CAS SciFinder^{n}

Quick Reference Guide

July 21st, 2021

Interface and Reference Search

Links to further CAS solutions, e.g. Analytical Methods, Formulus, or the STN IP Protection Suite

Click on the logo to go to the search landing page

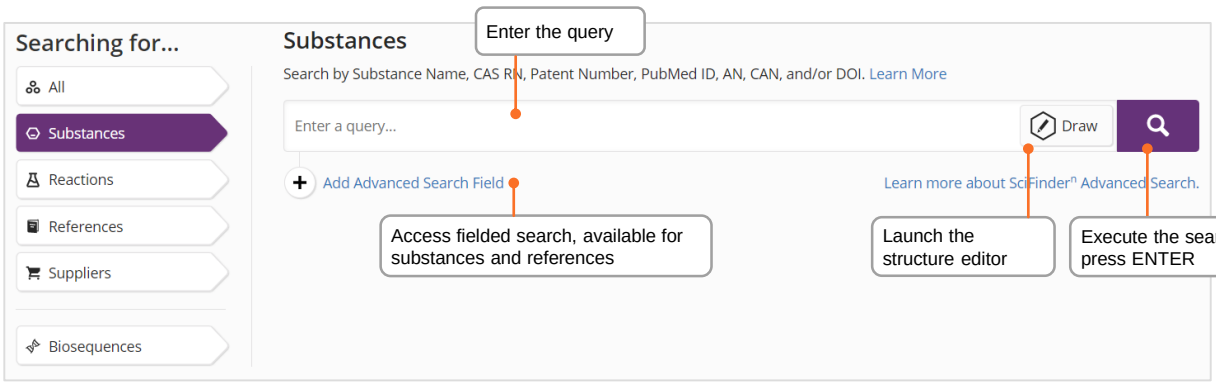
Access saved searches, Alerts and Combine. Migrate SF-web assets

Open prior searches

Open What's New, Settings Online Help or Log Out

Search Interface

SciFinder^n features a streamlined search interface.



Enter the query

Access fielded search, available for substances and references

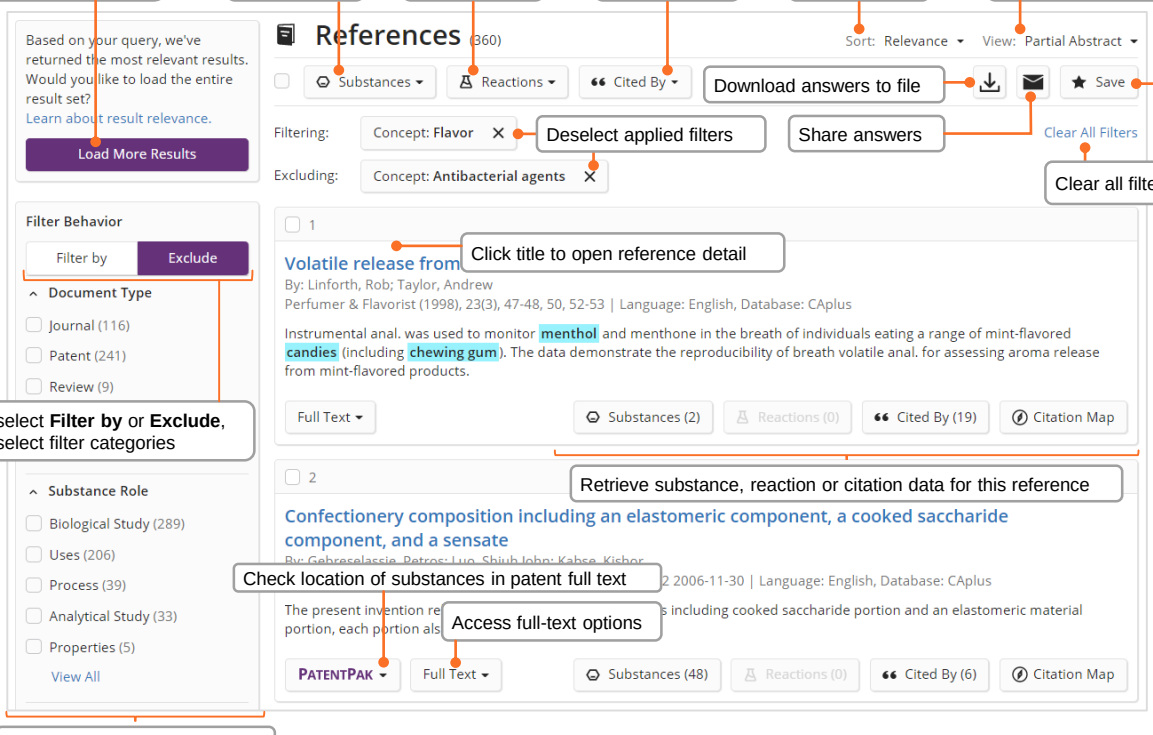
Launch the structure editor

Execute the search or press ENTER

Reference Search

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

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



Load further potentially relevant results for better comprehensiveness

View indexed substances

View indexed reactions

View forward citations

Sort answers

Change how answers are displayed

Download answers to file

Save results, set up alerts

Share answers

Deselect applied filters

Clear all filters

Click title to open reference detail

First select **Filter by** or **Exclude**, then select filter categories

Retrieve substance, reaction or citation data for this reference

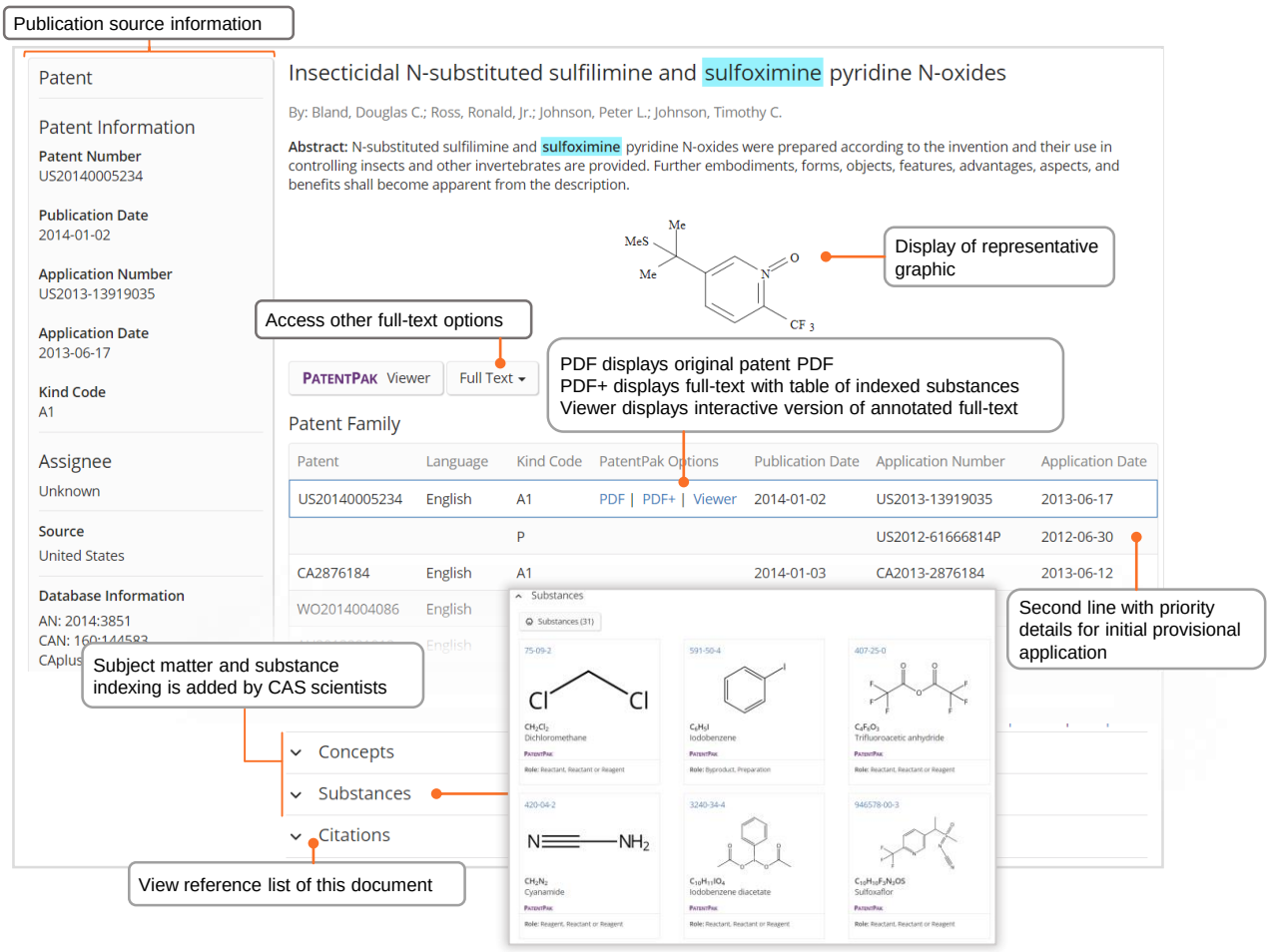
Check location of substances in patent full text

