

CAS SCIFINDER®

FOR ACADEMIA

# QUICK REFERENCE GUIDE

**CAS**



A division of the  
American Chemical Society

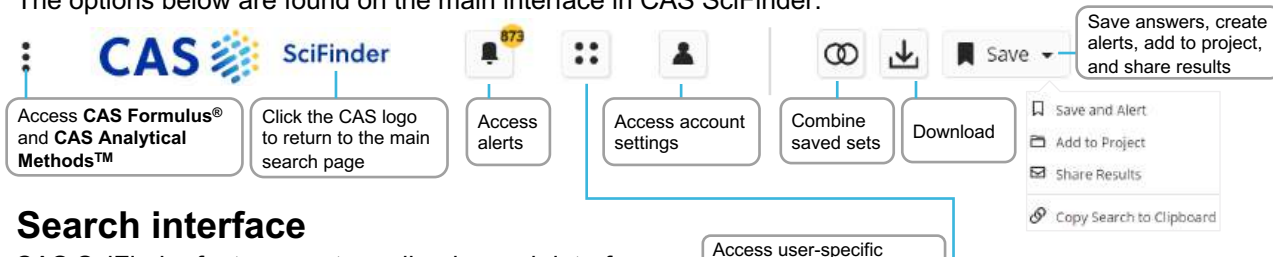
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# Solution interface and References search

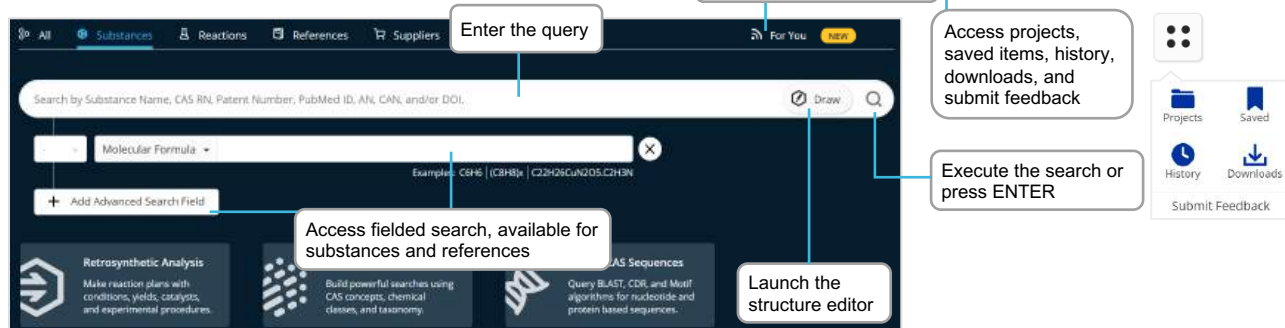
## Main interface

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



## Search interface

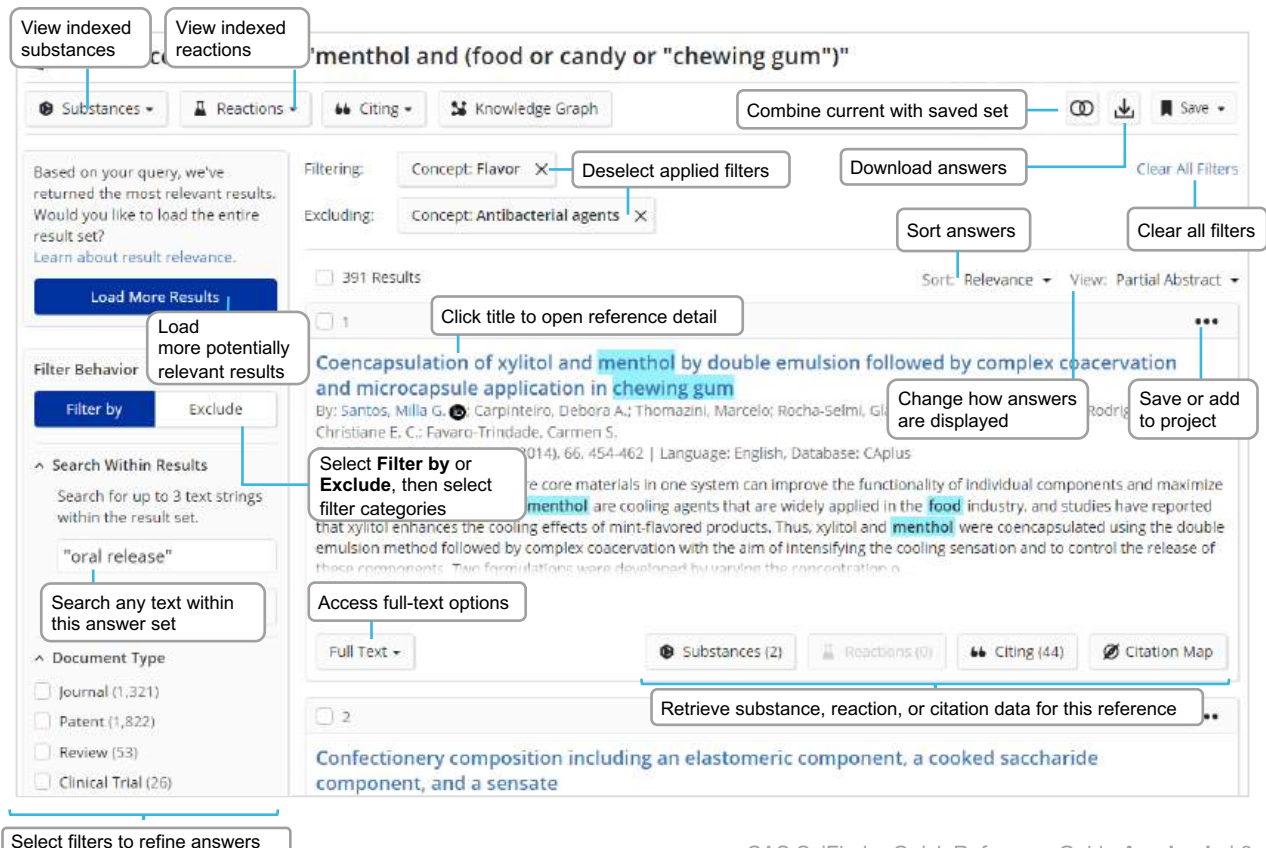
CAS SciFinder features a streamlined search interface.



