure

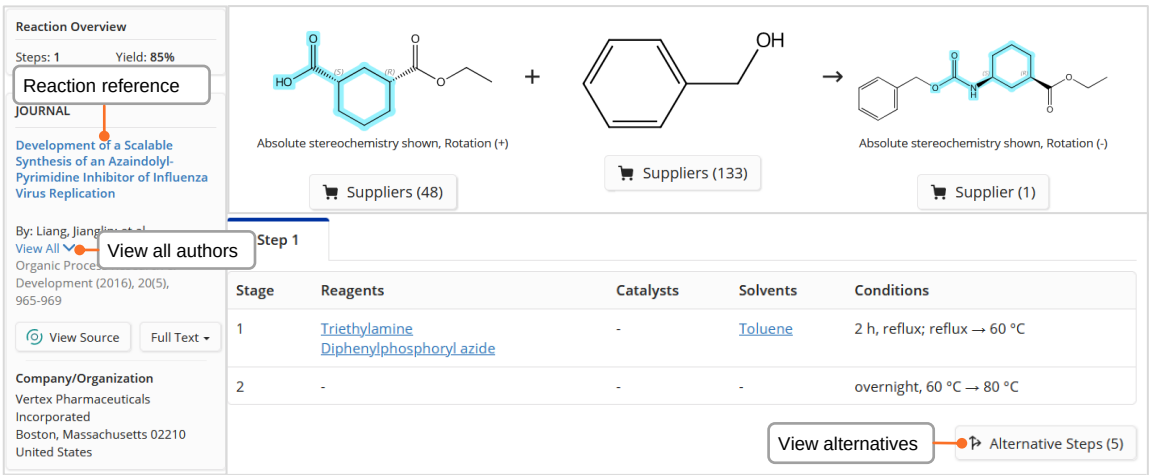
- Reactions are grouped
  - into schemes with identical reactants and products
  - into transformations
- Reactions are sorted by yield within a scheme