Access full-text options

Select filters to refine answers

CAS SciFinder^n

Reference detail and search



Boolean Operators

Logical operators define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.: (flavor or odor) and menthol

AND Requires both concepts to be present within the document

OR Requires either one or both concepts to be present
Connect synonyms with OR

NOT Excludes documents from an answer set containing the word after NOT

Wildcards

Wildcards allow for more comprehensive retrieval and more precision
Use in reference and substance name 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 phrase,
e.g.: "Programmed cell death protein"

Substance name and structure

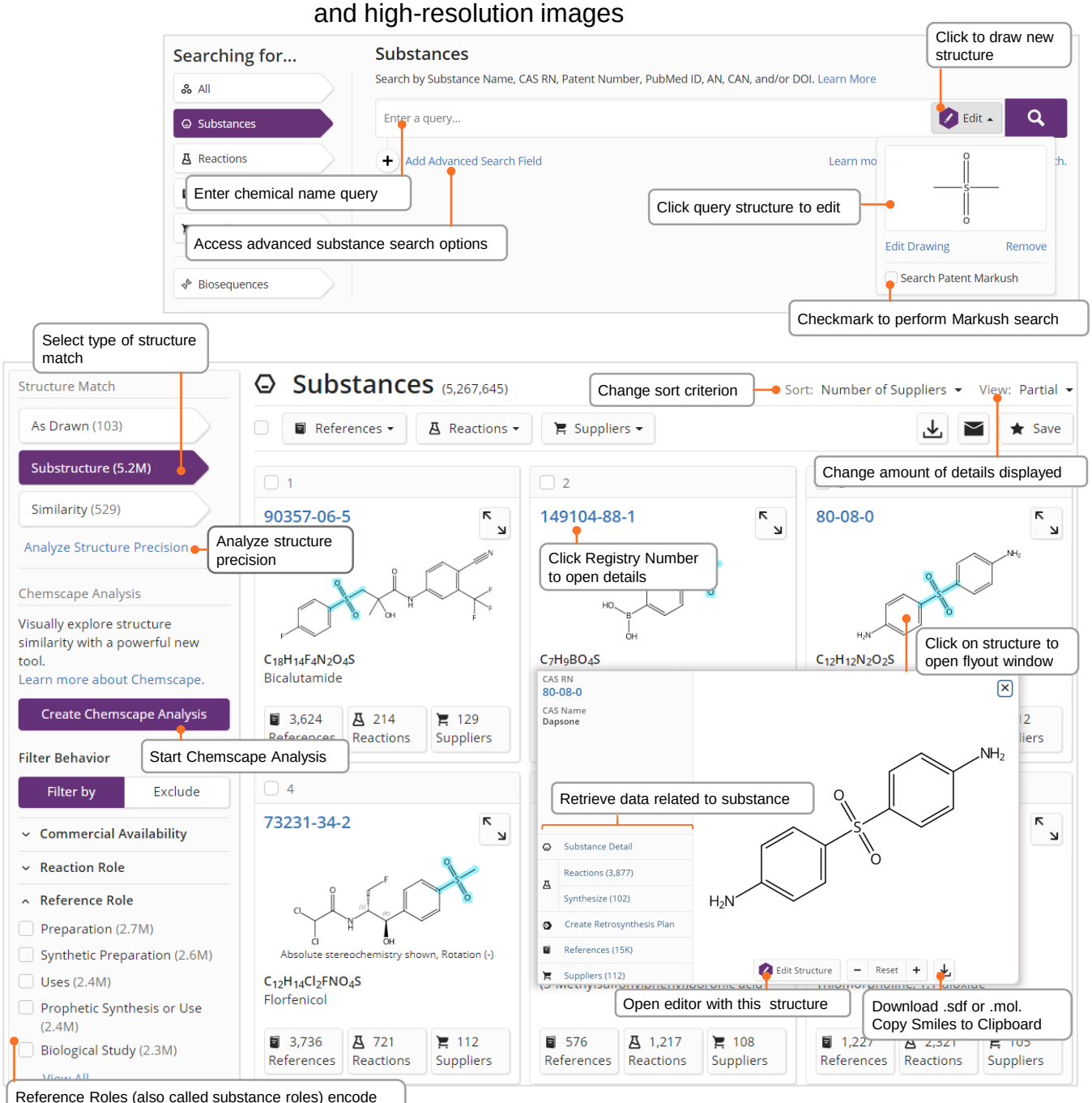
Name searches

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 with the stem Sulfoximin
WO2019234160	Finds all indexed substances for this patent

Structure searches

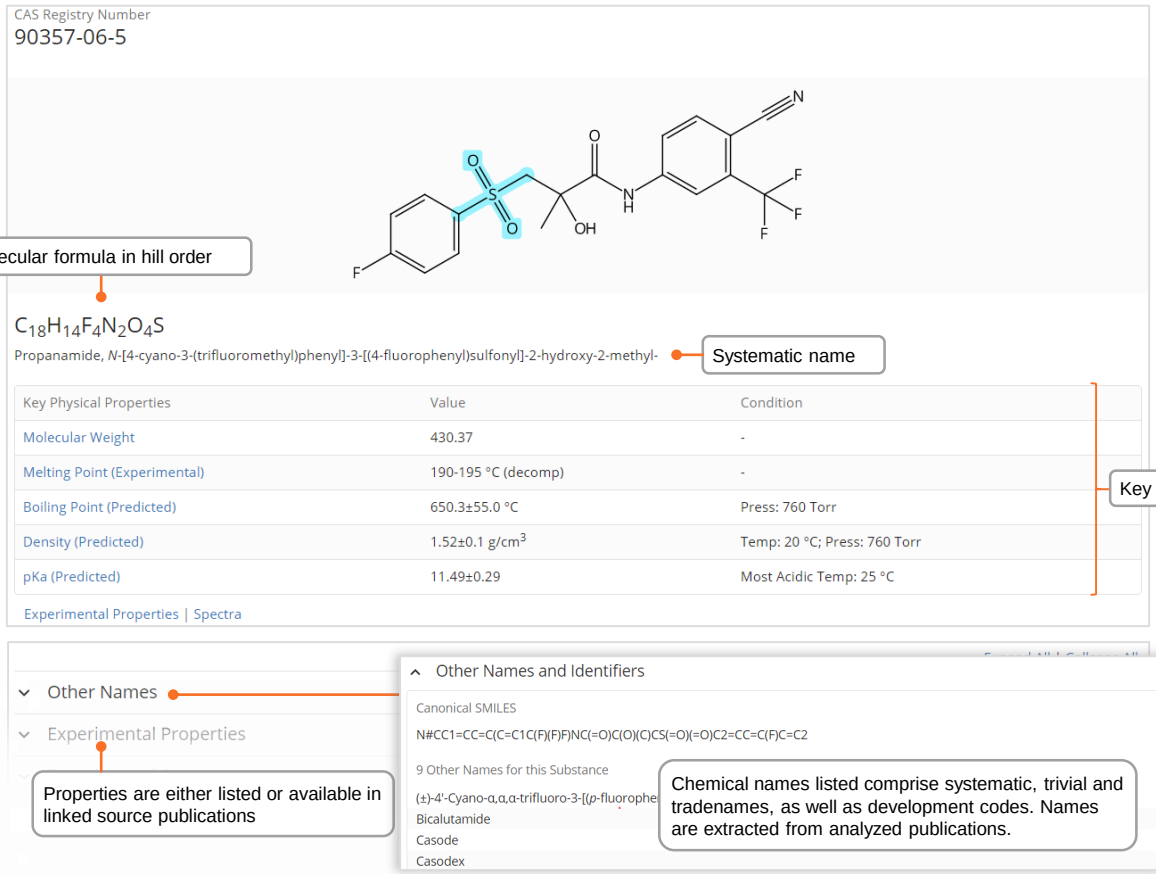
Substance searches returns results in an intuitive layout. The display highlights most relevant hits, critical property information and high-resolution images



