SciFinder^{n}

A CAS SOLUTION

Quick Reference Guide

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Login and Support

Login Details

- Login at https://scifinder-n.cas.org
- Use your existing SciFinder username and password
- Create a new SciFinder^{n} account for a new user:
  use the intranet SciFinder Registration URL of your institution

Learn More

- https://www.cas.org/support/training/scifinder-n

Training

- Contact aling@acs-i.org to organize your on-site or online session

Contact Customer Support

- Email help@cas.org to connect with a CAS Customer Center representative

Interface and Reference Search

Click on the logo to go to the home page

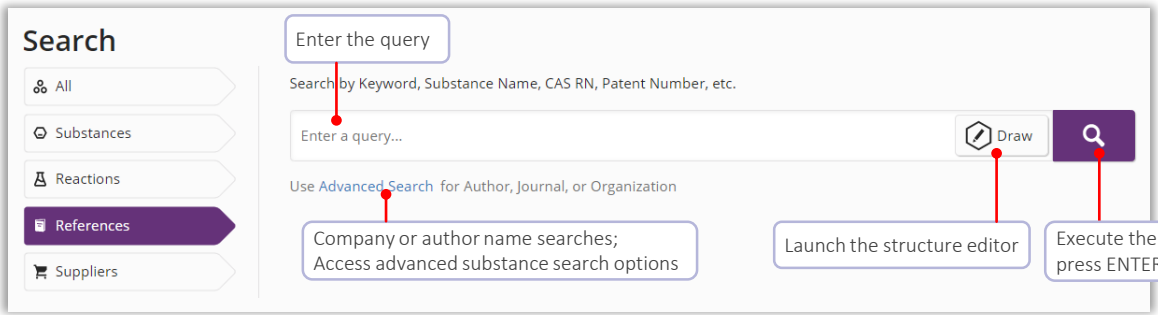
Access saved searches, Alerts and Combine. *Migrate SF-web assets*

Access prior searches

Open What's New, MyCASProfile (i.e. Settings) and Online Help

Search Interface

SciFinder^n features a streamlined search interface.



Enter the query

Company or author name searches; Access advanced substance search options

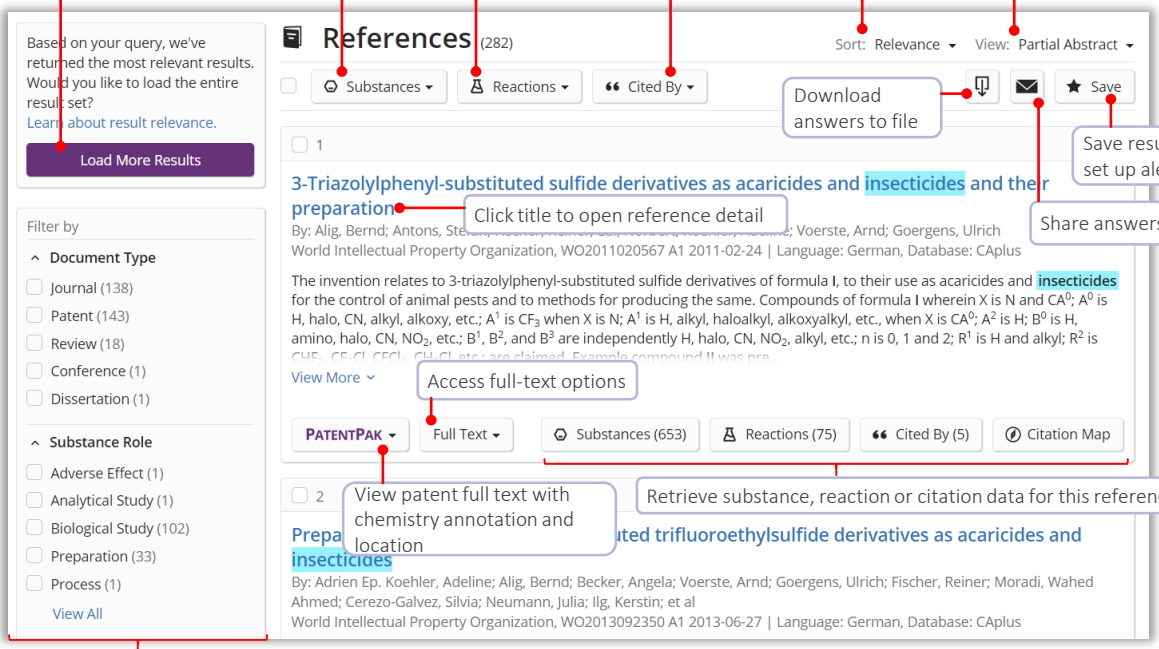
Launch the structure editor

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 by default
- 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 additional results for comprehensiveness