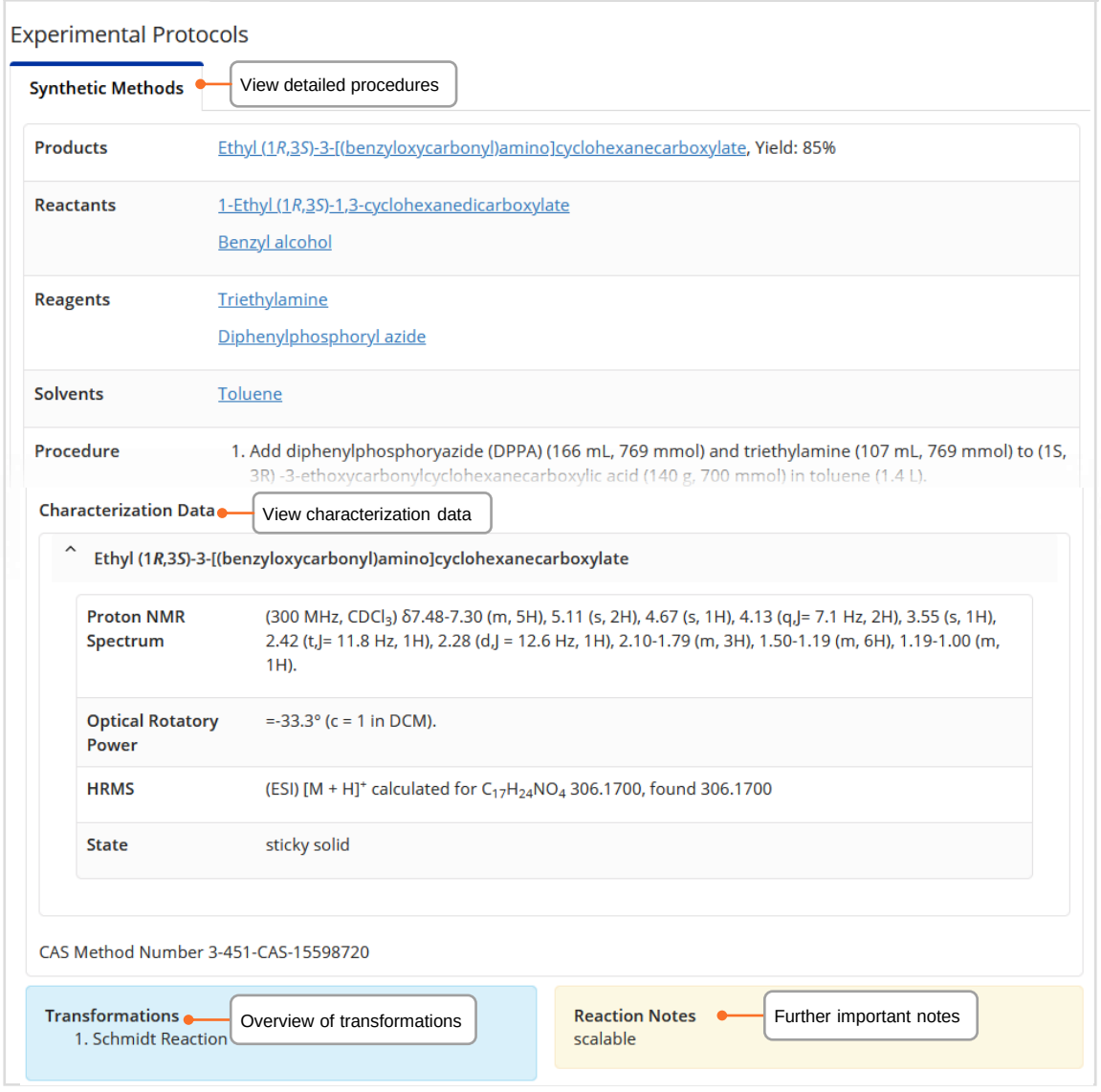


Reaction details

Reaction details

Details incl. solvents, catalysts, reagents, conditions and experimental protocols extracted from the publication and its supplement