Substance detail and structure editor

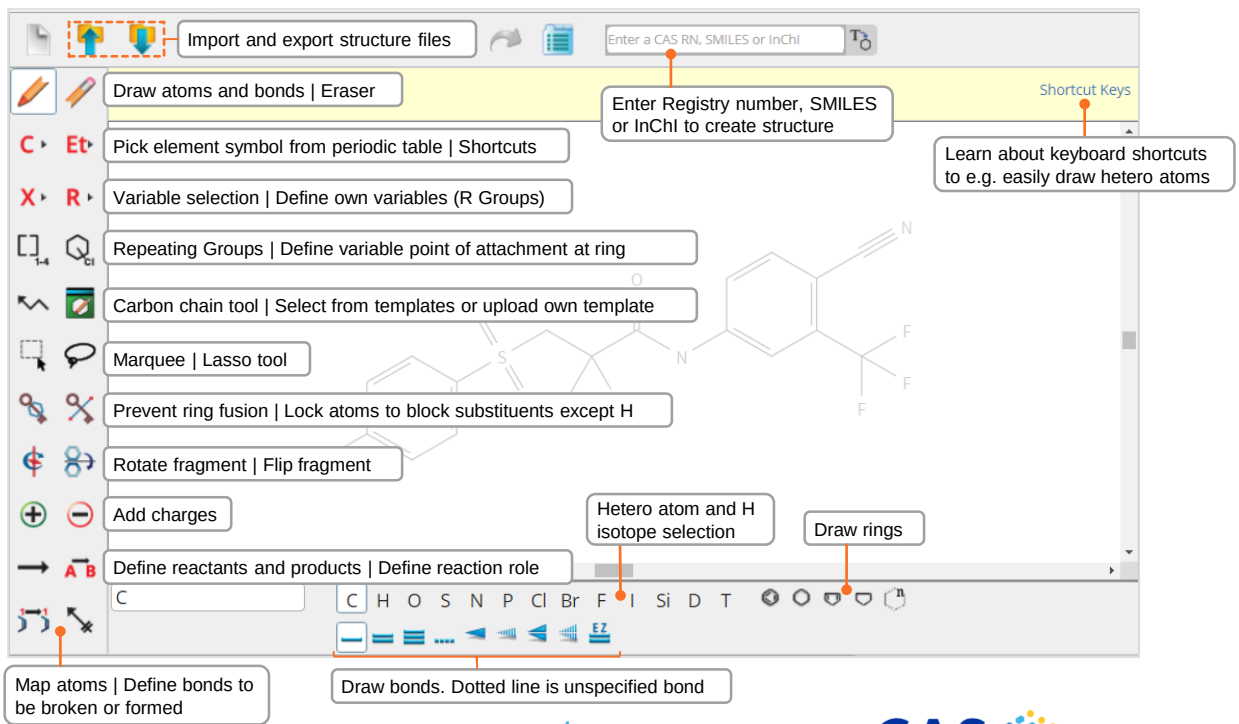
Substance detail

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



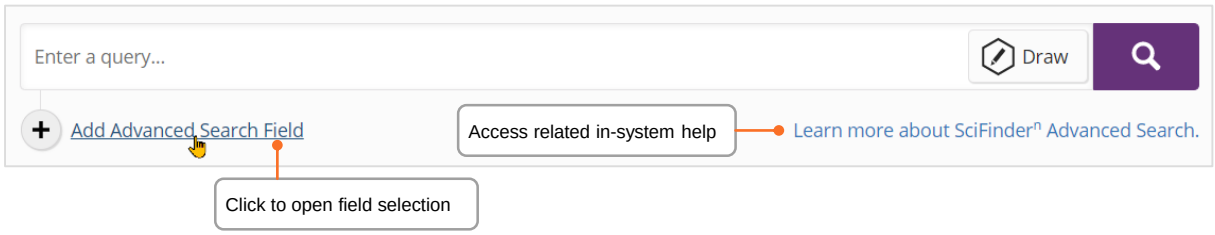
CAS SciFinder^n

Advanced search query builder

Advanced Search Query Builder

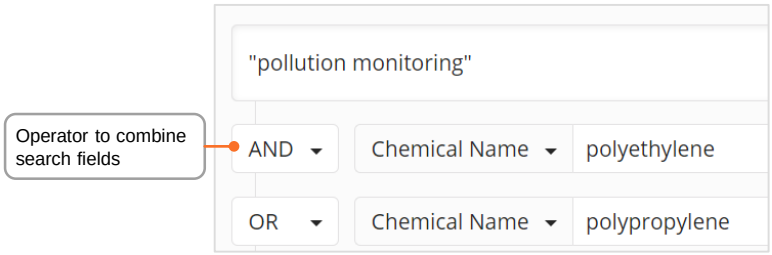
Provides specific reference and substance search fields from SciFinder^n's landing page

- 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)



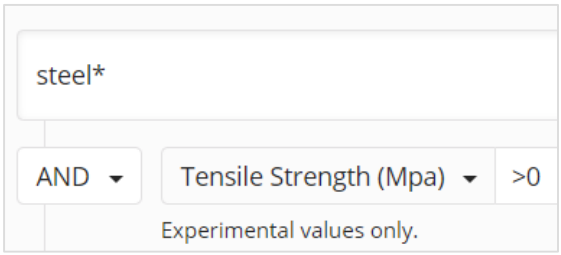
Examples

Reference Search

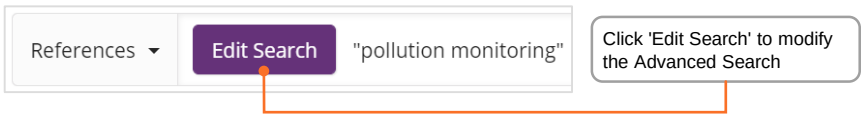


Query interpretation:
"pollution monitoring" and (polyethylene or polypropylene)

Substance Search



Query interpretation:
Steel with tensile strength property information



Advanced Search Fields

The below advanced search fields are available

Reference

- Author Name
- Journal Name
- Organization Name
- Title
- Concepts
- Substances
- Publication Year
- Document Identifier
- Patent Identifier

Substance

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

CAS Roles

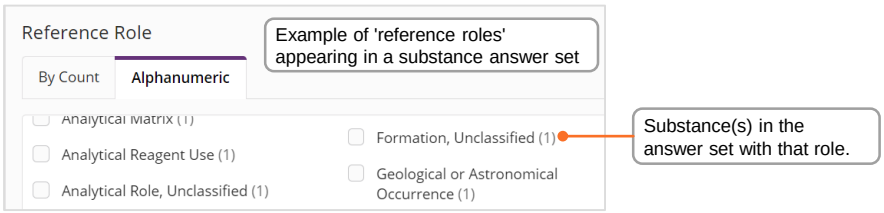
CAS Roles

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.

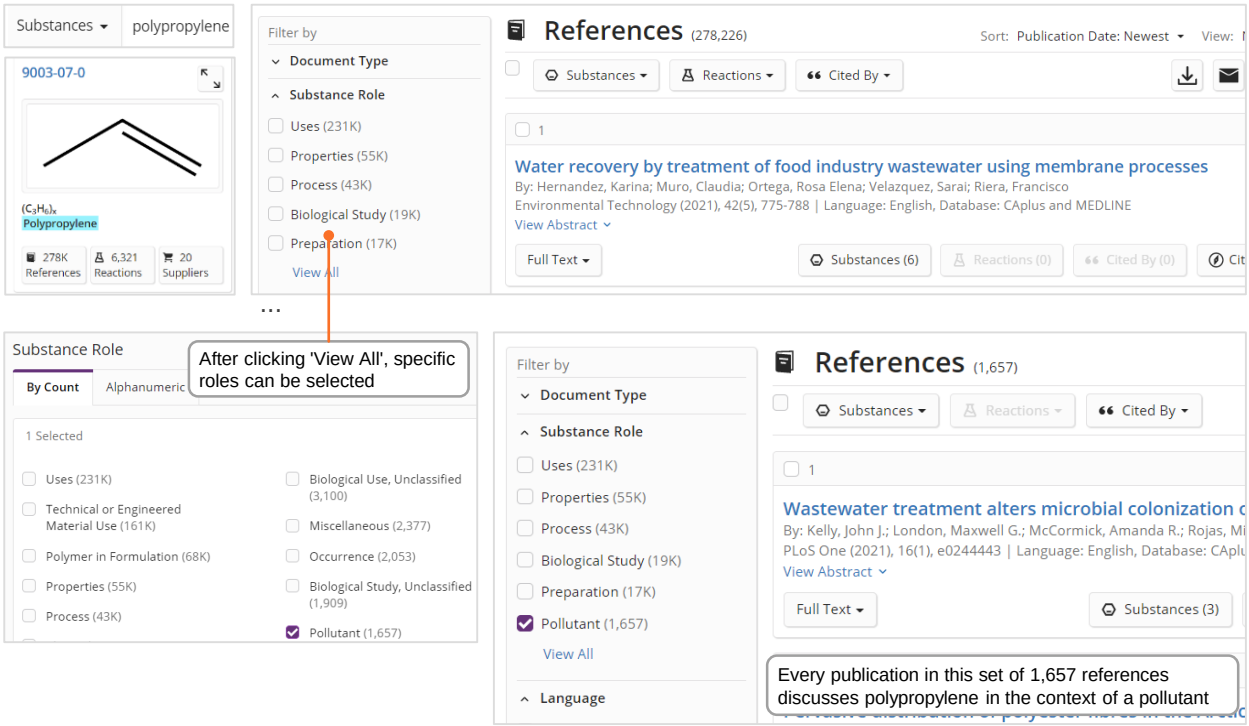


Roles in reference results

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 1648 publications that describe polypropylene as a pollutant.