View indexed substances

View indexed reactions

View forward citations

Sort answers

Change how answers are displayed

Download answers to file

Save results and set up alerts

Share answers by link

Click title to open reference detail

Access full-text options

View patent full text with chemistry annotation and location

Retrieve substance, reaction or citation data for this reference

Select filters to refine answers

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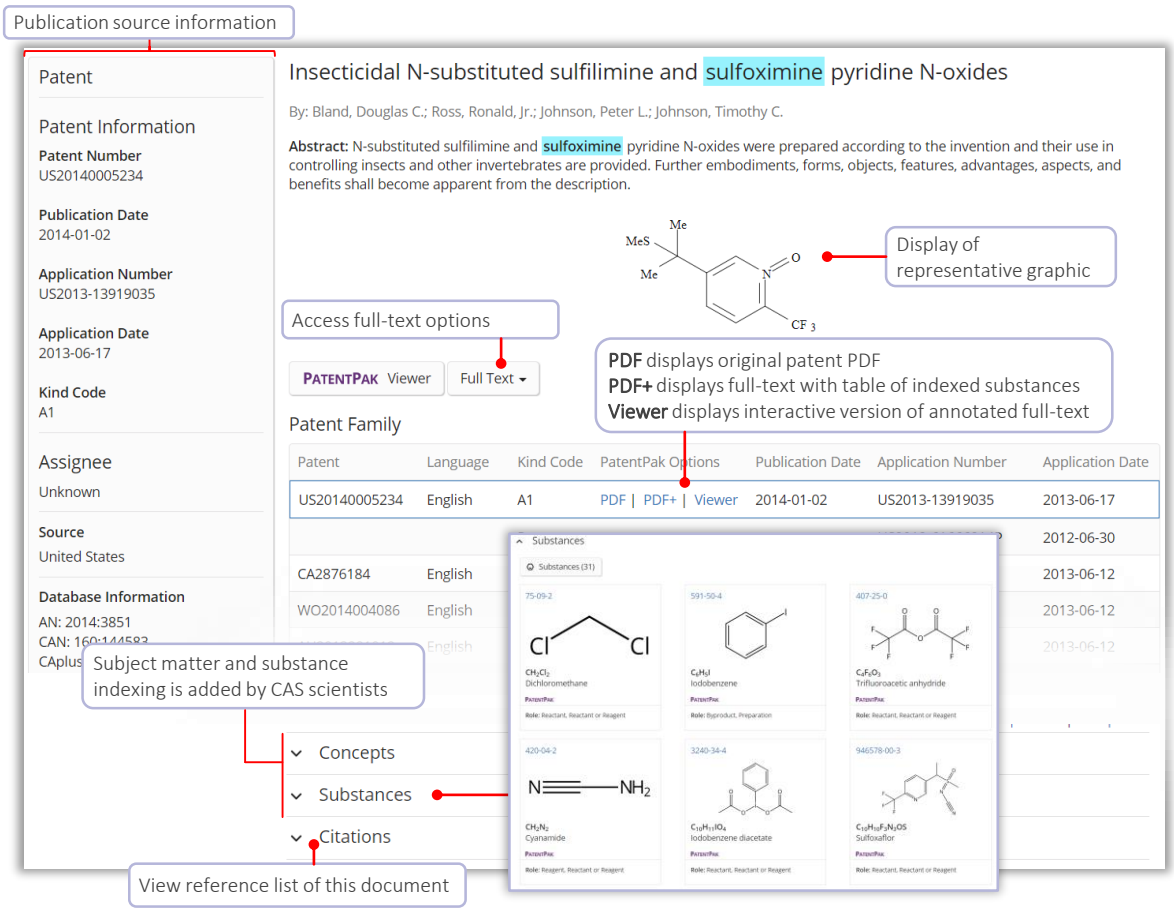
Reference Detail and Search Operators



Boolean Operators

Logical operators are available to define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.: (fungicide OR pesticide) AND strobilurin

AND Requires both words, phrases, or concepts to be present within the document

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

NOT Excludes documents from an answer set. Be careful when using the NOT operator, you cannot always assess the context of document texts

Wildcards, Masking

Wildcards and masking allow for more comprehensive retrieval and more precision respectively | 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.: 1,?-hexanediol

Terms masked with double quotes will be searched as a phrase, e.g.: "Programmed cell death protein"

Substance Name and Structure Searching

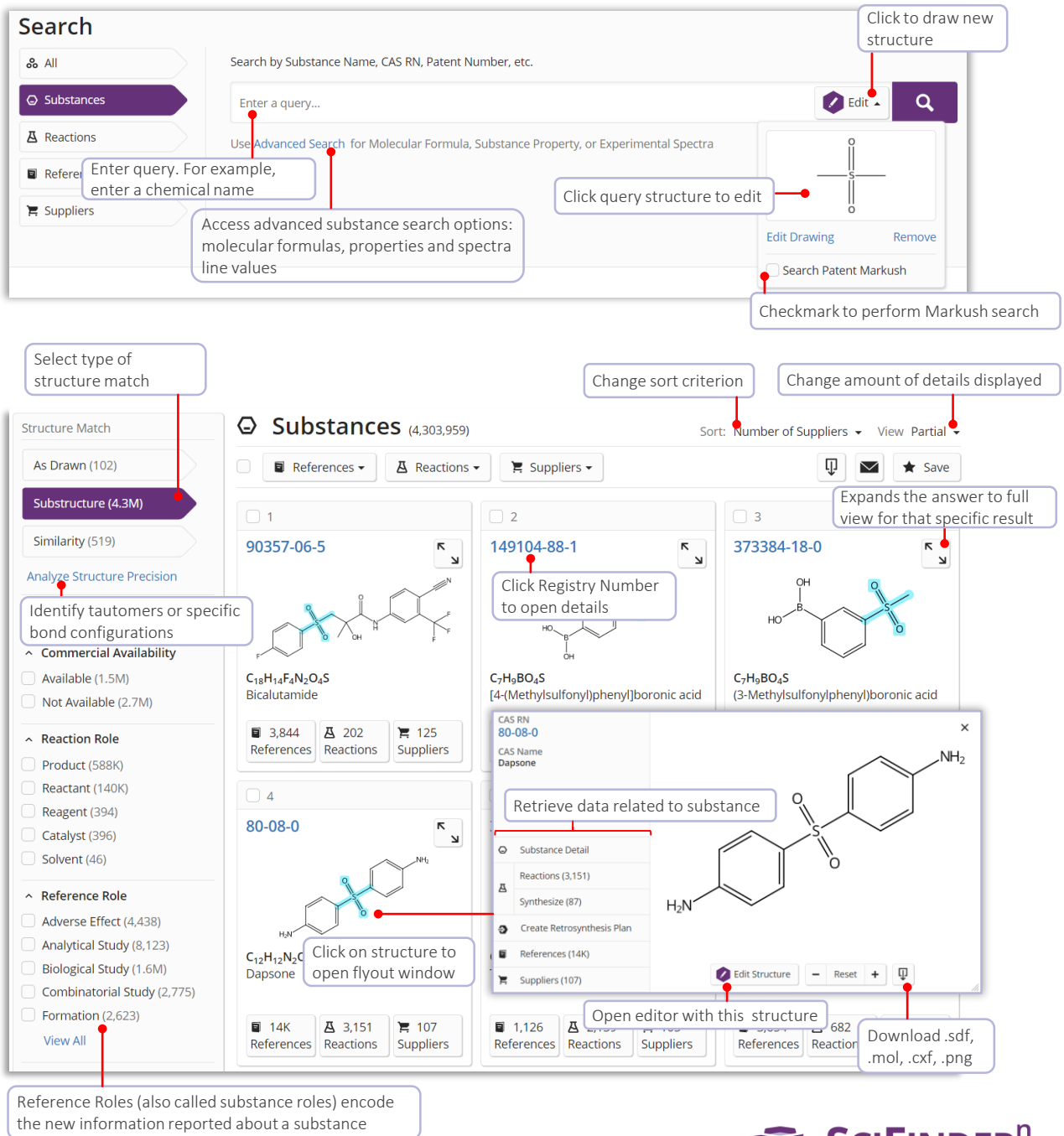
Name searches

Search with one or more substance names, identifiers, and document ID

Vanillin	Finds Vanillin record
57-92-1	Finds Vanillin record, uses CAS Registry number as identifier
Vanillin stearate	Finds 3 records: Vanillin, Vanillin stearate and Stearate
"Vanillin stearate" Vanillin	Finds 2 records: Vanillin stearate and Vanillin
Vanillin*	Finds all names that start with the term Vanillin
WO2019020773	Finds all indexed substances for this patent