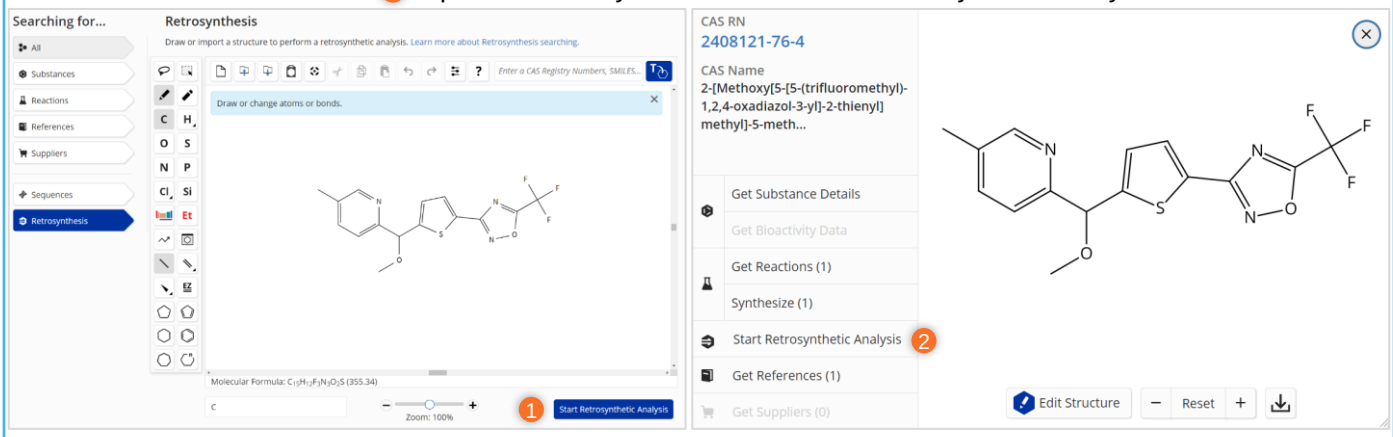


Retrosynthesis planner

Launch plan generation

There are two main options to launch CAS SciFinderⁿ's Retrosynthesis Planner

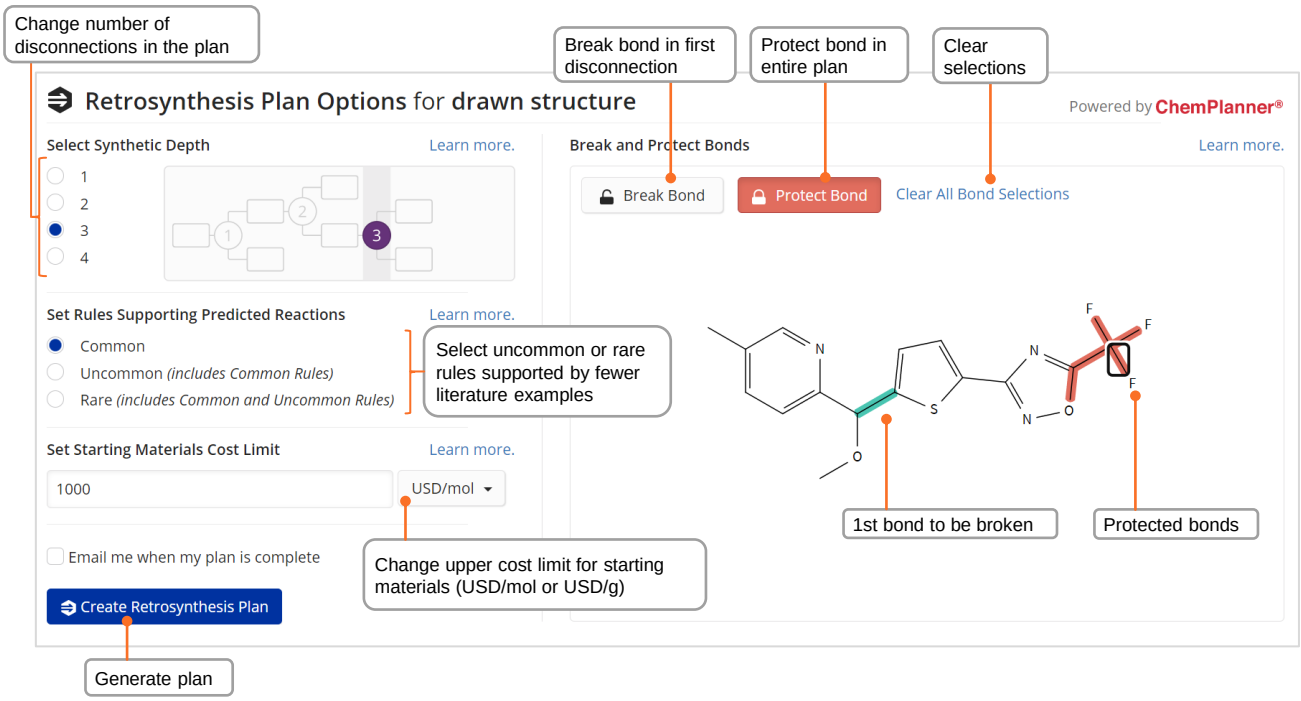
1. Draw structure in the Retrosynthesis editor from the landing page, substance can be novel
2. Open structure flyout window and start Retrosynthetic Analysis



Plan options

Edit plan options to...