Biosequence searching

Development

Sequence searching is developed in stages. June 2021 status:

- BLAST: Search similar sequences — **Implemented**
- CDR: Search antibodies via antigen binding sites — **Implemented**
- Motif: Search conserved shorter sequence patterns — **Implemented**
- Global crossover from sequences to patents — **Implemented**

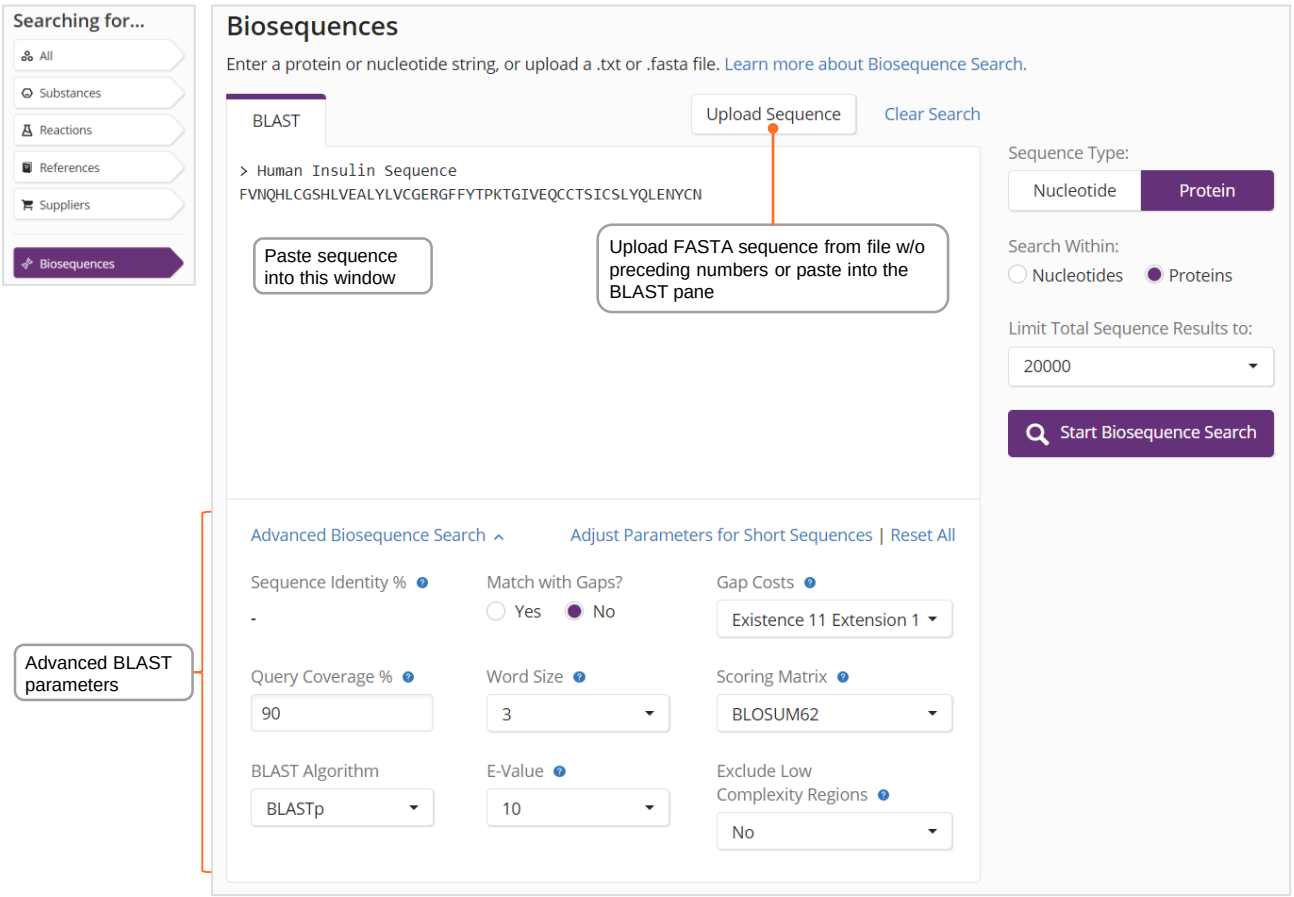
- Crossover from sequences to scientific literature — In development

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

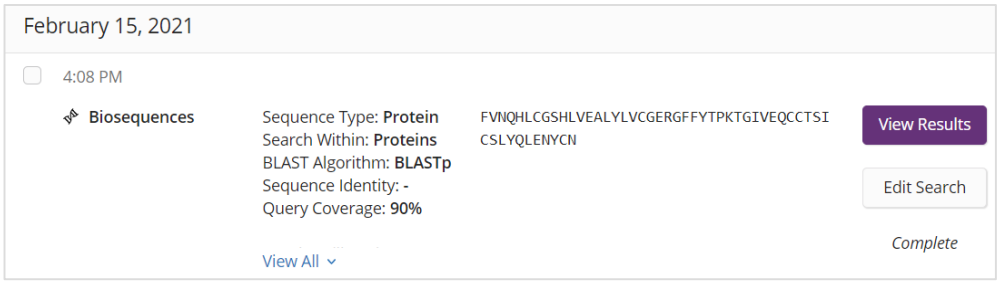
- Open the Biosequences module from the main SciFinder^{n} search page
- Load sequence from file or paste sequence
- Supported formats: Sequences containing residues represented by single-letter codes, e.g. in the FASTA format. Leading numbers are not allowed.
- Sequence input may contain header line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



BLAST result analysis

Access Results

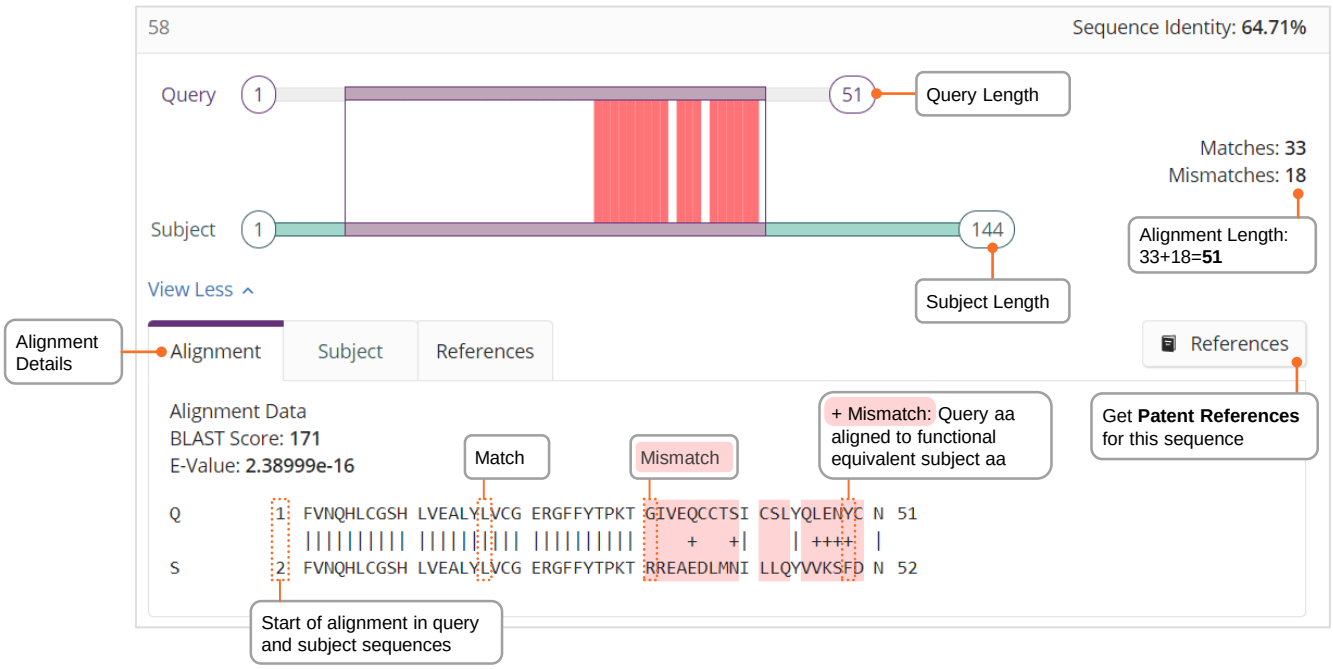
Biosequence search results appear in the Recent Search History and general Search History (History). Click 'View Results' to analyze answers. Refresh your browser to update the history.