## References search results

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.

### Fruit juice-containing **food** products with refreshing and cooling flavors

46 0 6 Citation Map View forward and backward citations Save

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder<sup>®</sup> users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®](#).

#### In this Reference

- IPC Data
- CAS Concepts
- Substances
- Formulations
- Cited Documents

By: Shimizu, Toru; Shigeta, Yoshinari; Kunieda, Satomi

A fruit juice-containing **food** product contains, in addition to a fruit component and a sweet base, (a) one or more refreshing substances selected from the group consisting of **menthol**, menthone, camphor, pulegol, isopulegol, pulegone, cineol, mint oil, peppermint oil, spearmint oil, eucalyptus oil, and fractions thereof, and (b) one or more cool-tasting substances selected from the group consisting of 3-(1-menthoxy)propane-1,2-diol, N-ethyl-p-menthane-3-carboxamide, 3-(1-menthoxy)-2-methylpropane-1,2-diol, p-menthane-3,8-diol, 2-(1-menthoxy)ethan-1-ol, 3-(1-menthoxy)propan-1-ol, 4-(1-menthoxy)butan-1-ol, cyclic carboxamides, acyclic carboxamides, N,2,3-trimethyl-2-iso-Pr butanamide, a menthoxy alkanol (alkyl group having 2-6 carbons), a menthoxy alkyl ether (alkyl group having 1-6 carbons), and a menthoxy alkanediol (alkyl group having 3-6 carbons). Thus, an orange juice beverage may contain **menthol** as the refreshing component and 3-(1-menthoxy)-1,2-propanediol as the cool-tasting component.

Table of contents provides a quick overview and navigation to content

Keywords: fruit juice flavor **food** beverage **menthol**

PatentPak Viewer Get Prior Art Analysis Full Text

View bibliographic details

Patent Number	Publication Date	Application Number	Application Date	Kind Code
WO2005048743	2005-06-02	WO2004-JP17524	2004-11-18	A1

Assignee	Source	Database Information	Language
Takasago International Corporation, Japan	World Intellectual Property Organization	AN: 2005:470226 CAN: 143:25602	English

#### Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2005048743	English	A1	PDF   PDF+   Viewer	2005-06-02	WO2004-JP17524	2004-11-18
JP2005143461	Undetermined	A				2003-11-19

PDF displays original patent PDF  
PDF+ displays the full text with a table of marked-up substances  
Viewer displays the interactive version of annotated full text

## Boolean operators

You can use logical operators to create precise text queries.

Use parentheses to group logical expressions, such as related terms using "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 in reference searching

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

The screenshot shows the top navigation bar with tabs for All, Substances, Reactions, References, and Suppliers. The search bar contains the text "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and "Enter chemical name query". Callouts include: "Click to draw new structure" pointing to the Edit icon; "Add Advanced Search Field" pointing to the plus icon; "Add advanced search fields" pointing to the "Add Advanced Search Field" button; "Click query structure to edit" pointing to the structure editor; "Check to perform Markush search" pointing to the "Search Patent Markush" checkbox; and "Click to draw new structure" pointing to the structure editor.

## Substances search results

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 structure images.

The screenshot shows the search results interface. Callouts include: "Select type of structure match" pointing to the "Structure Match" section; "Change sort criterion" pointing to the "Sort: Number of Suppliers" dropdown; "Change amount of details displayed" pointing to the "View: Partial" dropdown; "Click CAS Registry Number to open details" pointing to the CAS RN "80-08-0"; "Click on structure to open flyout window" pointing to the structure of Dapsone; "Retrieve data related to substance" pointing to the "Retrieve data related to substance" dropdown; "Search a (sub)structure within this set of substances" pointing to the "Search Within Results" section; "Reference Roles show which new information was reported about a substance in the literature" pointing to the "Reference Role" section; "Open editor with this structure" pointing to the "Edit Structure" button; and "Download .sdf or .mol. Copy Smiles to Clipboard" pointing to the download icon.

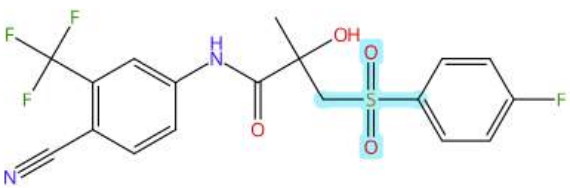
# Substance detail and structure editor

## Substance details

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 Registry Number: 90357-06-5

4,364 233 116



**C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>4</sub>S** — Molecular formula in hill order

Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[[4-fluorophenyl]sulfonyl]-2-hydroxy-2-methyl- (9CI, ACI) — Systematic name

GHS Hazard pictograms, full list in tab at bottom of page

Key Physical Properties	Value	Condition
Molecular Weight	430.38	-
Melting Point (Experimental)	190-195 °C (decomp)	-
Boiling Point (Predicted)	650.3±55.0 °C	Press: 760 Torr
Density (Predicted)		

Key properties

Other Names

Experimental Properties

Experimental Spectra

Properties and spectra are either listed or available in linked source publications

The chemical identifier list contains SMILES, InChI, systematic, trivial, and trade names. Names are extracted from analyzed publications

Canonical SMILES  
N#CC1=CC=C(C1C(F)(F)F)N(C(=O)C(O)C(C)S(=O)(=O)C2=CC=CC=C2)