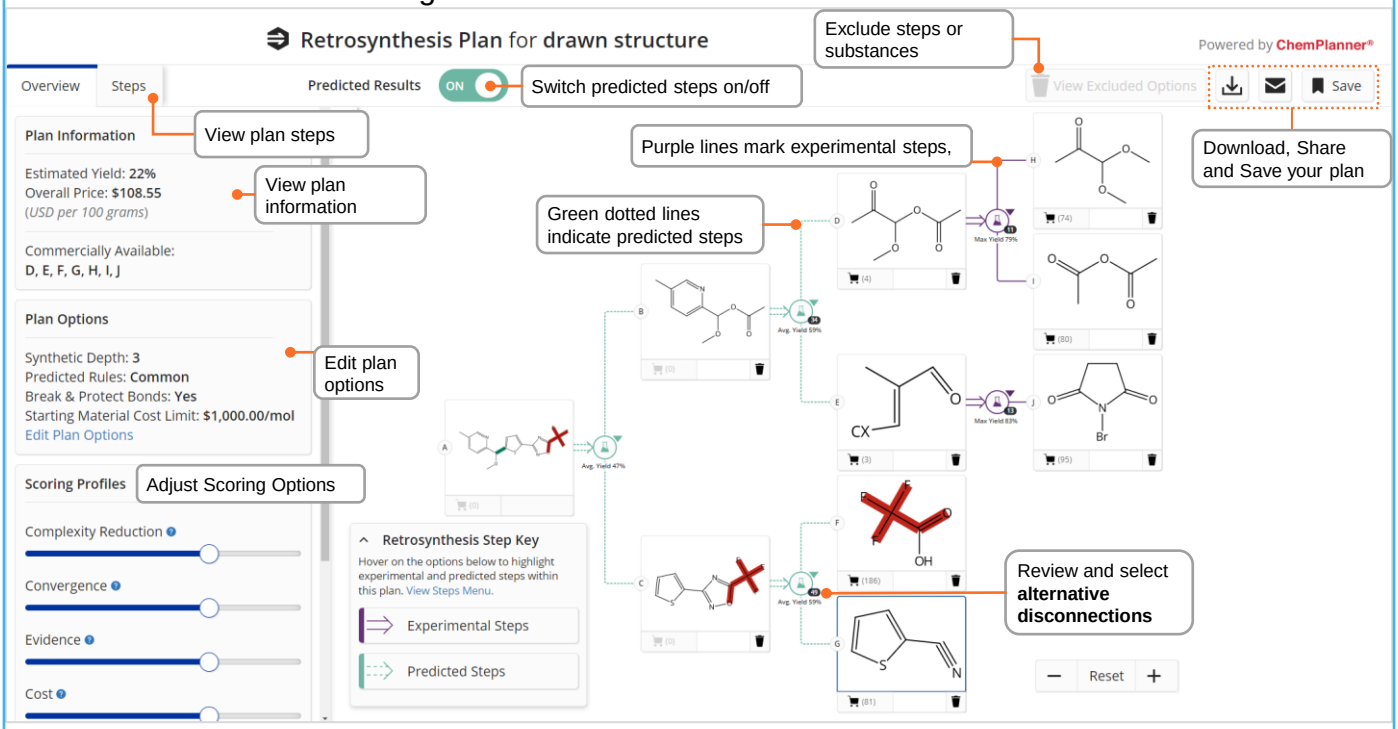
- increase the synthetic depth
- protect bonds through the entire synthetic route
- define bonds to be broken in the first disconnection
- change the starting material cost limit
- create a predictive plan with more meaningful alternatives, e.g. for poly- or heterocyclic molecules



Retrosynthesis plan and alternative steps

Open plan

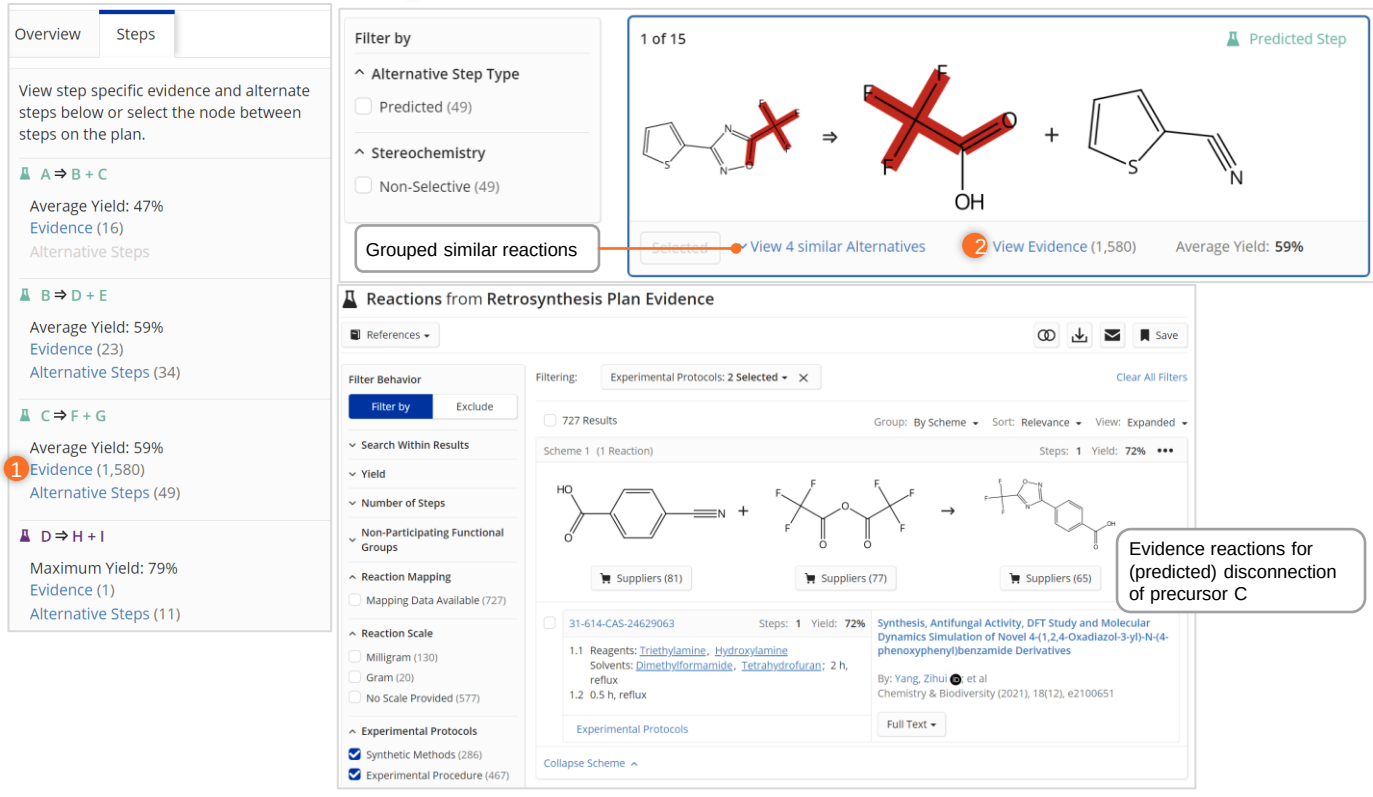
The Experimental Plan is available within a few seconds, the calculation of the Predictive Retrosynthesis Plan will take a bit longer