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 patent references
- XLSX result download available



Filter Results

Filtering dynamically changes the result set

$$Expectation\ Value$$

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

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

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

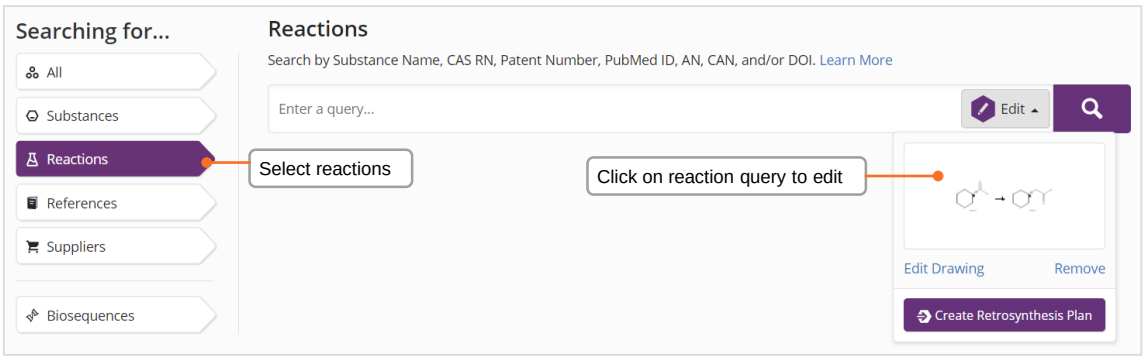
CAS SciFinder^n

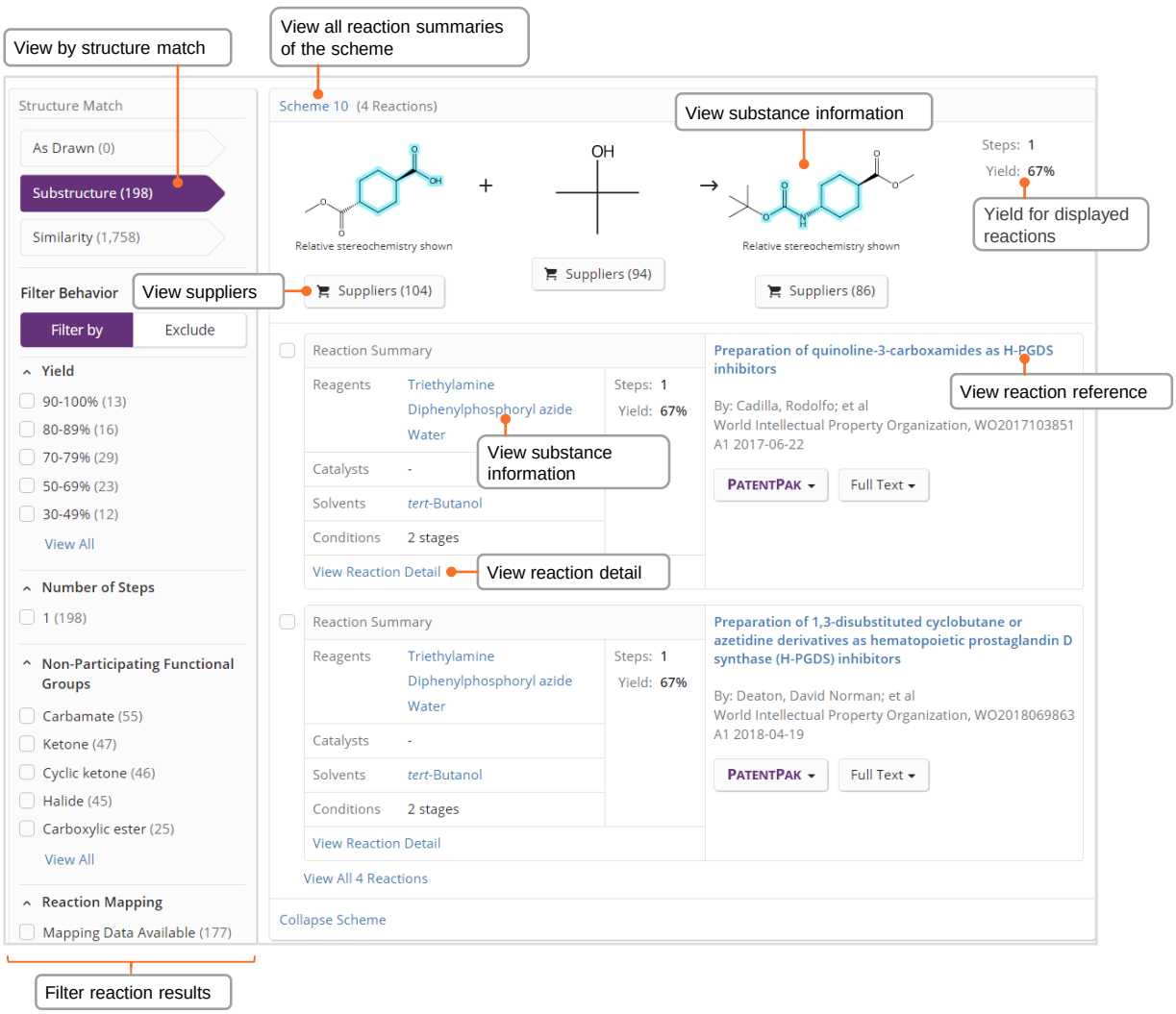
Reaction searching

Reaction searches

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

- Reactions are grouped into schemes with identical reactants and products
- Reactions are sorted by yield within a scheme
- Find reactions by substance name, registry number, document identifier or chemical structure