Structure searches

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



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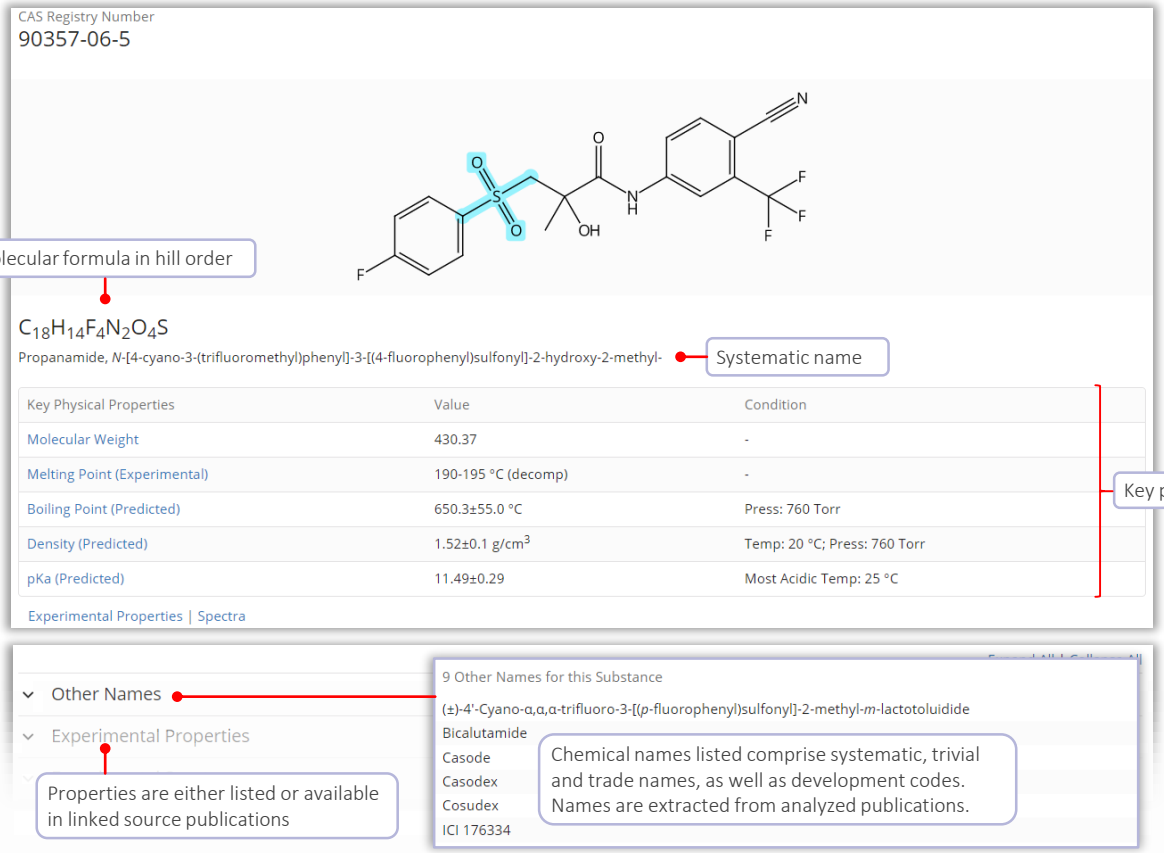
Substance Detail and Structure editor