Alternative steps

Provide an overview of all experimental and predicted disconnections
Evidence reactions are displayed as a reaction answer set

- Access Evidence Reactions from the 1 link in the steps overview or 2 the alternative reaction scheme



Scoring Options

Scoring Options

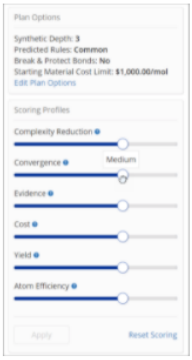
For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

- 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

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.

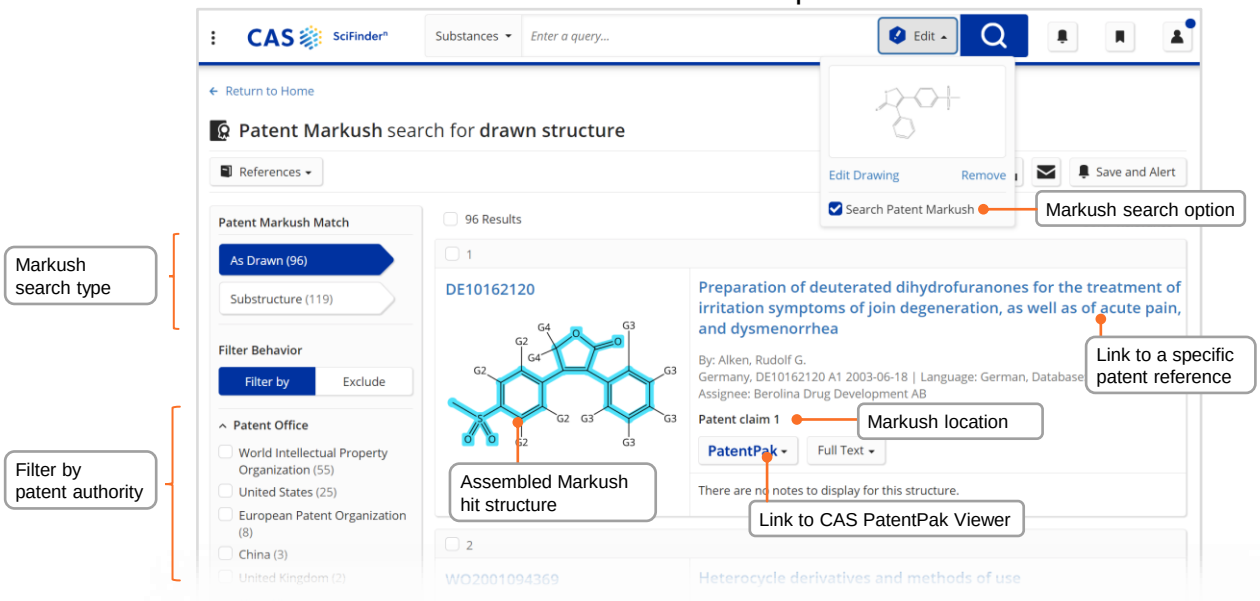
Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.