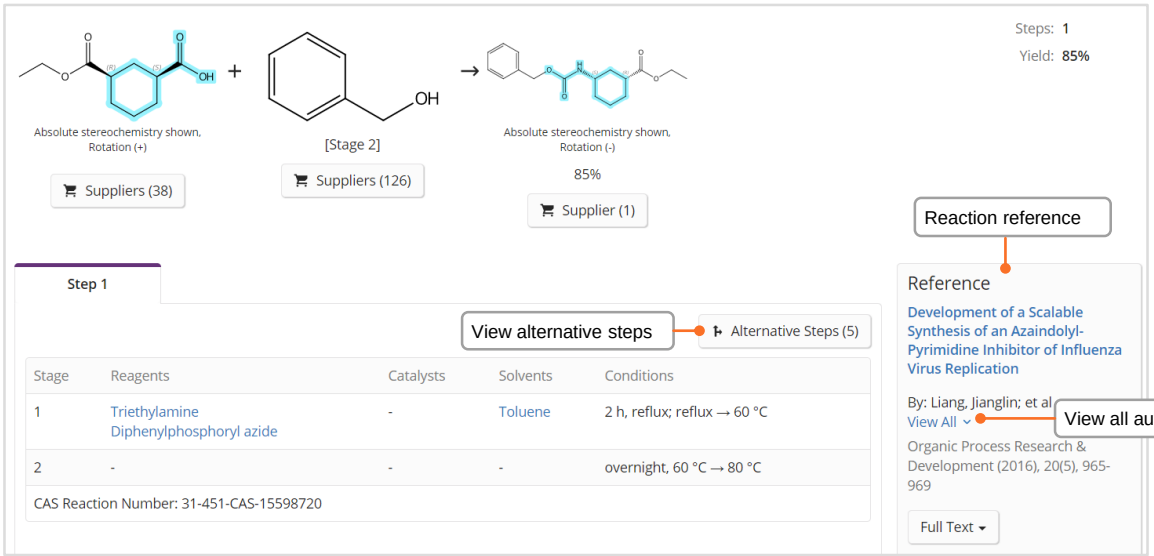


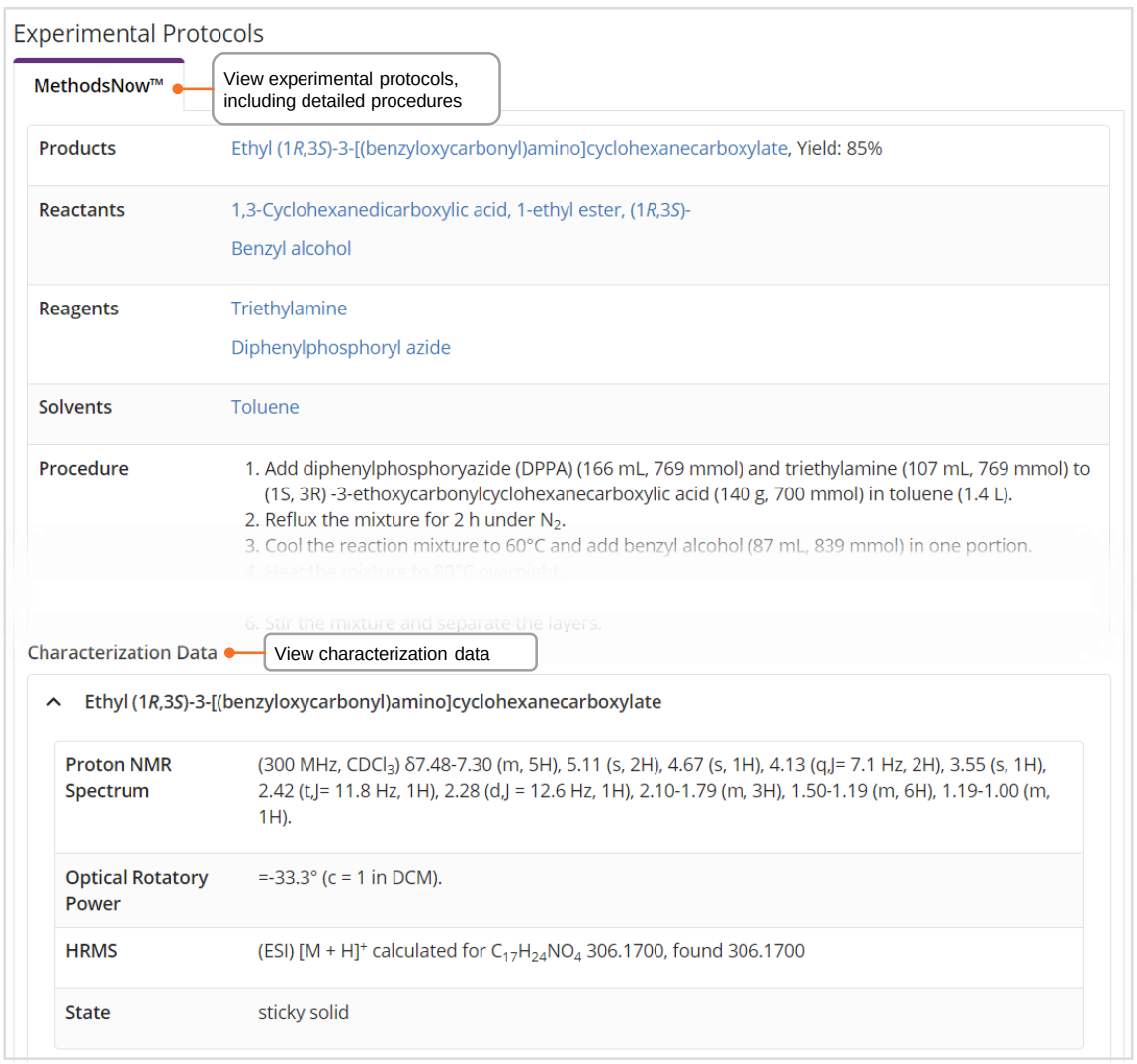


Reaction details

Reaction details

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



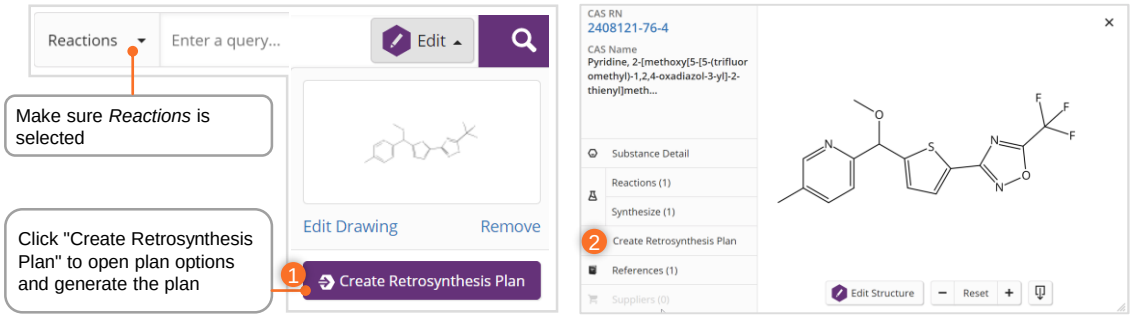


Retrosynthesis planner

Launch plan generation

There are two options to launch SciFinderⁿ's Retrosynthesis Planner

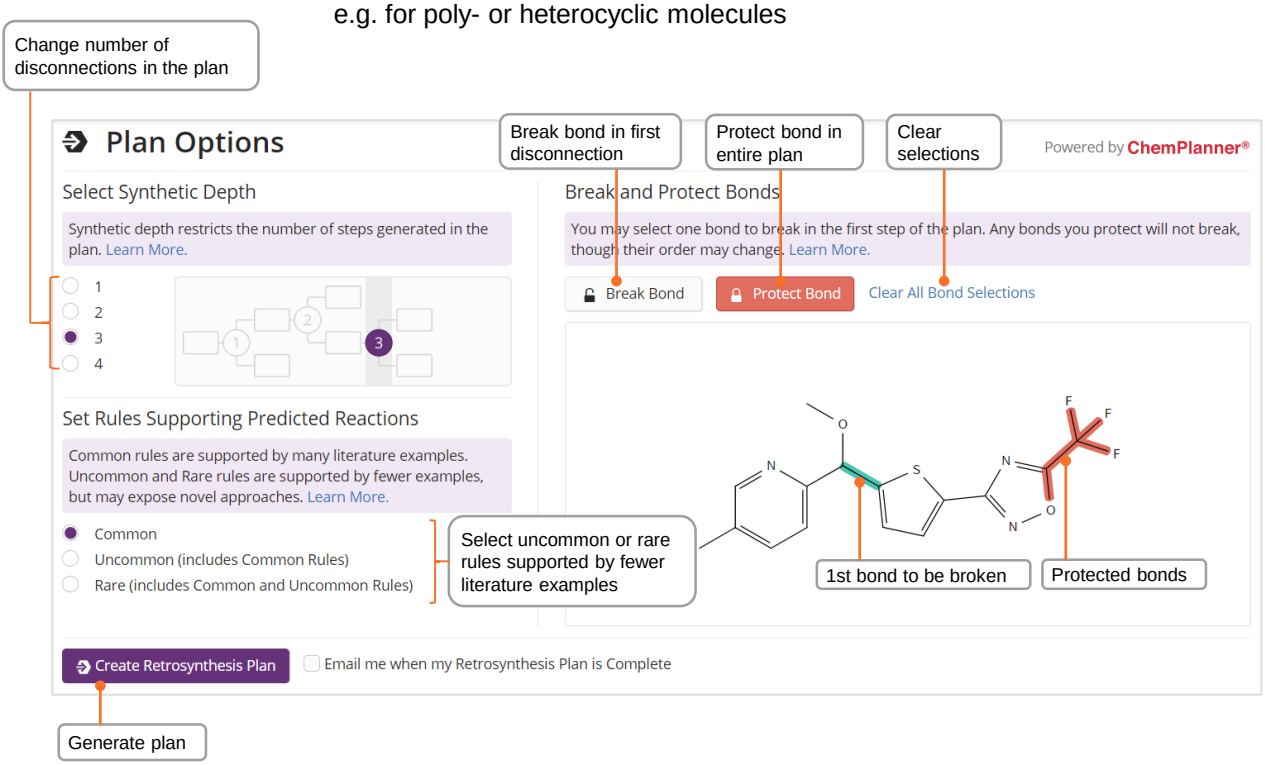
1. Draw reaction structure and create plan from Edit icon
2. Open structure flyout window and start plan generation



Plan options

Edit plan options to...

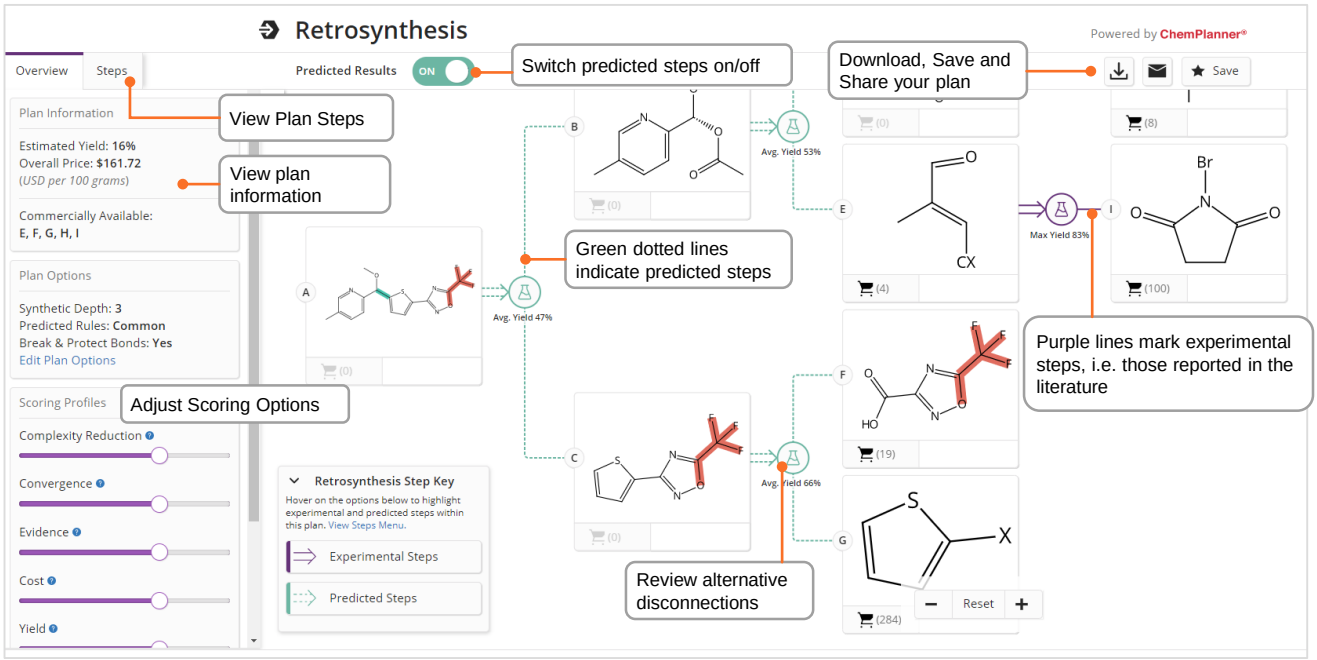
- increase the synthetic depth
- protect bonds through the entire synthetic route
- define bonds to be broken in the first disconnection
- create a plan with more meaningful alternatives, e.g. for poly- or heterocyclic molecules