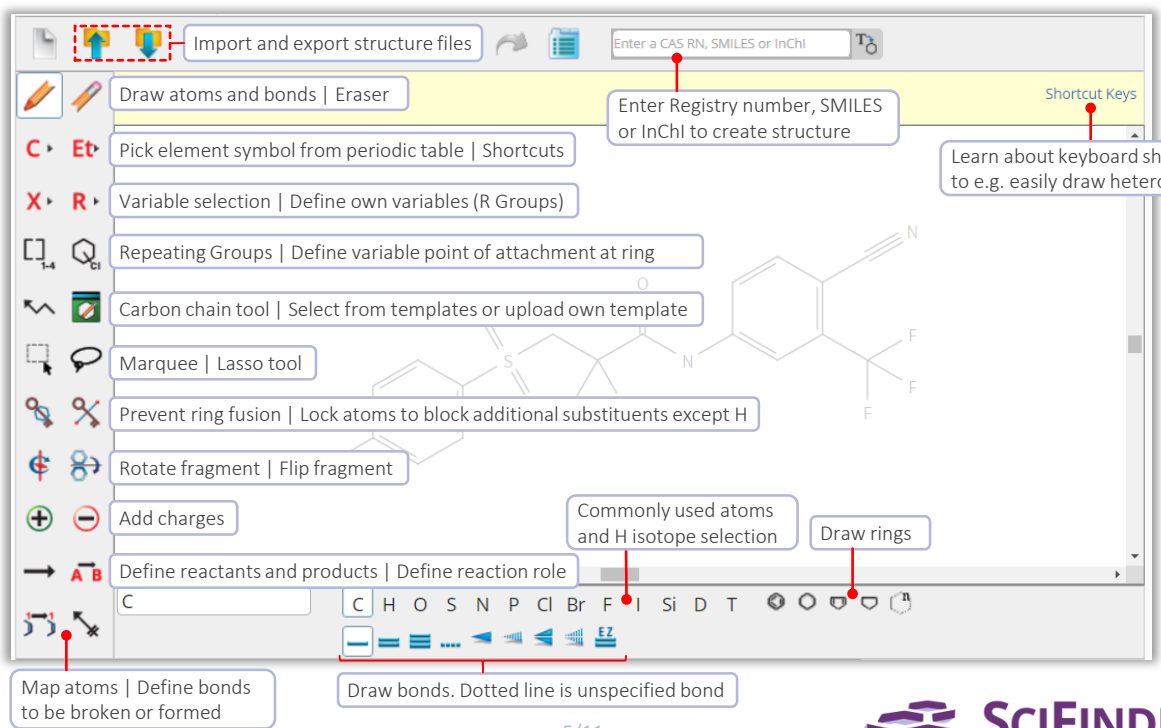
Substance detail

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



CAS Draw editor

Define structure and reaction queries with the structure editor



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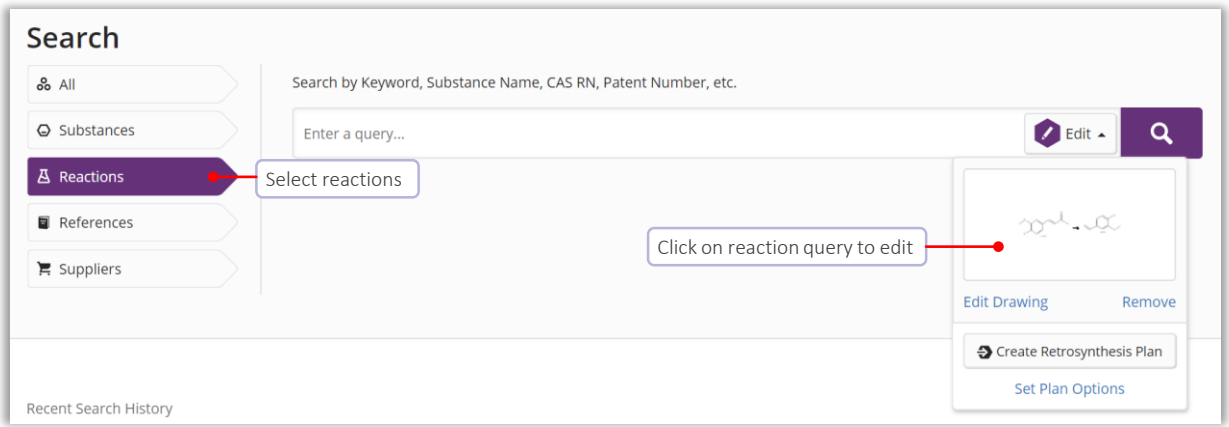
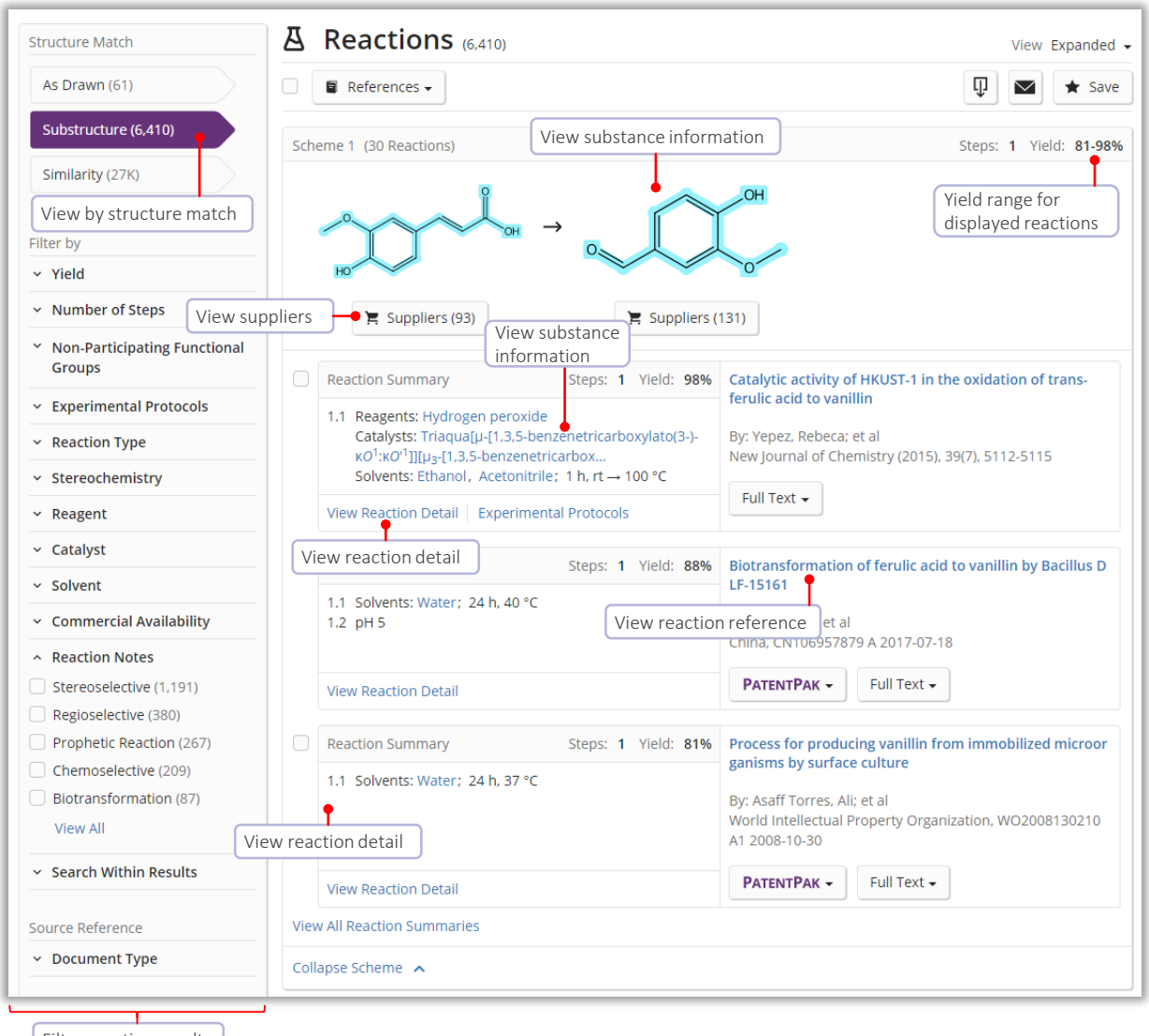
Reaction Searching

