

CAS SCIFINDER®

QUICK REFERENCE GUIDE

CAS



A Division of the
American Chemical Society

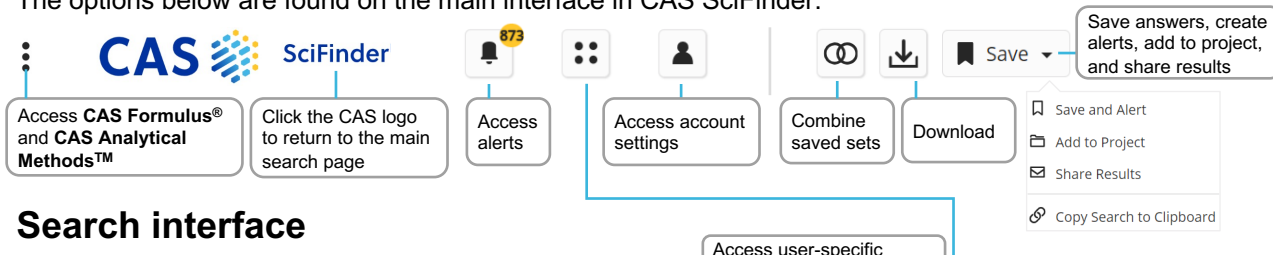
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Solution interface and References search

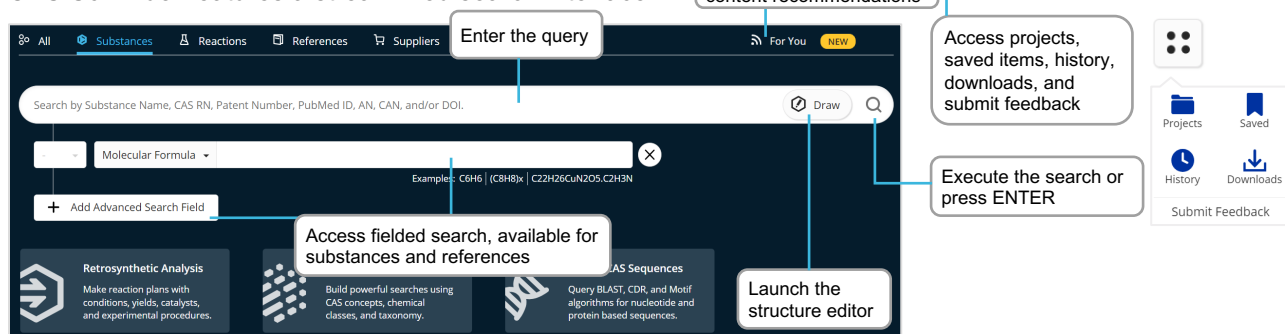
Main interface

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



Search interface

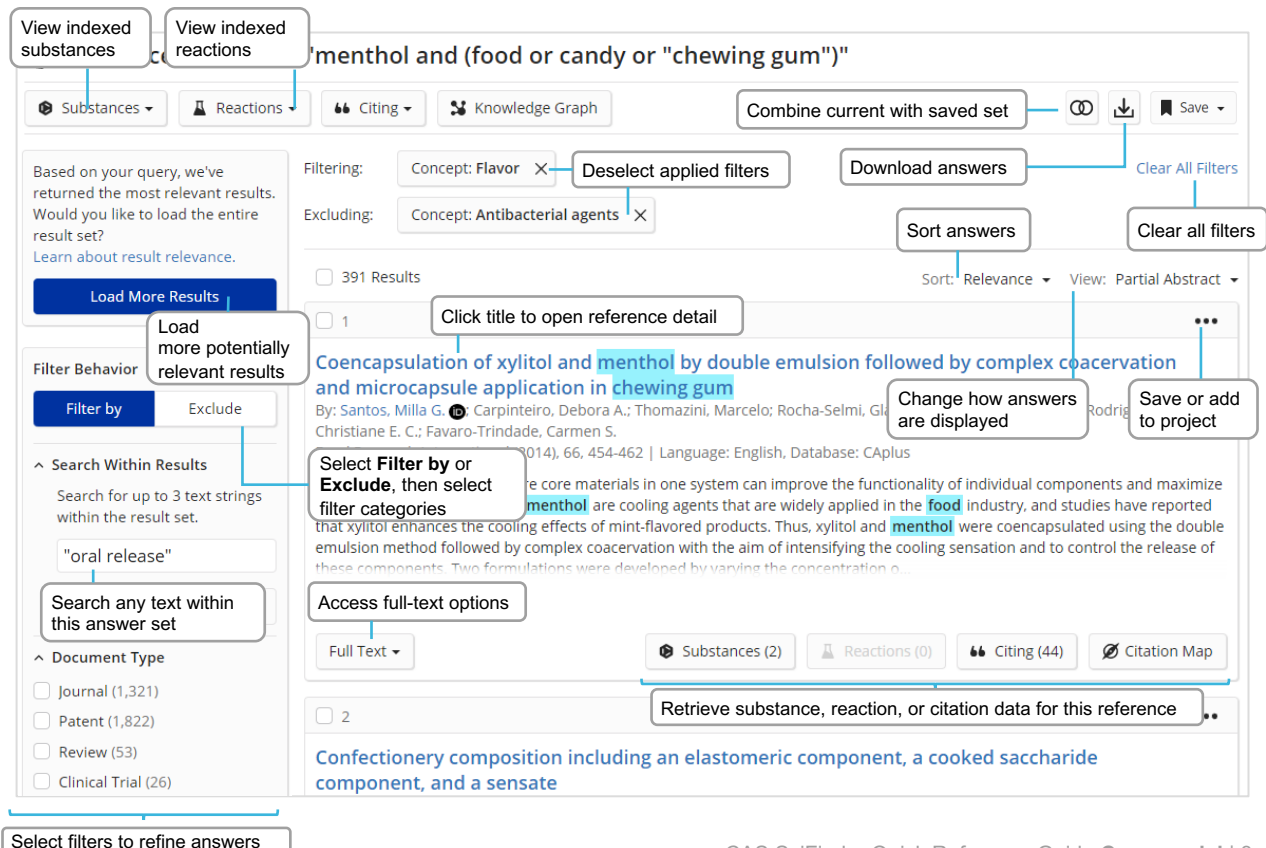
CAS SciFinder features a streamlined search interface.