InChI  
InChI=1S/C18H14F4N2O4S/c1-17(26,10-29(27,28)14-6-3-12(19)4-7-14)16(25)24-13-5-2-11(9-23)15(8-13)18(20,21)22/h2-8,26H,10H,14H,19,24,25

InChI Key  
LKIJPYSCBVHEWU-UHFFFAOYSA-N

5 Other Names for this Substance

N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[[4-fluorophenyl]sulfonyl]-2-hydroxy-2-methylpropanamide (ACI)  
Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[[4-fluorophenyl]sulfonyl]-2-hydroxy-2-methyl-, (±)- (ZCI)  
(±)-4'-Cyano-α,α,α-trifluoro-3-[[p-fluorophenyl]sulfonyl]-2-methyl-*m*-lactoluidide  
Bicalutamide

## CAS Draw editor

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

CAS Draw

Import and export structure files

Enter CAS Registry Number, SMILES, or InChI to create structure

Enter a CAS Registry Number, SMILES, or InChI...

Lasso | Marquee tool

Learn about keyboard shortcuts (e.g., drawing hetero atoms easily)

Hetero atom and H isotope selection

Draw atoms and bonds | Eraser

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Add attachment point to fragment | Select from templates

Add positive charge | Add negative charge

Repeating groups | Carbon chain tool

Define variable point of attachment at ring | Lock rings

Lock atoms | Rotate/Flip fragment

Reaction role | Atom mapping

Bond mapping | Draw reaction arrow

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw

OK Cancel

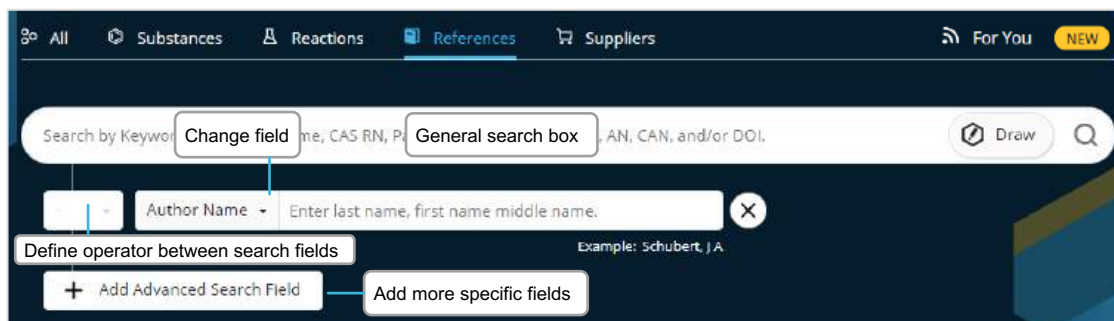
Zoom: 90%

# 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.

- 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, relating to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in an organism (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.

Reference Role

By Count | **Alphanumeric**

Example of 'reference roles' appearing in a substance answer set

Number of substance(s) in the answer set with that role

Role	Count
<input type="checkbox"/> Adverse Effect	15
<input type="checkbox"/> Agricultural Use	29
<input type="checkbox"/> Analyte	17
<input type="checkbox"/> Diagnostic Use	3
<input type="checkbox"/> Food or Feed Use	120
<input type="checkbox"/> Formation, Non-preparative	
<input type="checkbox"/> Pharmacological Activity	10
<input type="checkbox"/> Physical, Engineering, or Chemical Process	888

## Roles in reference results

Roles will appear as a filter in reference results 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.

Substances - Polypropylene

9003-07-0

(C3H6)x  
**Polypropylene**

321K References | 7,909 Reactions | 27 Suppliers

Filter Behavior: Filter by | Exclude

456,514 Results | Sort: Relevance | View: Full Abstract

1

**Microstructure of polypropylene**  
By: Busico, Vincenzo; Capullo, Roberto  
Progress in Polymer Science (2001), 26(3), 443-533 | Language: English, Database: CAlpha

A review, with 175 references, on catalyst technologies for manufacture of polypropylene with well-controlled microstructure and properties for advanced applications. The development of transition metal catalysts with tunable structure and selectivity is discussed. Polypropylene products with novel and well-controlled microstructure are described. The use of high-field <sup>13</sup>C NMR methods to study the stereochem. of polypropylene is also discussed.

Full Text | Substance (1) | Reactions (0) | Citing (385) | Citation Map

After clicking 'View All', more specific roles can be selected

Substance Role

By Count | **Alphanumeric**

1 Selected

<input type="checkbox"/> Uses (268K)	<input type="checkbox"/> Biological Use, Unclassified (3,793)
<input type="checkbox"/> Technical or Engineered Material Use (191K)	<input checked="" type="checkbox"/> <b>Pollutant (3,661)</b>
<input type="checkbox"/> Polymer in Formulation (81K)	<input type="checkbox"/> Biological Study, Unclassified (2,558)
<input type="checkbox"/> Properties (61K)	<input type="checkbox"/> Miscellaneous (2,444)
<input type="checkbox"/> Process (52K)	

Microplastics in marine environment review of methods for identification and quantification  
By: Pellegrini, Valerio; Gualini, Irene; Thompson, Richard C.; Thié, Henry  
Environmental Science & Technology (2012), 46(4), 3960-3975 | Language: English, Database: CAlpha and MEDLINE

This review of 68 studies compares the methodologies used for the identification and quantification of microplastics from the marine environment. Three main sampling strategies were identified: selective, coarse-meshed, and total sampling. About 6000 samples came from sandy beaches at the high tide line, and most seawater samples were taken at the sea surface using neuston nets. Four steps were distinguished during sample processing: digestion, filtration, sieving, and visual sorting of microplastics. Visual sorting was one of the most commonly used methods for the identification of microplastics (using type, shape, degradation stage, and color as criteria). Chem. and phys. characteristics (eg. specific IR) were also used. The most reliable method to identify the chem. composition of microplastics by IR spectroscopy. Most studies reported that plastic fragments were polyethylene and polypropylene polymers. Uses commonly used for abundance estimates are "items per m<sup>3</sup>" for sediment and sea surface studies and "items per m<sup>3</sup>" for water column studies. Mesh size of sieves and filters used during sampling in sample processing enhance abundance estimates. Most studies reported two main size ranges of microplastics: 6300 µm < size, which are retained by a 500 µm sieve, and 16-1300 µm, or fractions thereof that are retained on filters. We recommend that future programs of monitoring continue to distinguish these size fractions, but we suggest standardized sampling procedures which allow the spatiotemporal comparison of microplastic abundance across marine environments.