Retrosynthesis plan and alternative steps

Open plan

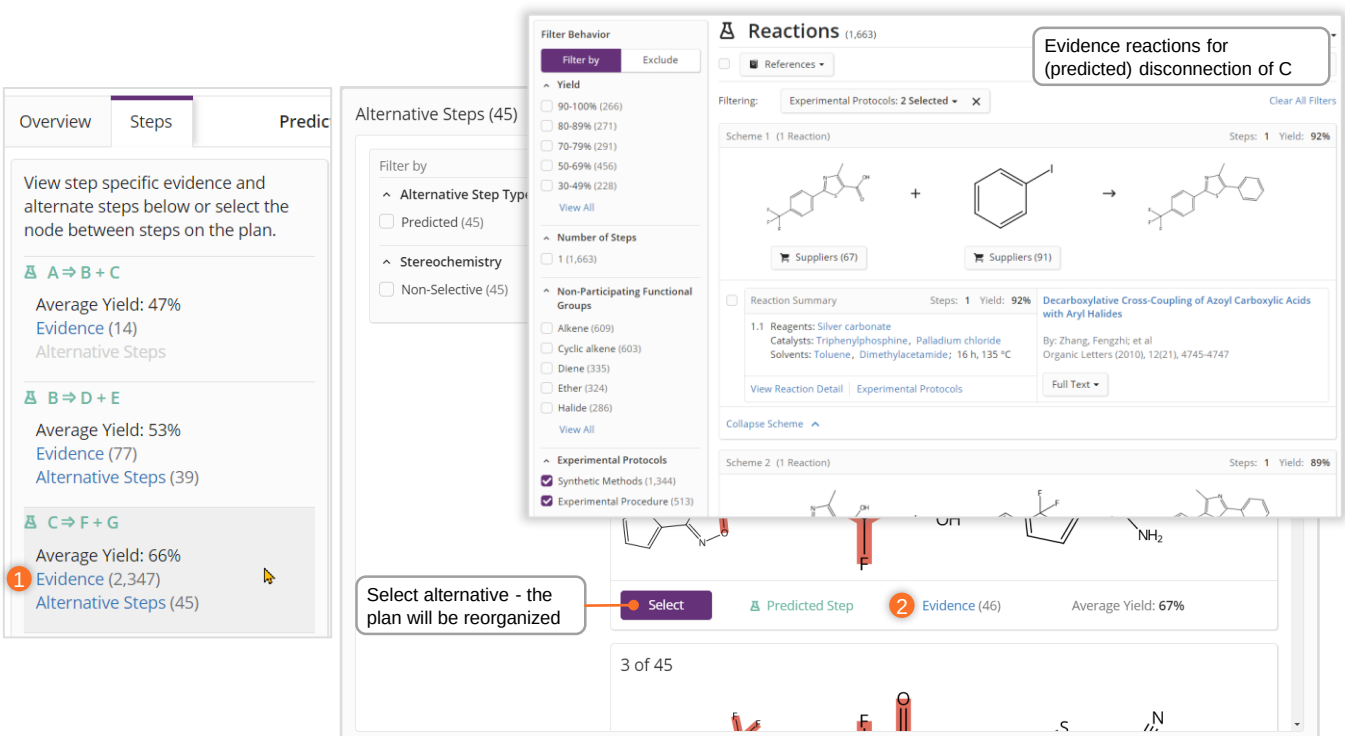
The Experimental Plan is available within a few seconds, the calculation of the Predictive Retrosynthesis Plan will take a bit longer



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

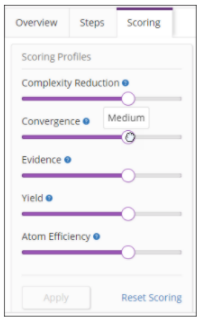


Scoring Options

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



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.

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.

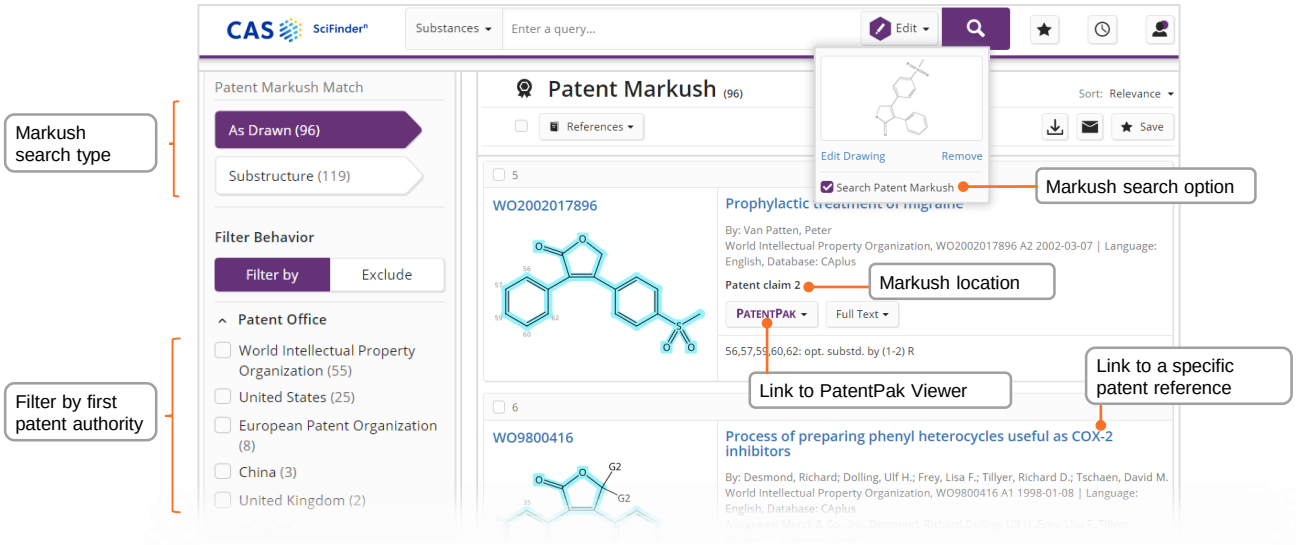
Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.