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[®] users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®](#).

In this Reference

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

- [IPC Data](#)
- [CAS Concepts](#)
- [Substances](#)
- [Formulations](#)
- [Cited Documents](#)

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-(l-menthoxy)propane-1,2-diol, N-ethyl-p-menthane-3-carboxamide, 3-(l-menthoxy)-2-methylpropane-1,2-diol, p-menthane-3,8-diol, 2-(l-menthoxy)ethan-1-ol, 3-(l-menthoxy)propan-1-ol, 4-(l-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

Patent family and priority application information

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 "Enter chemical name query". Below the search bar are several search options: "Add Advanced Search Field", "Add advanced search fields" (with a sub-option for "Retrosynthetic Analysis"), "Search CAS Lexicon", "Search CAS Sequences", and "Search Patent Markush". A "Click to draw new structure" button is located in the top right corner. A chemical structure editor is visible, showing a simple structure with a central sulfur atom bonded to two oxygen atoms. A "Click query structure to edit" button is positioned above the editor. A "Check to perform Markush search" checkbox is located at the bottom right of the search options area.

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 displays the search results interface. On the left, there are filters for "Structure Match" (As Drawn (117), Substructure (6.2M), Similarity (1,052)), "Analyze Structure Precision", "Chemscape Analysis", and "Filter Behavior". The main results area shows a list of substances with their CAS RNs and chemical structures. Callouts point to various features: "Select type of structure match", "Change sort criterion" (Sort: Number of Suppliers), "Change amount of details displayed", "Click CAS Registry Number to open details", "Click on structure to open flyout window", "Search a (sub)structure within this set of substances", "Retrieve data related to substance", "Open editor with this structure", and "Download .sdf or .mol. Copy Smiles to Clipboard". A detailed view of a substance is shown on the right, including its CAS RN (149104-88-1), CAS Name ([4-(Methylsulfonyl)phenyl]boronic acid), and a chemical structure. A "Reference Role" section is also visible, showing "Preparation (3.1M)" and "Synthetic Preparation (3M)".

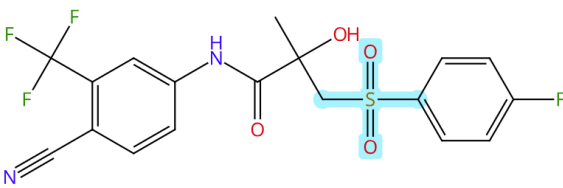
Substance detail and structure editor

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



Molecular formula in hill order: C₁₈H₁₄F₄N₂O₄S

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

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)		

Other Names

- Experimental Properties
- Experimental Spectra

Key properties

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

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

Canonical SMILES: N#CC1=CC=C(C=C1C(F)(F)F)NC(=O)C(O)C(C)S(=O)(=O)C2=CC=C(F)C=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,10H2,1H3,(H,24,25)

InChI Key: LKJPYSCBVHEWU-UHFFFAOYSA-N

9 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-lactotoluidide
- 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: Selects. Ctrl-click to select or deselect individual objects.