Full Text | Substance (3) | Reactions (0) | Citing (239) | Citation Map

Every publication in this set of 3,661 references discusses polypropylene in the context of a pollutant

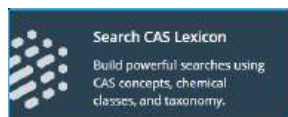
# CAS Lexicon

## CAS Lexicon overview

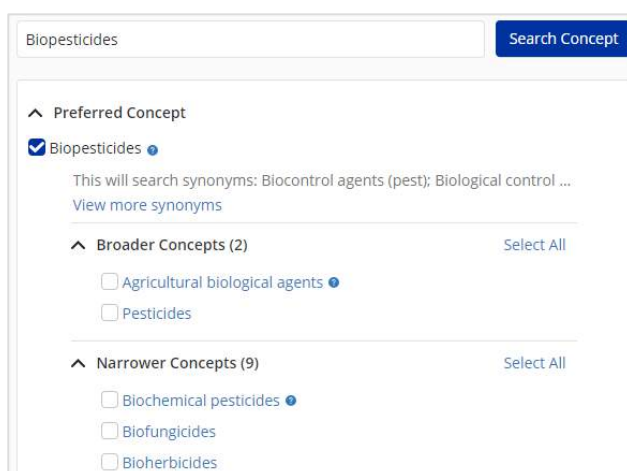
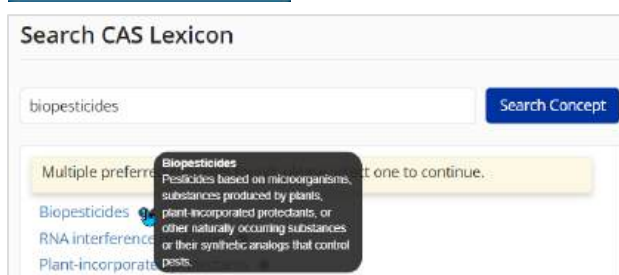
The CAS Lexicon is an ideal tool to understand CAS concept hierarchies, identify scientific expressions, gather relevant keyword synonyms for query building, or perform narrow and focused Lexicon searches.

The CAS Lexicon is an ontology of CAS Concepts. CAS Concepts are controlled terms describing the focus of a publication. They are added manually by CAS scientists, based on full-text analysis. The CAS Lexicon contains subject, chemical class, and taxonomic indexing terms in a hierarchy with broader and narrower terms. Concept indexing will be done on the highest level of detail possible, given the information present in the source document. Broader terms do not include more detailed concepts.

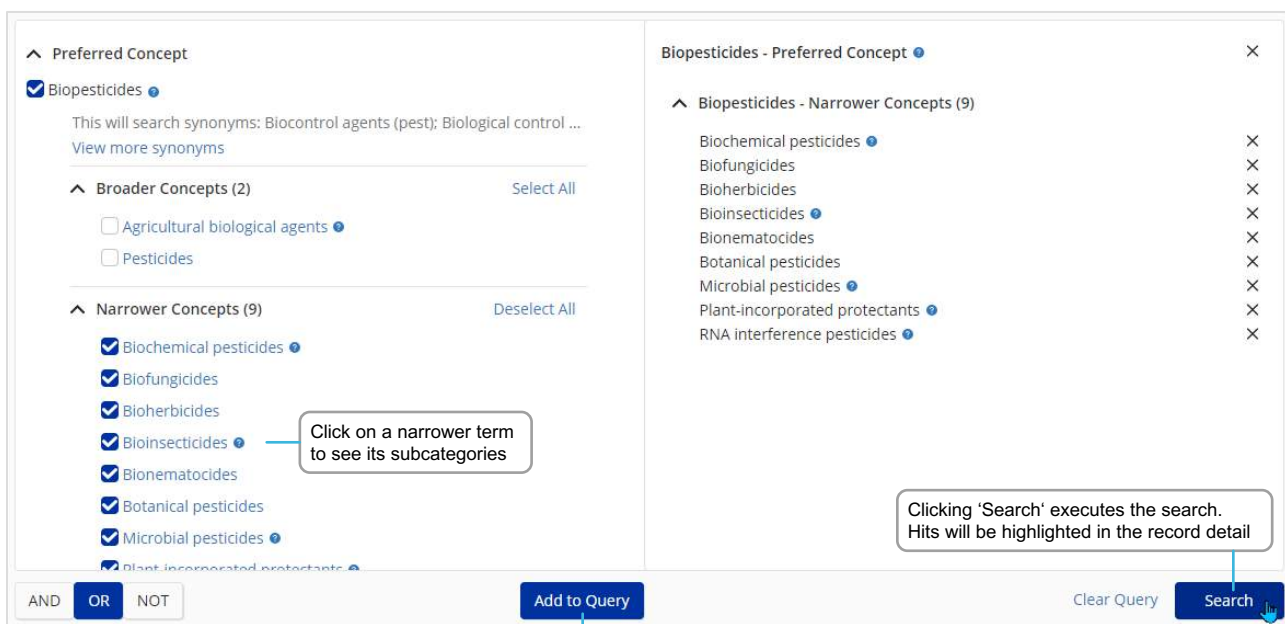
## Access and navigation



Start by clicking on 'CAS Lexicon' on the landing page, enter a concept or synonym and navigate through the hierarchy of broader and narrower terms. Only one hierarchy level is shown at a time.