Reaction searches

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

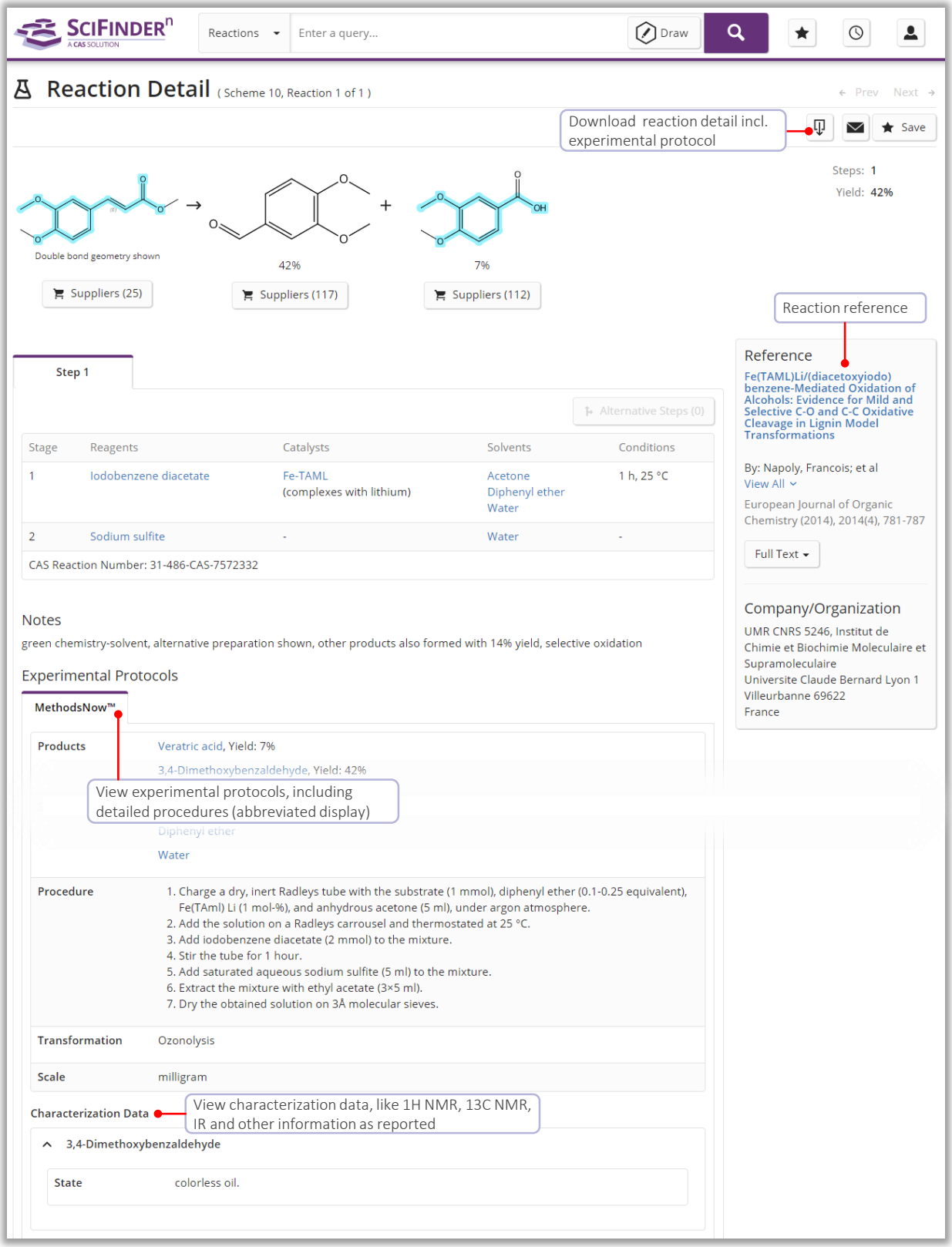
- Reactions are grouped into schemes with identical reactants and products
- Reactions are sorted by yield within a scheme
- Find reactions by substance name, registry number, document identifier, chemical structure or reaction scheme





Reaction Details

Detailed information includes solvents, catalysts, reagents, conditions and experimental protocols extracted from the publication and its supplemental information.

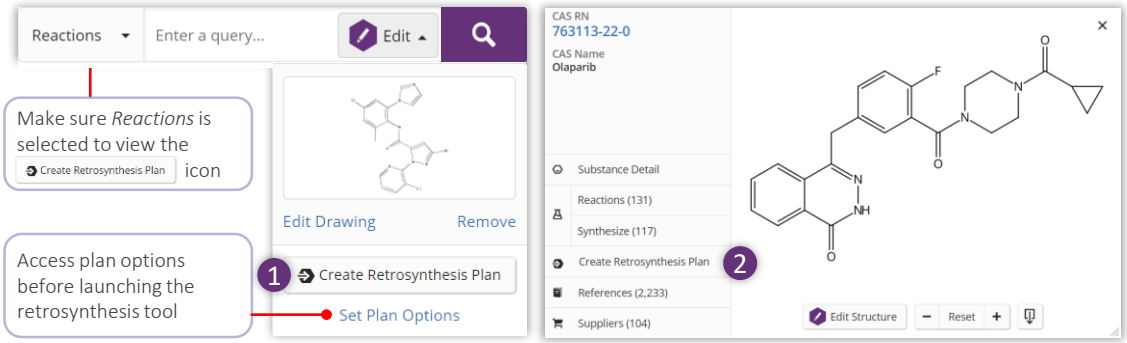


Retrosynthesis Planner

Launch plan generation

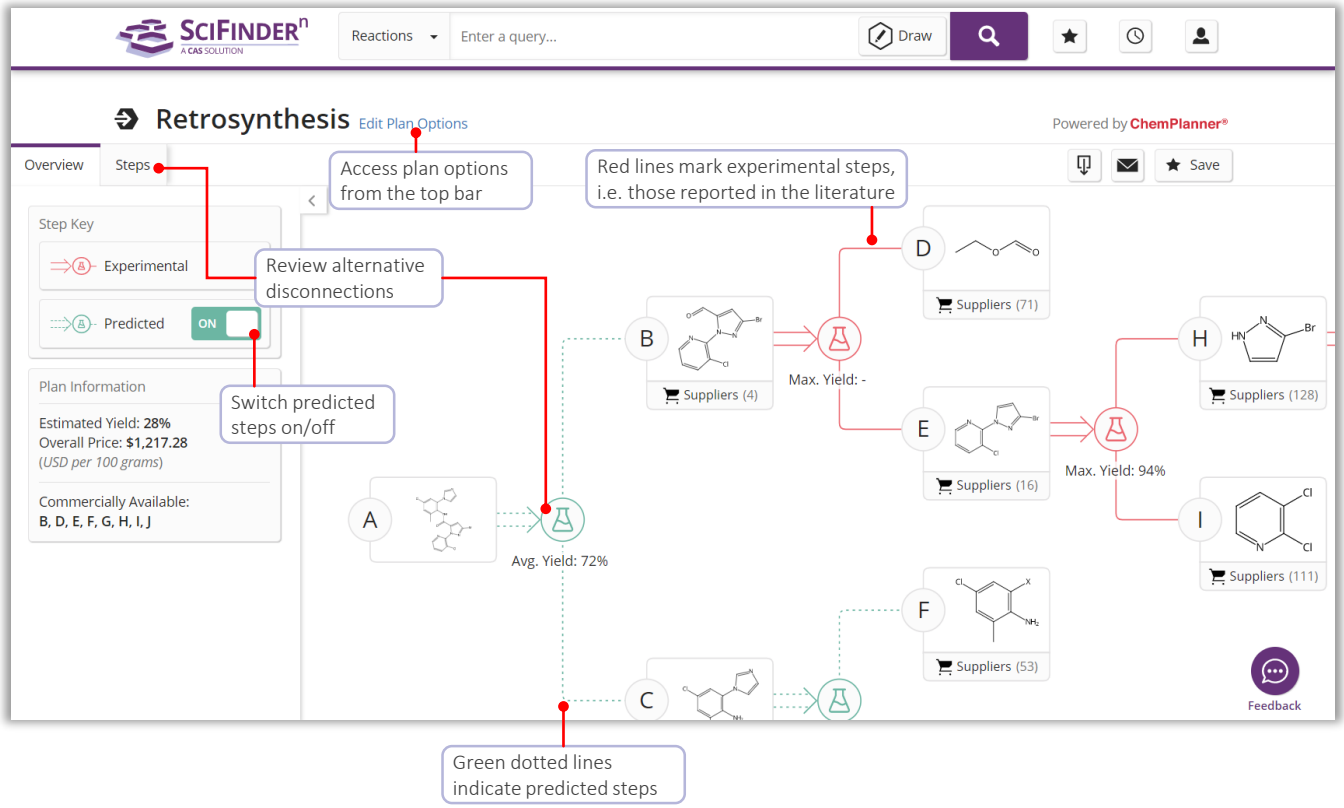
There are three options to launch SciFinder^n's retrosynthesis planner