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

Markush Searching and PatentPak

Markush searching

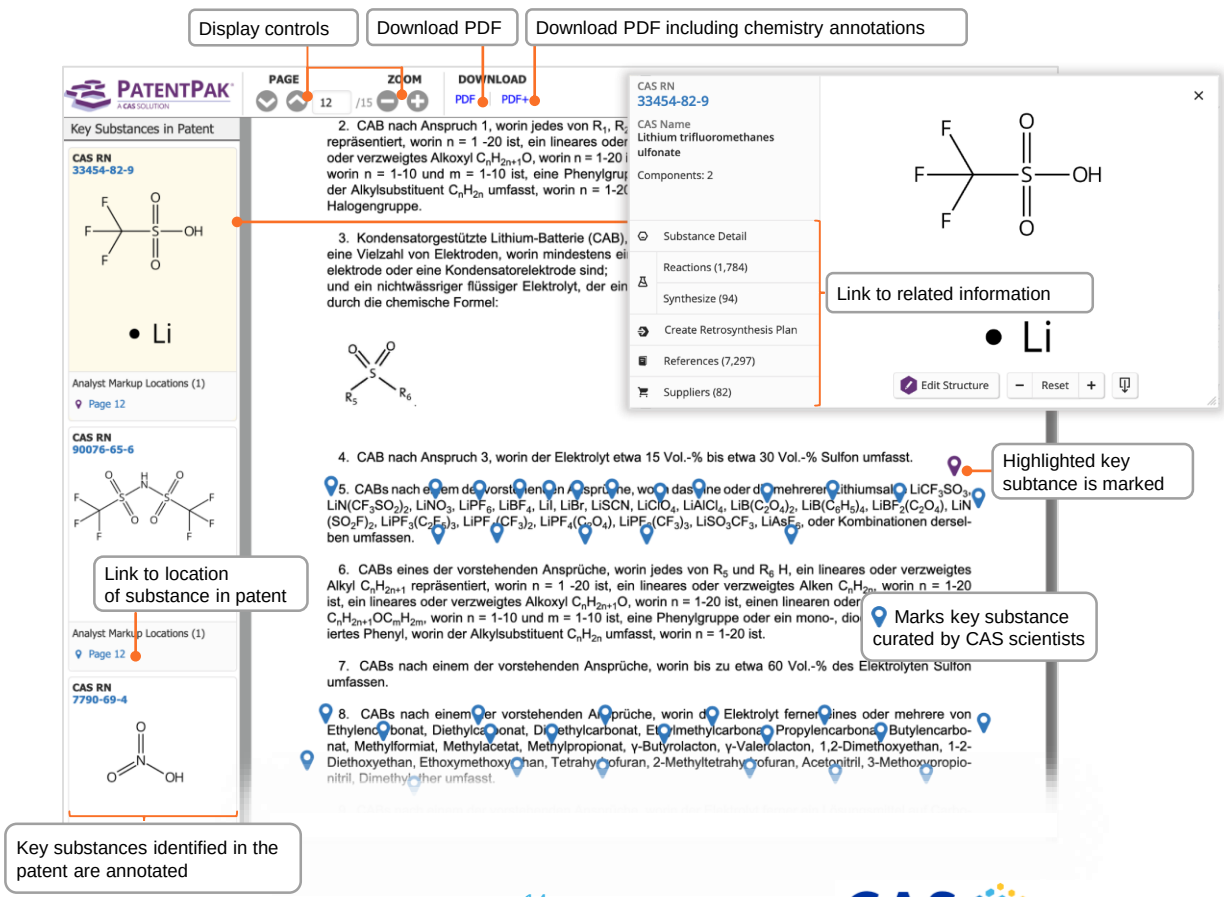
Markush structure searches can be performed by using the Search Patent Markush option while in Substances search mode



PatentPak

Up to three PatentPak Options for viewing a patent PDF:

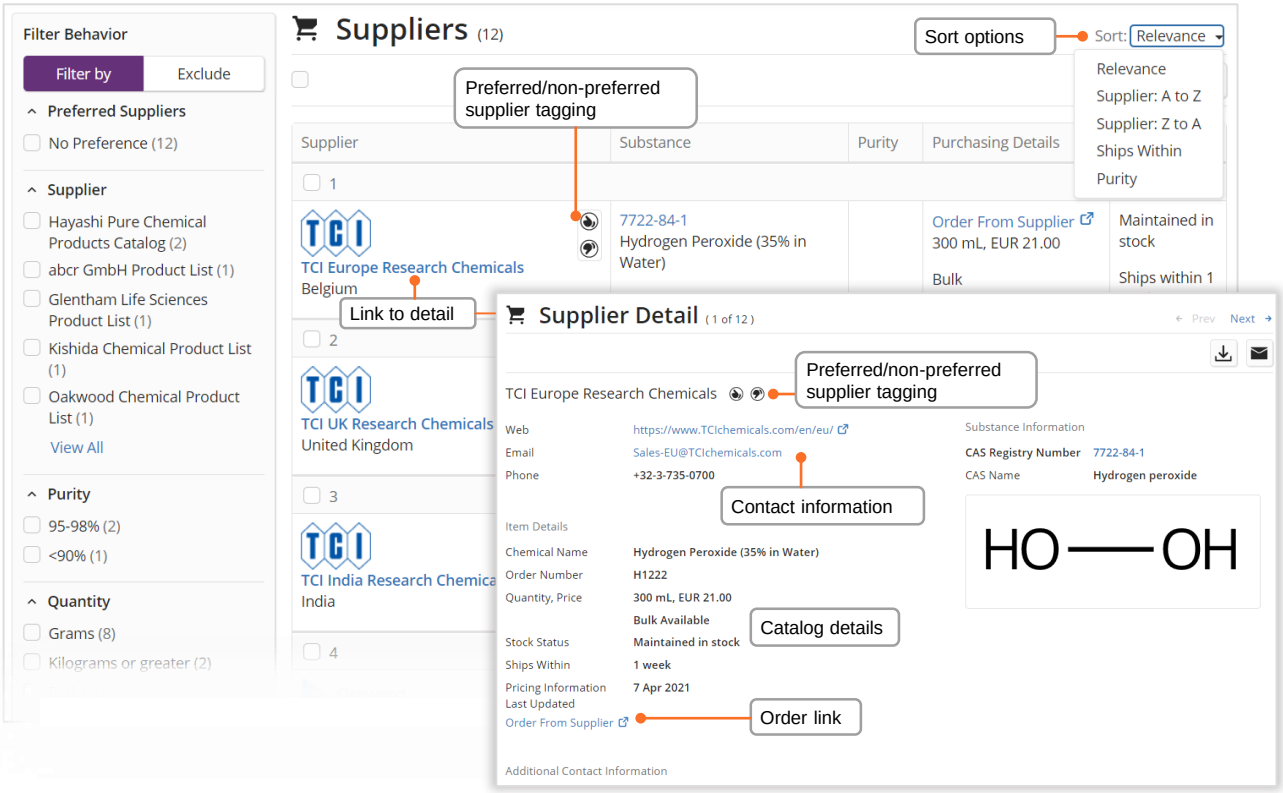
- **PDF**: Full-text patent PDF only; text-searchable PDF
- **PDF+**: Full-text patent PDF with marked-up Key Substances; text-searchable PDF
- **Viewer**: Patent PDF with linked markups of Key Substances; see below:



Supplier Searching and ChemDoodle®

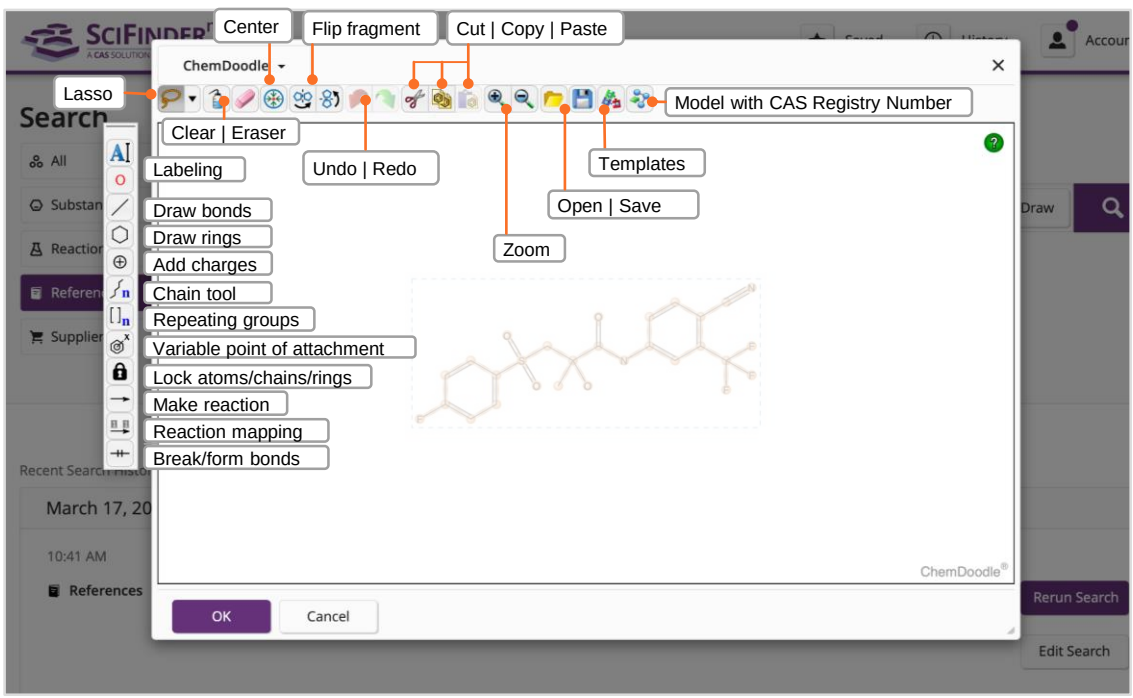
Suppliers searching

Suppliers searching allows for direct access to chemical catalog information based on chemical structure, names or other identifiers



ChemDoodle®

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



Login, Feedback and Support

Login Details

- Login at http://scifinder-n.cas.org
- Use your existing SciFinder username and password

Feedback Button

Provide direct feedback to CAS 

Learn More

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

Upcoming and recorded SciFinder^{n} webinars:
https://www.cas.org/about/events/scifinder-webinars

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