Users can build highly specific CAS Lexicon search queries by selecting concepts and adding them to the query window on the right. Only the selected CAS Concepts will be searched.



Operators can be used to combine different concepts

Click 'Add to Query' to populate the pane on the right with selected terms

# Search CAS Sequences

## Search options

You can search sequences using three different modalities:

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

## BLAST similarity search

BLAST allows you 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.

To perform a BLAST search:

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



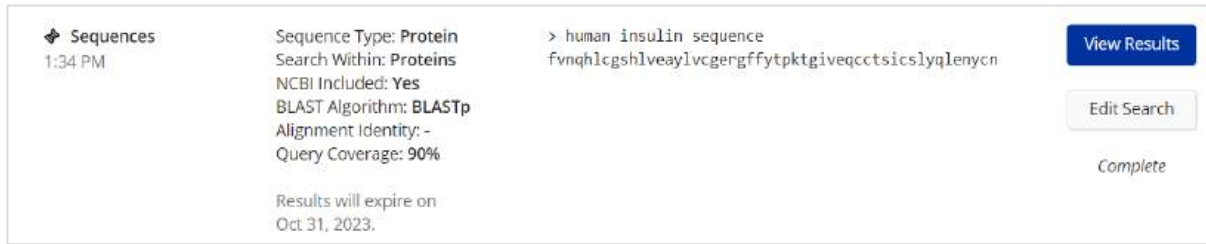
The screenshot shows the BLAST search interface with the following components and callouts:

- Sequence Search options:** A callout box pointing to the tabs for BLAST, CDR, and Motif.
- Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane:** A callout box pointing to the "Upload Sequence (.fasta or .txt)" button.
- Paste sequence into this window:** A callout box pointing to the text input area containing the sequence: `> human insulin sequence  
fvnqhlcghshlveaylvcgergffytptkgiveqcctscicslyqlenycn`
- Include NCBI sequences:** A callout box pointing to the "Include NCBI Sequences" checkbox, which is checked.
- Advanced BLAST parameters:** A callout box pointing to the "Advanced Sequence Search" section, which includes:
  - Alignment Identity %: -
  - Match with Gaps?:  Yes  No
  - Gap Costs: Existence 11 Extension 1
  - Query Coverage %: 90
  - Word Size: 3
  - Scoring Matrix: BLOSUM62
  - BLAST Algorithm: BLASTp
  - E-Value: 10
  - Exclude Low Complexity Regions:  Yes  No

# BLAST results analysis

## Access results

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



Sequences 1:34 PM

Sequence Type: Protein  
Search Within: Proteins  
NCBI Included: Yes  
BLAST Algorithm: BLASTp  
Alignment Identity: -  
Query Coverage: 90%


> human insulin sequence  
fvnqhlcgshlveaylvcgergffypktgiveqcctsiclslyqlenycn

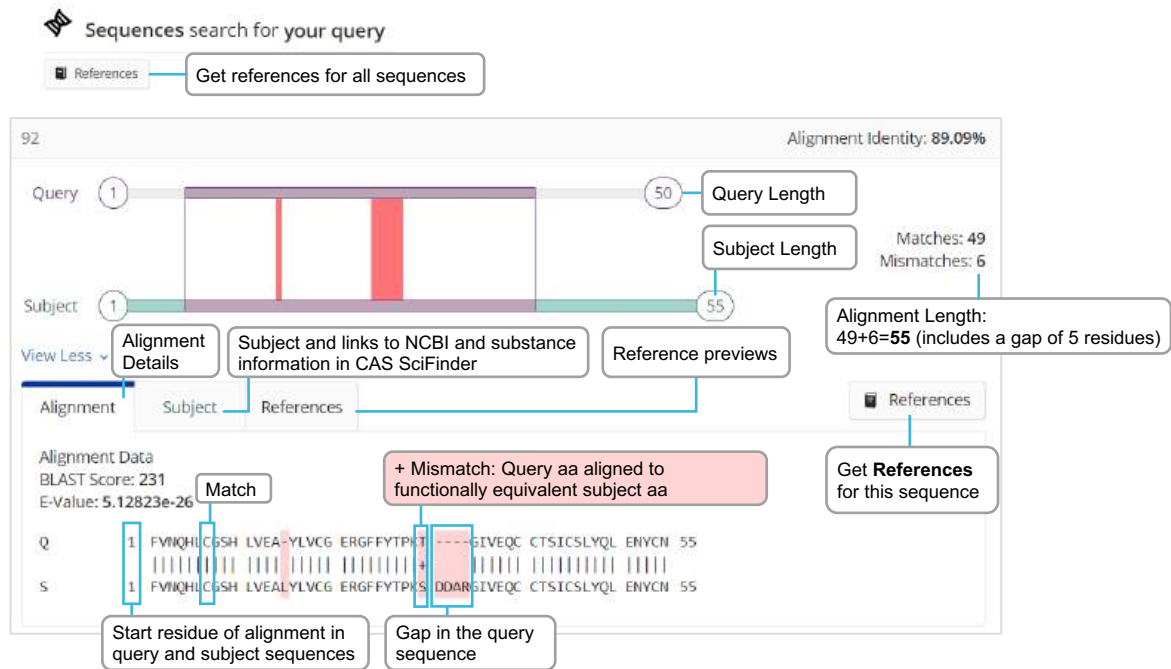
View Results  
Edit Search  
Complete

Results will expire on Oct 31, 2023.

## View results

When viewing 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 the 'Alignment' tab.
- Subject details and patent previews are available in separate tabs.
- Click  References to retrieve related references.
- XLSX result download  is available.