1. Draw reaction structure and create plan from Edit icon
2. Open structure flyout window and start plan generation
3. Structured based reaction query without any results (not pictured)



Open plan

The Experimental Plan is available within a few seconds. As soon as the calculation of the Predictive Retrosynthesis Plan is finished, a notification will pop up in that retrosynthetic plan. You will also be informed via email.



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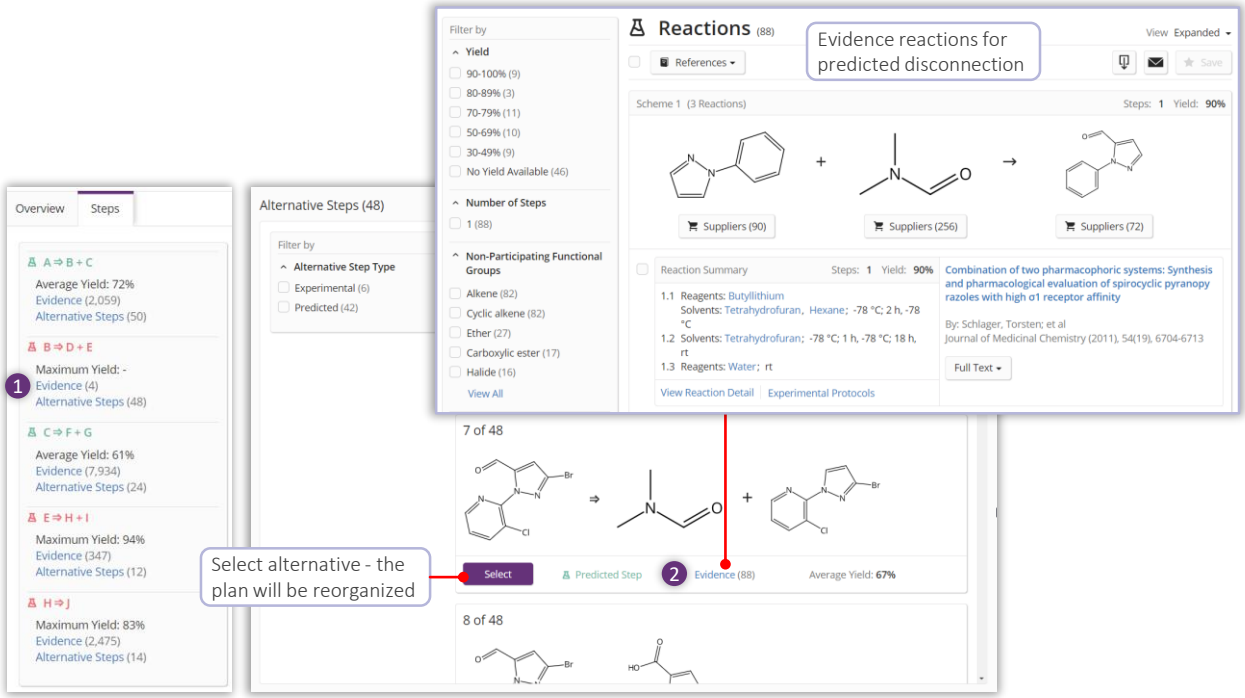
Alternative Steps and Plan Options

Alternative steps

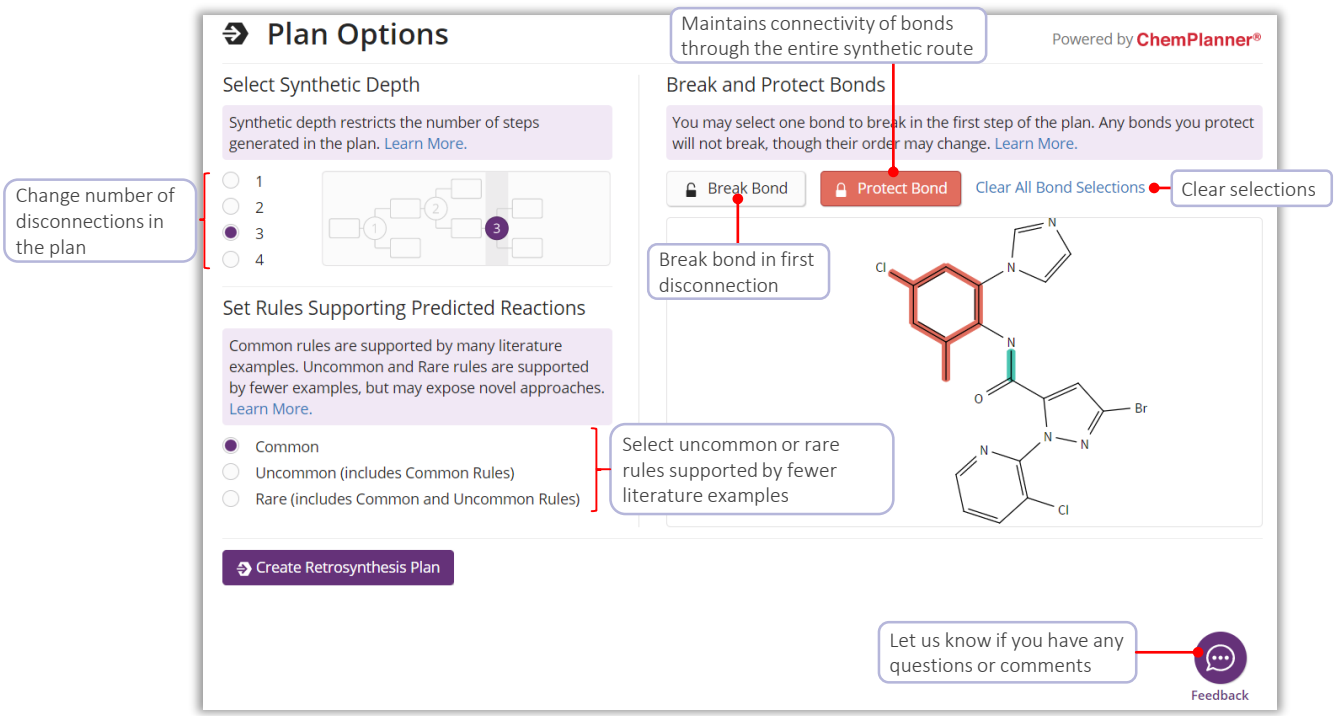
Provide an overview of all experimental and predicted disconnections
Evidence reactions are displayed as a reaction answer set
Access Evidence Reactions from the 1 link in the steps overview or
2 the alternative reaction scheme



Plan options

Edit plan options to...