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

Markush Searching and CAS PatentPak®

Markush searching

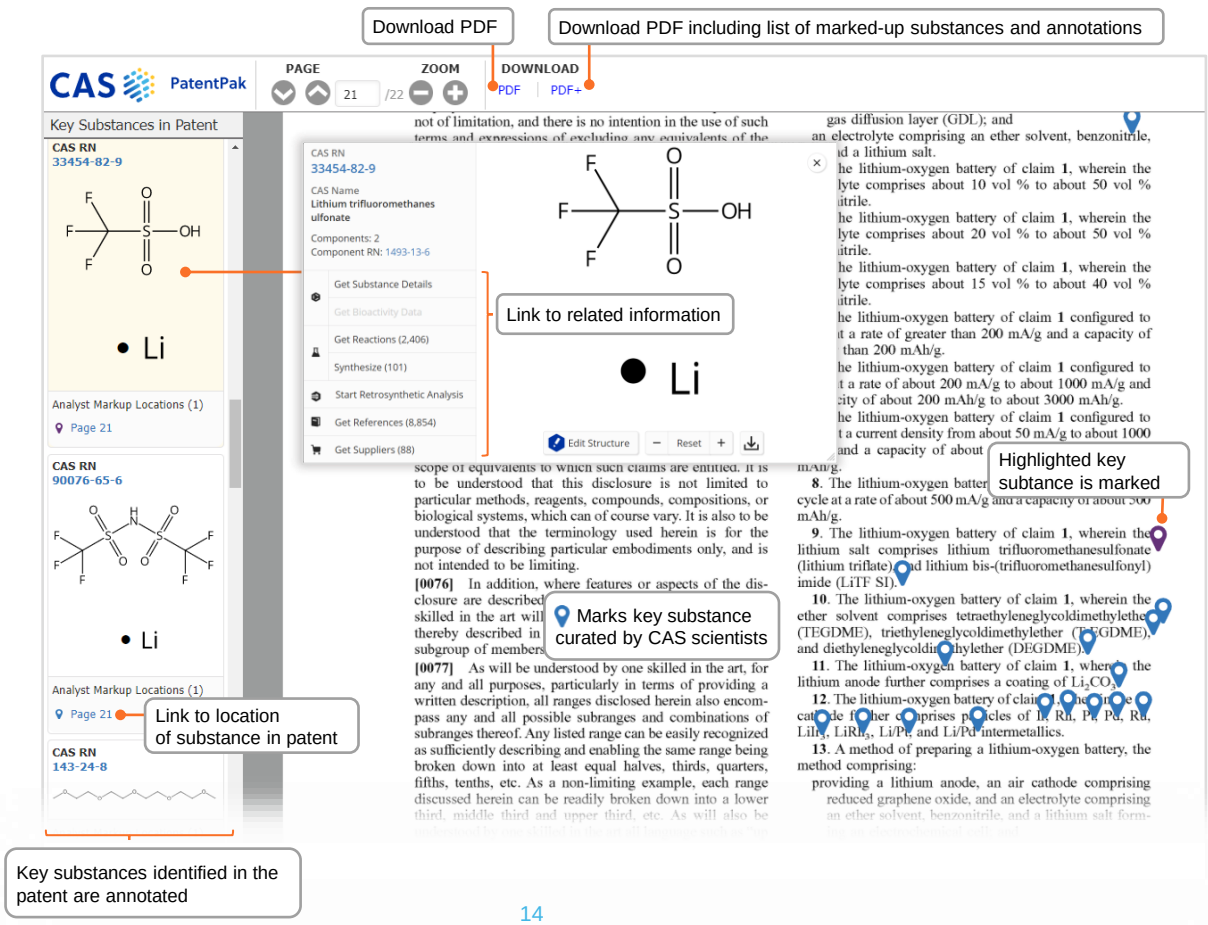
Markush structure searches can be performed by using the Search Patent Markush option while in Substances search mode