Sequences search for your query

References Get references for all sequences

92 Alignment Identity: 89.09%

Query 1 50 Query Length

Subject 1 55 Subject Length

Matches: 49  
Mismatches: 6

Alignment Length: 49+6=55 (includes a gap of 5 residues)

Alignment Details Subject and links to NCBI and substance information in CAS SciFinder Reference previews

Alignment Data  
BLAST Score: 231  
E-Value: 5.12823e-26

Match + Mismatch: Query aa aligned to functionally equivalent subject aa

Get References for this sequence

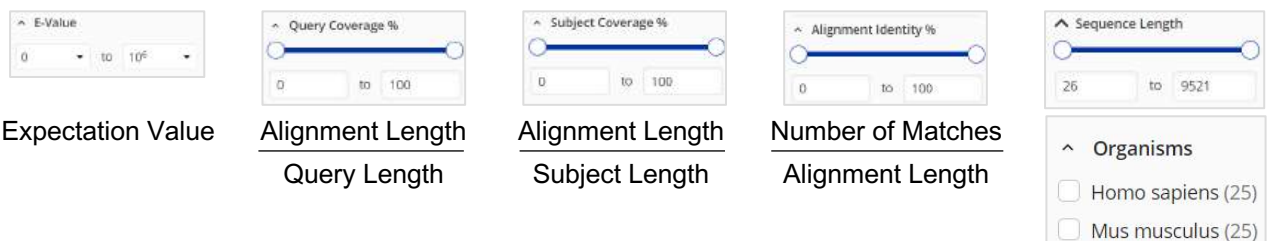
Start residue of alignment in query and subject sequences

Gap in the query sequence

Q 1 FVNQHLCGSHLVEA-YLVCG ERGFFYPTK T ----GIVEQC CTSICSLYQL ENYCN 55  
S 1 FVNQHLCGSHLVEALYLVCG ERGFFYPTK S DDARGIVEQC CTSICSLYQL ENYCN 55

## Filter results

Filtering dynamically changes your results.



E-Value 0 to 10<sup>6</sup>

Query Coverage % 0 to 100

Subject Coverage % 0 to 100

Alignment Identity % 0 to 100

Sequence Length 26 to 9521

Organisms  
 Homo sapiens (25)  
 Mus musculus (25)

Expectation Value

Alignment Length  
Query Length

Alignment Length  
Subject Length

Number of Matches  
Alignment Length

# Bioactivity data

## Searching for targets, ligands, and diseases

The advanced search fields in Substances and References search allow you to find targets, ligands, and diseases with the according bioactivity data. This will search for substance and/or literature within the CAS Life Sciences accordion.

The first screenshot shows the 'Substances' search page with a callout: 'Substances with bioactivity data are searched'. The second screenshot shows the 'References' search page with a callout: 'Literature with bioactivity data is searched'. The third screenshot shows the 'References' search page with a callout: 'Enter a target' and 'Select target, ligand, or disease (further bioactivity search field can be added and combined)'. The search field contains 'Renin receptor ATP6IP2'.

## Bioactivity data filter in reference and substance search

The left screenshot shows the 'Bioactivity Data' filter with a callout: 'Filter to refine by the availability of SAR, ADME, and Toxicity data'. The right screenshot shows the 'Bioactivity Data' filter with a callout: 'Filter to refine by the availability of SAR, ADME, and Toxicity data'. The filter options include Structure Activity Relationships (527), Absorption, Distribution, Metabolism, Excretion (110), and Toxicity (5).

## Bioactivity data in Substance details

The screenshot shows the 'Structure Activity Relationships' section with a callout: 'Filter functionality'. Below it is a table with columns: Target, Function, Parameter, Value, Disease, Organism, Assay, Source. The first row shows: Target: 17-beta-hydroxysteroid dehydrogenase type 2, Function: Inhibitor, Parameter: Activity, Value: 111 %, Disease: -, Organism: HOMO SAPIENS, Assay: View Detail, Source: (1) CAS. There are also buttons for 'Excel download', 'Clear All Filters', and 'Knowledge Graph'. Below the table are sections for 'Absorption, Distribution, Metabolism, and Excretion Data' and 'Toxicity'. A callout 'Shows full assay details' points to an 'Assay Data' pop-up window showing details for the target and assay.

## Bioactivity data in Reference details

The screenshot shows the 'Structure Activity Relationships' section with a callout: 'Shows full assay details'. Below it is a table with columns: Ligand, Target, Function, Parameter, Value, Disease, Organism, Assay. The first row shows: Ligand: 2460481-54-1, Target: Transforming growth factor-beta-induced protein ig-h3, Function: Binder, Parameter: Ka, Value: No interaction, Disease: Neoplasm, Organism: -, Assay: View Detail.

# Reactions search

## Performing a Reactions search

Reaction queries can be set up using CAS Reaction Numbers, substance names, CAS Registry Numbers, document identifiers, a chemical structure, or text-based reaction searching.

## Reactions search results

By default, reaction search results are grouped into schemes with identical reactants and products. A panel of filters, including yield and steps, allows for further refinement.