- Change the synthetic depth
- Maintains connectivity of bonds through the entire synthetic route
- Define bonds to be broken in the first disconnection
- Create a plan with potentially more alternatives, e.g. for poly- or heterocyclic molecules



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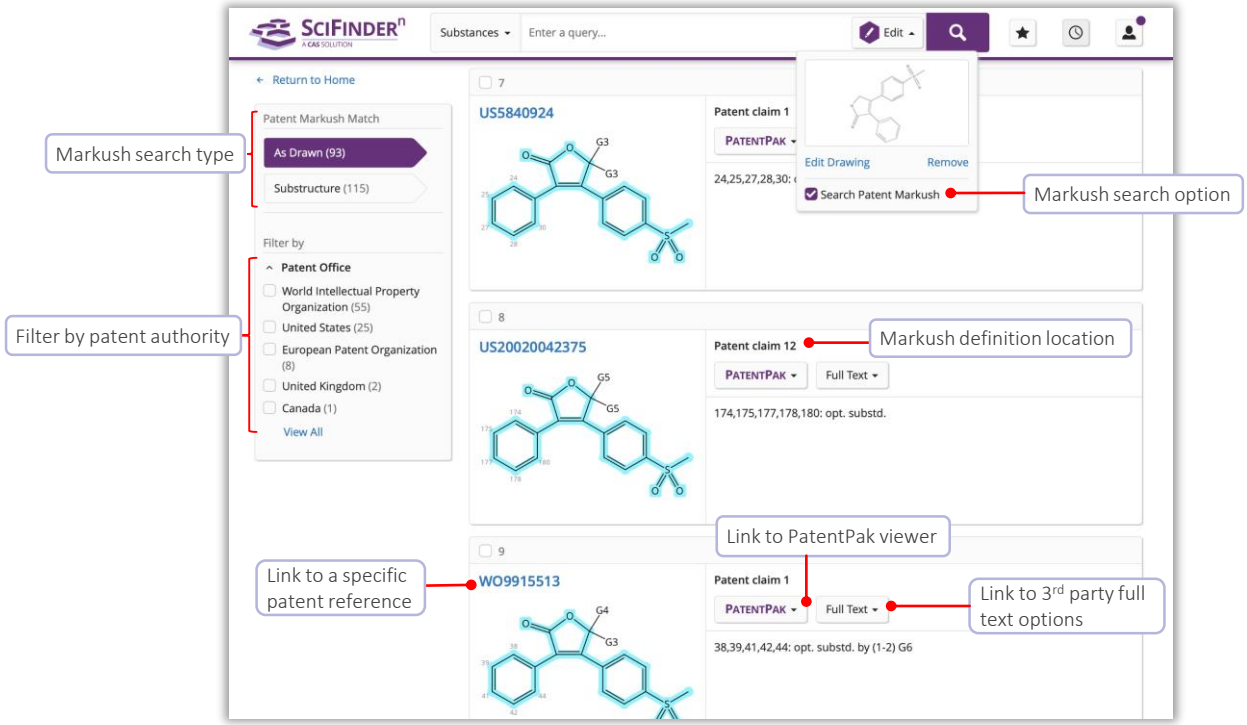
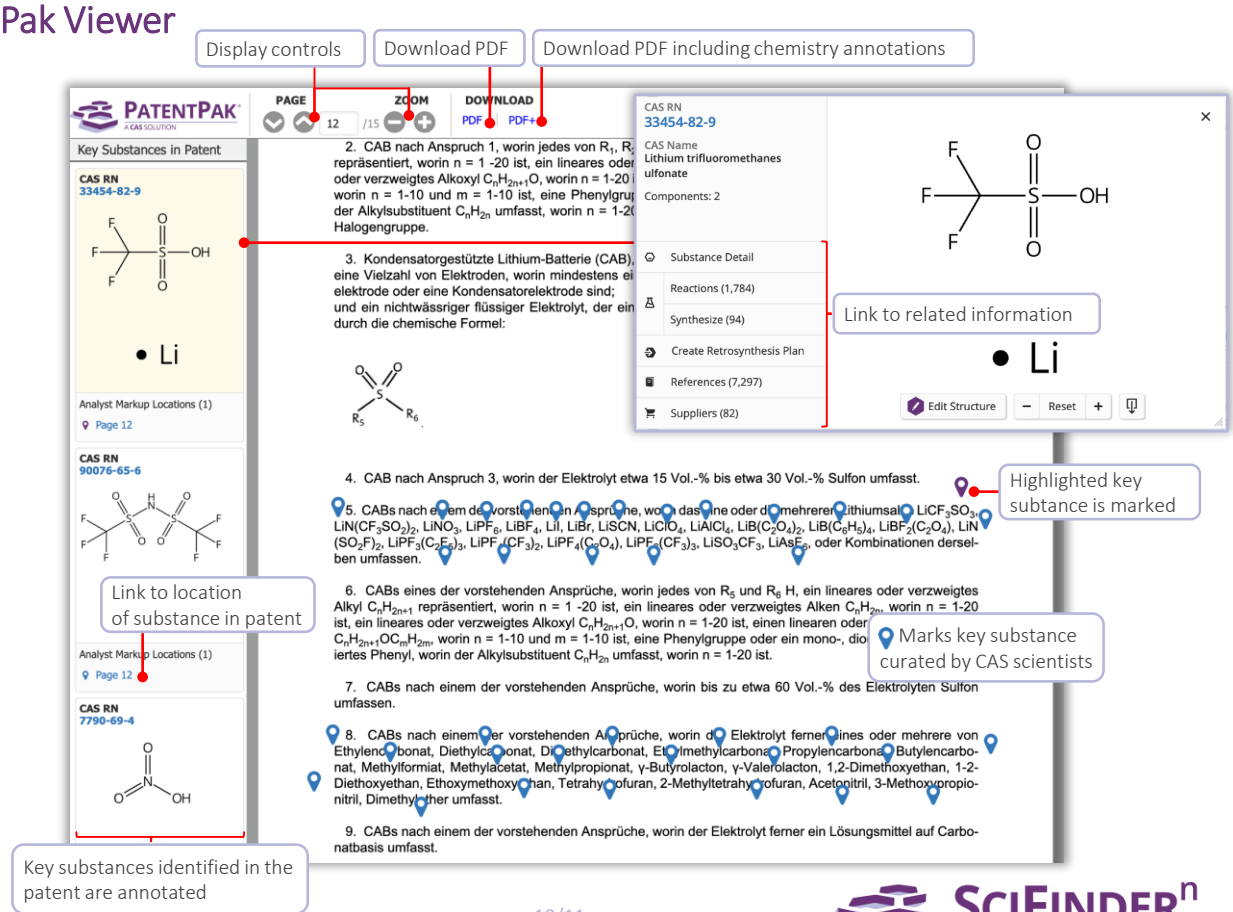
Markush Searching and PatentPak