CAS PatentPak

Up to three CAS PatentPak Options for viewing a patent PDF:

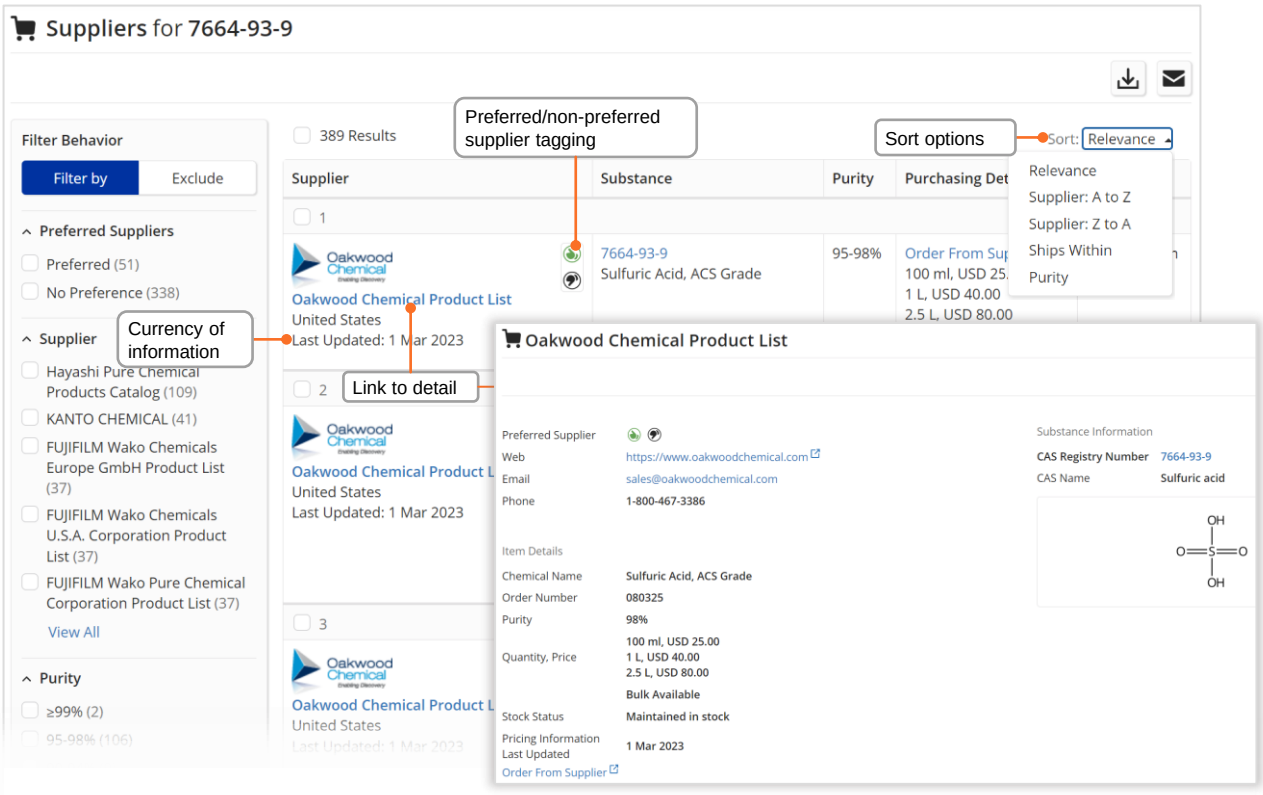
- **PDF**: Full-text patent PDF only; text-searchable PDF
- **PDF+**: Full-text patent PDF with marked-up Key Substances; text-searchable PDF
- **Viewer**: Patent PDF with linked markups of Key Substances; see below:



Supplier Searching and ChemDoodle®

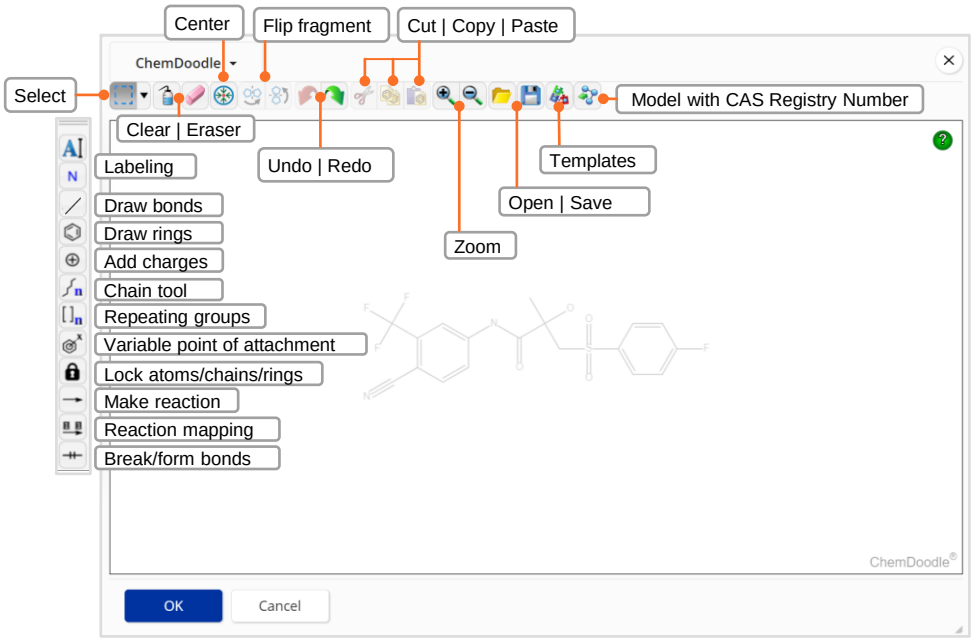
Suppliers searching

Suppliers searching allows for direct access to 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.

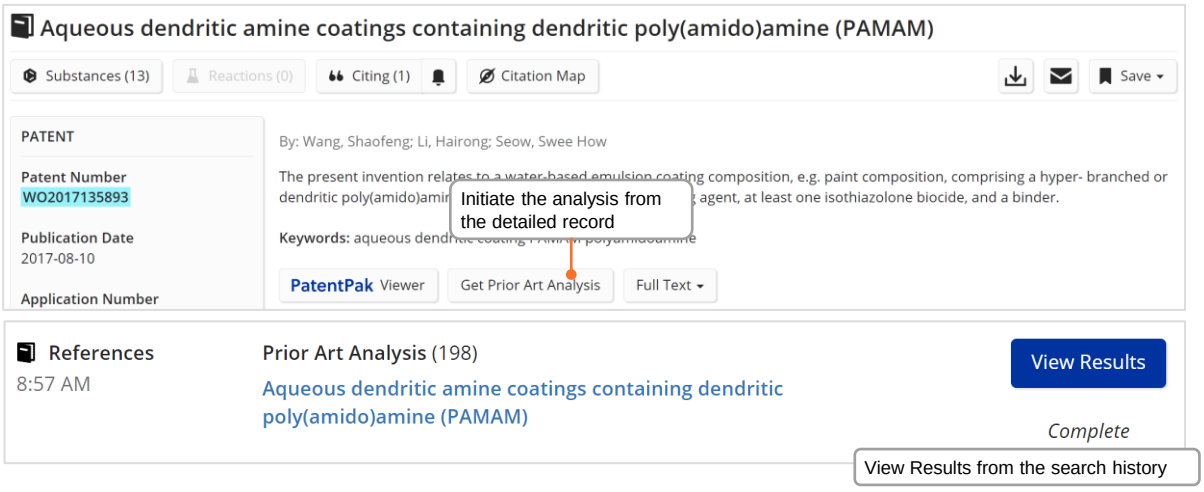


Prior Art Analysis

Prior Art Analysis

Upon viewing a patent Reference Detail page, an option to Get Prior Art Analysis is available. Results appear in the search history.

- AI-based relevance prediction
- Based on a single patent document as the starting point
- Analysis of CAS concepts, indexed substances, IPC codes and additional full-text
- Generates list of relevance-ranked previously known documents, comprising patents and non-patent literature



Login, Feedback and Support

Login Details

- Register for an account and login at your library's database website
- Use your existing CAS SciFinder^{n} username and password

Feedback Button

Provide direct feedback to CAS 

Learn More

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

Recorded events and webinars:
https://www.cas.org/about/events/scifinder-webinars

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

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