For single-step, single-stem reactions, you may view similar reactions based on the similarity 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 Azaindole-Pyrimidine Inhibitor of Influenza Virus Replication  
By: Liang, Jiang  
View All [View all authors](#)  
Organic Process Development (2016), 20(5), 955-969  
[View Source](#) [Full Text](#)

Company/Organization  
Vertex Pharmaceuticals Incorporated  
Boston, Massachusetts 02210  
United States

Suppliers (48) [Stage 2] Suppliers (149) Suppliers (2)

Stage	Reagents	Catalysts	Solvents	Conditions
1	<a href="#">Triethylamine</a> <a href="#">Diphenylphosphoryl azide</a>	-	<a href="#">Toluene</a>	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 \(1R,3S\)-3-\(\(benzyloxycarbonyl\)amino\)cyclohexanecarboxylate](#), Yield: 85%

**Reactants** [1-Ethyl \(1R,3S\)-1,3-cyclohexanedicarboxylate](#)  
[Benzyl alcohol](#)

**Reagents** [Triethylamine](#)  
[Diphenylphosphoryl azide](#)

**Solvents** [Toluene](#)

**Procedure** 1. Add diphenylphosphoryl azide (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 (1R,3S)-3-((benzyloxycarbonyl)amino)cyclohexanecarboxylate

**Proton NMR Spectrum** (300 MHz, CDCl<sub>3</sub>) δ: 7.48-7.30 (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]<sup>+</sup> calculated for C<sub>17</sub>H<sub>24</sub>NO<sub>4</sub> 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 '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.

The screenshot displays the CAS SciFinder interface. At the top, a navigation bar includes 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. A search bar is present with the text 'Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' Below the search bar are three main action buttons: 'Retrosynthetic Analysis', 'Search CAS Lexicon', and 'Search CAS Sequences'. The 'Retrosynthetic Analysis' button is highlighted with a blue '1' and a red arrow. Below this, the 'Retrosynthetic Analysis' window is open, showing a chemical structure of a complex molecule. The window includes a toolbar with icons for drawing and editing, a text input field for 'Enter a CAS Registry Number, SMILES, or INCHI', and a 'Start Retrosynthetic Analysis' button. The molecular formula is displayed as  $C_{17}H_{17}F_3N_5O_2S$  (355.34). To the right, a substance flyout window is open, showing the CAS RN '2408121-76-4' and the CAS Name '2-[Methoxy(5-[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-2-thienyl)methyl]-5-meth...'. A blue '2' and a red arrow point to the 'Start Retrosynthetic Analysis' option in the flyout window. The flyout window also includes options for 'Get Substance Details', 'Get Bioactivity Data', 'Get Reactions (1)', 'Synthesize (1)', 'Start Retrosynthetic Analysis', 'Get References (1)', and 'Get Suppliers (0)'. A chemical structure of the substance is shown in the flyout window, and there are 'Edit Structure', 'Reset', and download icons at the bottom.

# 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, e.g., poly or heterocyclic molecules.

Once you have selected the desired options, click the 'Create Retrosynthesis Plan' button.

**Retrosynthesis Plan Options for drawn structure** Powered by ChemPlanner®

**Select Synthetic Depth** Learn more.

1  
2  
3  
4

**Break and Protect Bonds** Learn more.

Break Bond Protect Bond Clear All Bond Selections

**Set Rules Supporting Predicted Reactions** Learn more.

Common  
Uncommon (includes Common Rules)  
Rare (includes Common and Uncommon Rules)

**Set Starting Materials Cost Limit** Learn more.

1000 USD/mol

Email me when my plan is complete

Create Retrosynthesis Plan

Change the number of disconnections in the plan

Break bond in first disconnection

Protect bond(s) in entire plan

Clear selections

Select uncommon or rare rules supported by fewer literature examples

First bond to be broken

Protected bonds

Change upper cost limit for starting materials (USD/mol or USD/g)

Generate plan

# 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 longer.

Retrosynthesis Plan for drawn structure

View plan information

Plan Information

Estimated Yield: 22%  
Overall Price: \$48.62  
(USD per 100 grams)

Scoring Profiles

Complexity Reduction

Convergence

Evidence

Cost

Yield

Atom Efficiency

Apply Reset Scoring

Experimental Steps

Predicted Steps

Edit Plan Options

Exclude steps or substances

Download, Share, and Save your plan

View plan steps

Show experimental steps

Switch predicted steps on/off

Adjust scoring options

Blue lines mark experimental steps

Green dotted lines indicate predicted steps

Review and select alternative disconnections

Powered by ChemPlanner®

## 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.

Step Evidence

A → B + C 1,1 Reagents: Butyllithium  
Average Yield: 47%  
Evidence (16)  
Alternative Steps

B → D + E 1,1 Reagents: Potassium *tert*-butoxide  
Solvents: Tetrahydrofuran  
Average Yield: 59%  
Evidence (22)  
Alternative Steps (34)  
[Experimental Protocols](#) 1

C → F + G 1,1 Reagents: Diisopropylethylamine  
Ammonium chloride  
*D*-(7-Azabenzotriazol-1-yl)-*N,N,N,N*-tetramethyluronium hexafluoro phosphate  
Solvents: Dimethylformamide; 2 d, rt  
Average Yield: 50%  
Evidence (38)  
Alternative Steps (48)  
[Experimental Protocols](#)

D → H + I Predicted Step Only  
No reaction summary  
Maximum Yield: 79%  
Evidence (1)  
Alternative Steps (11)  
[Experimental Protocols](#)

E → J 1,1 Solvents: Carbon tetrachloride  
Maximum Yield: 83%  
Evidence (1)  
Alternative Steps (14)

Filter by

Alternative Step Type

Predicted (48)

Stereochemistry

Non-Selective (48)

5 of 15

[Select](#) [View 8 similar Alternatives](#) [View Evidence](#) 2

Average Yield: 63%

Grouped similar reactions

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (2)

80-89% (3)

70-79% (10)

50-69% (15)

30-49% (2)

View All

Number of Steps

1 (55)

Non-Participating Functional Groups

55 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1

Suppliers (49) Suppliers (51) Suppliers (61)

31-614-CAS-29434160 Steps: 1

Preparation of piperidine-containing compounds for treating and preventing metabolic and cerebrovascular diseases

By: Rodriguez, Martha E., et al  
World Intellectual Property Organization,  
WO201008964 A1 2010-07-15

PatentPak Full Text

Evidence reactions for (predicted) disconnection of precursor C

# 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.

## 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.

The screenshot shows a 'Plan Information' section with 'Estimated Yield: 78%' and 'Overall Price: \$188.28 (USD per 100 grams)'. Below is the 'Scoring Profiles' section with sliders for Complexity Reduction, Convergence (set to Medium), Evidence, Cost, Yield, and Atom Efficiency. At the bottom are 'Apply' and 'Reset Scoring' buttons. The 'Apply' button is highlighted with a green border.