Markush searching

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



PatentPak Viewer



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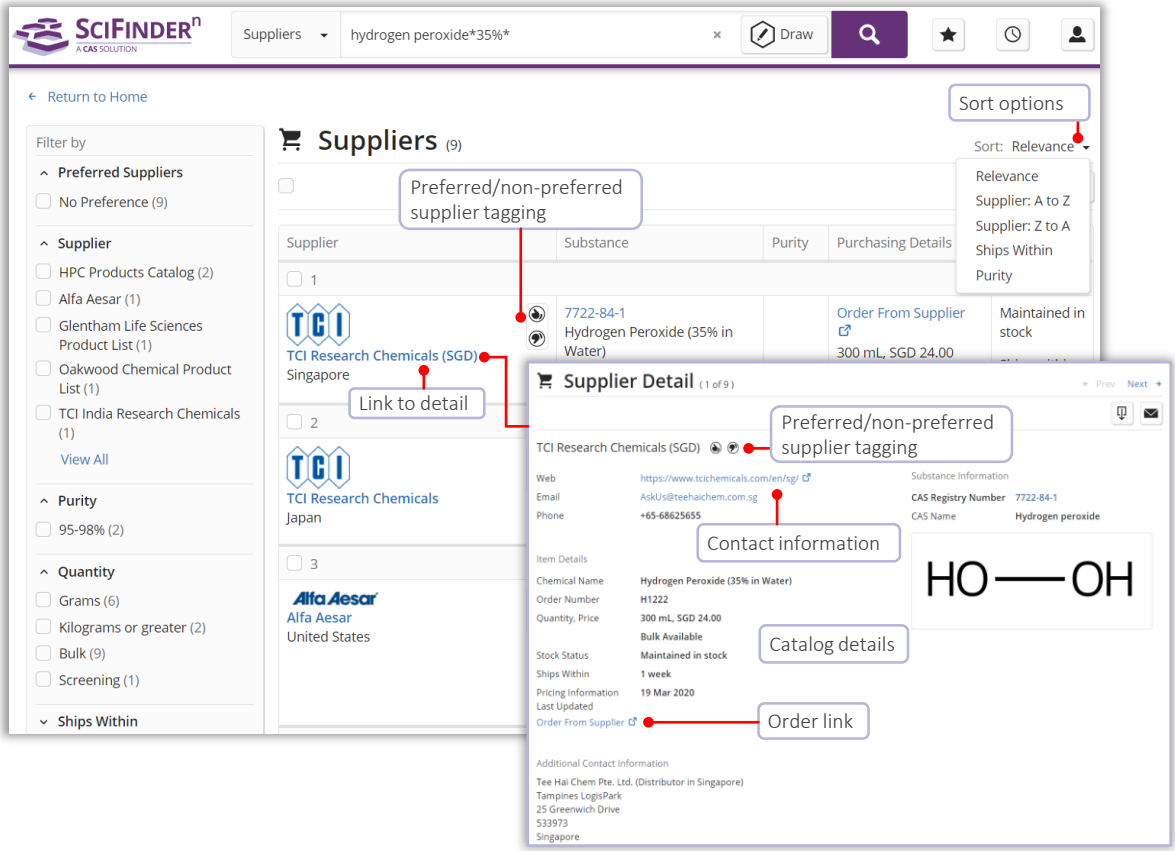
Suppliers Searching and ChemDoodle®

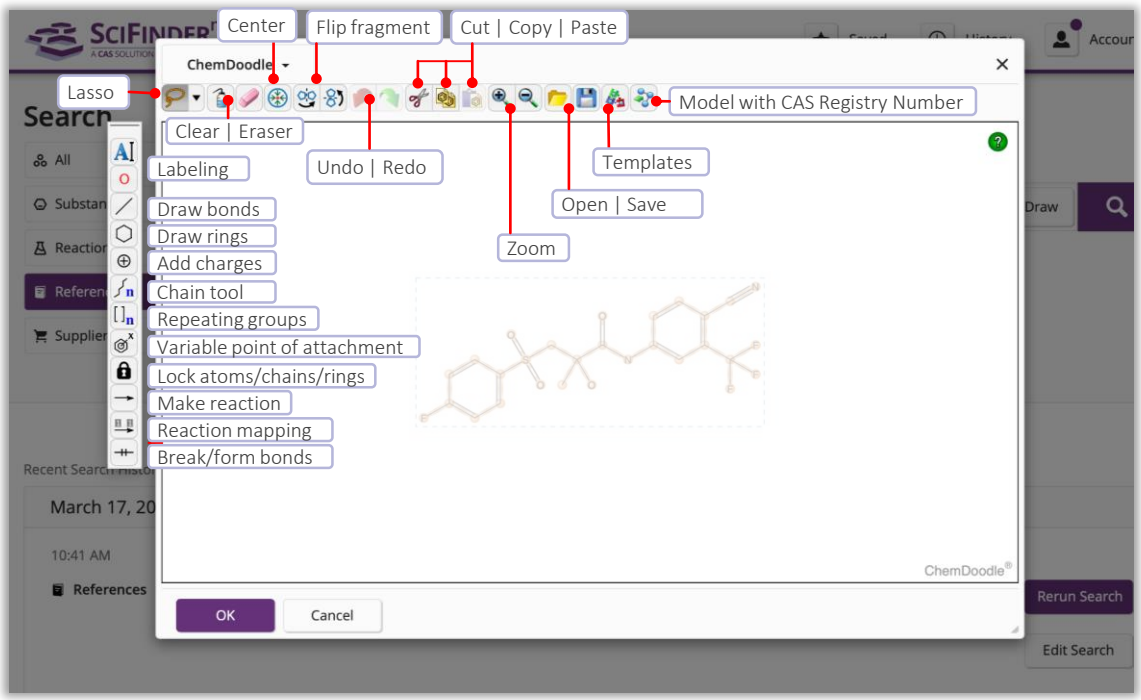
Suppliers searching

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.



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