### 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.

A close-up of the 'Apply' and 'Reset Scoring' buttons. The 'Apply' button is highlighted with a green border.

# Markush search and CAS PatentPak

## Markush search

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

Patent Markush search for drawn structure

96 Results

As Drawn (96)

Substructure (119)

Filter Behavior

Filter by Exclude

Patent Office

- World Intellectual Property Organization (55)
- United States (25)
- European Patent Organization (5)
- China (3)
- United Kingdom (2)

View All

Markush search option

Markush structure search type

Assembled Markush hit structure

Filter by patent authority

Markush location

Link to a specific patent reference

Link to CAS PatentPak Viewer

## 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)

Download PDF including list of marked-up substances and annotations

Download PDF

Link to location of substance in patent

Highlighted key substance is marked

Link to related information

Marks key substance curated by CAS scientists

Key substances identified in the patent are annotated

# Suppliers search and ChemDoodle

## Suppliers search

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

The screenshot shows a search results page for the CAS number "7664-93-9". The interface includes a filter sidebar on the left, a main results table, and a detailed product list for the first result.

**Filter Behavior:** Filter by (selected), Exclude. Preferred Suppliers: Preferred (52), No Preference (438). Supplier: Hayashi Pure Chemical Products Catalog (106), Thermo Fisher Scientific Product List (66), KANTO CHEMICAL (43), Aladdin Scientific Product Listing (37), FUJIFILM Wako Chemicals Europe GmbH Product List (37). Purity: ≥99% (8), 95-98% (132), 90-94% (9), <90% (14).

**Search Results Table:**

Supplier	Substance	Purity	Purchasing Det
1. Oakwood Chemical Product List United States Last Updated: 1 Mar 2024	7664-93-9 Sulfuric Acid, ACS Grade	95-98%	Order From Sup 100 ml, USD 25.00 1 L, USD 40.00 2.5 L, USD 80.00
2. Oakwood Chemical Product List United States Last Updated: 1 Mar 2024			
3. Oakwood Chemical Product List United States Last Updated: 1 Mar 2024			

**Oakwood Chemical Product List Details:**

- Preferred Supplier:
- Web: <https://www.oakwoodchemical.com>
- Email: [sales@oakwoodchemical.com](mailto:sales@oakwoodchemical.com)
- Phone: 1-800-467-3386
- Item Details: Chemical Name: Sulfuric Acid, ACS Grade; Order Number: 25494; Purity: 98%; Quantity, Price: 100 ml, USD 25.00; 1 L, USD 40.00; 2.5 L, USD 80.00; Bulk Available; Stock Status: Maintained in stock; Pricing Information Last Updated: 1 Mar 2024; Order from Supplier
- Substance Information: CAS Registry Number: 7664-93-9; CAS Name: Sulfuric acid
- Chemical Structure:

## ChemDoodle

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

The screenshot shows the ChemDoodle software interface with a toolbar and a chemical structure being edited. The toolbar includes various tools for drawing and editing molecules.

**Toolbar Tools:** Select, Center, Flip fragment, Cut | Copy | Paste, Clear | Eraser, Labeling, Draw bonds, Draw rings, Add charges, Chain tool, Repeating groups, Variable point of attachment, Lock atoms/chains/rings, Add attachment point to fragment, Make reaction, Reaction mapping, Break/form bonds, Undo | Redo, Templates, Open | Save, Zoom, Model with CAS Registry Number.

**Chemical Structure:** A complex organic molecule is shown in the center of the workspace, consisting of a benzene ring with various substituents, including a carbonyl group and a hydroxyl group.

# 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 is how it works:

- 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.

The screenshot displays the SciFinder interface. The top section shows a patent reference detail page for 'Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)'. It includes a citation map, a list of references, and a 'Get Prior Art Analysis' button. A callout box points to this button with the text 'Initiate the analysis from the detailed record view'. Below this, a search history entry is shown, listing the same patent title and a 'View Results' button. A callout box at the bottom right of the search history entry says 'View Results from the search history'.

## Login, feedback, training, and support

### Login details

Log in at [scifinder-n.cas.org](https://scifinder-n.cas.org)

Use your existing CAS SciFinder username and password.

### Feedback button

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

### Training

Upcoming events and webinars:

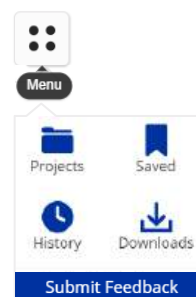
[www.cas.org/cas-webinars](https://www.cas.org/cas-webinars)

Recorded events and webinars:

[www.cas.org/cas-past-webinars](https://www.cas.org/cas-past-webinars)

CAS SciFinder training topics:

[www.cas.org/support/training/scifinder-n](https://www.cas.org/support/training/scifinder-n)



### Support contact

Email [help@cas.org](mailto: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>

CAS connects the world's scientific knowledge to accelerate breakthroughs that improve lives. We empower global innovators to efficiently navigate today's complex data landscape and make confident decisions in each phase of the innovation journey. As a specialist in scientific knowledge management, our team builds the largest authoritative collection of human-curated scientific data in the world and provides essential information solutions, services, and expertise. Scientists, patent professionals, and business leaders across industries rely on CAS to help them uncover opportunities, mitigate risks, and unlock shared knowledge so they can get from inspiration to innovation faster. CAS is a division of the American Chemical Society.

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SCIACDENREF101245240414 - A4