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

Zoom: 90%

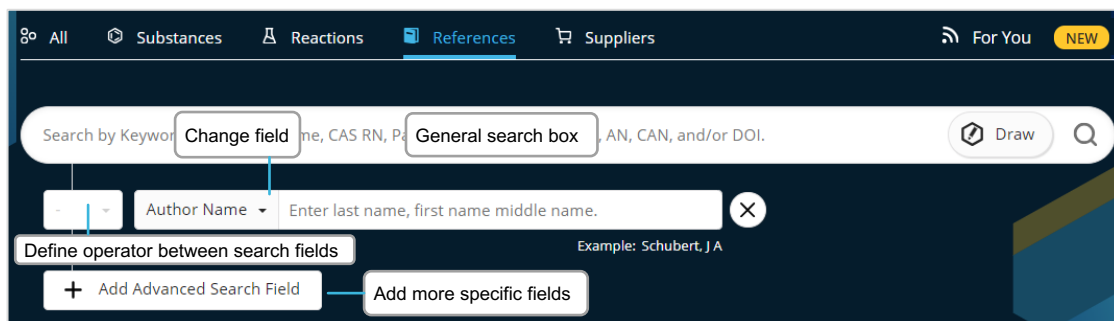
OK Cancel

Advanced Search

Performing an Advanced Search

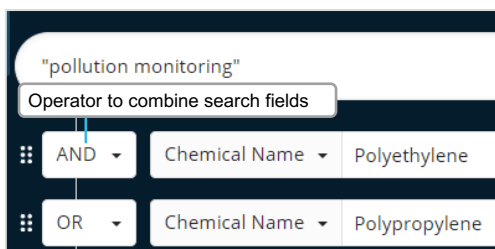
You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinder.

- 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)



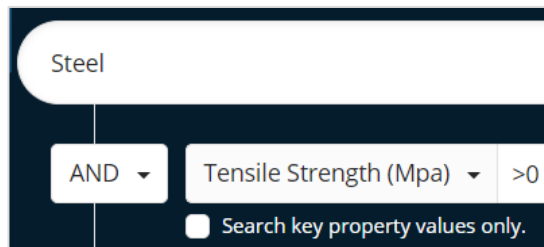
Advanced Search examples

Advanced References Search

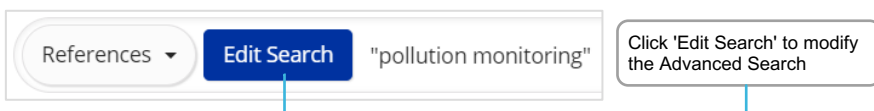


Query interpretation:
"pollution monitoring" and (polyethylene or polypropylene)

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
Adverse Effect	15
Agricultural Use	29
Analyte	17
Diagnostic Use	3
Food or Feed Use	120
Formation, Non-preparative	
Pharmacological Activity	10
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

Search Within Results

Document Type

Substance Role

- Uses (268K)
- Properties (61K)
- Process (52K)
- Biological Study (23K)
- Preparation (19K)

View All

Language

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

1

Microstructure of polypropylene

By: Busico, Vincenzo; Cipullo, Roberto
Progress in Polymer Science (2001), 26(3), 443-533 | Language: English, Database: CPlus

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 ¹³C 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

- Uses (268K)
- Technical or Engineered Material Use (191K)
- Polymer in Formulation (81K)
- Properties (61K)
- Process (52K)
- Biological Use, Unclassified (3,793)
- Pollutant (3,661)**
- Biological Study, Unclassified (2,558)
- Miscellaneous (2,444)

View All

Publication Year

1974 to 2023

Microplastics in marine environment review of methods for identification and quantification

By: Hidalgo-Ruz, Valeria; Gutwirth, Lars; Thompson, Richard C.; The, Martin
Environmental Science & Technology (2012), 46(6), 3060-3075 | Language: English, Database: CPlus 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, volume-reduced, and bulk sampling. Most sediment 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: separation, 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 (e.g. specific ft.) were also used. The most reliable method to identify the chem. composition of microplastics is by IR spectroscopy. Most studies reported that plastic fragments were polyethylene and polypropylene polymers. Units commonly used for abundance estimates are "items per m³" for sediment and sea surface studies and "items per m³" for water column studies. Mesh size of sieves and filters used during sampling or sample processing influence abundance estimates. Most studies reported two main size ranges of microplastics: (i) 500 µm $$mm, which are retained by a 500 µm sieve/net, and (ii) 1-500 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 - Substances (3) | Reactions (0) | Citing (2,289) | Citation Map

9003-53-6

Substances

Substances (3)

CAS RN | Chemical Name | Role

9003-53-6
PP/PL
Polypropylene

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

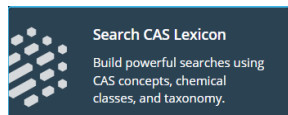
CAS Lexicon

CAS Lexicon overview

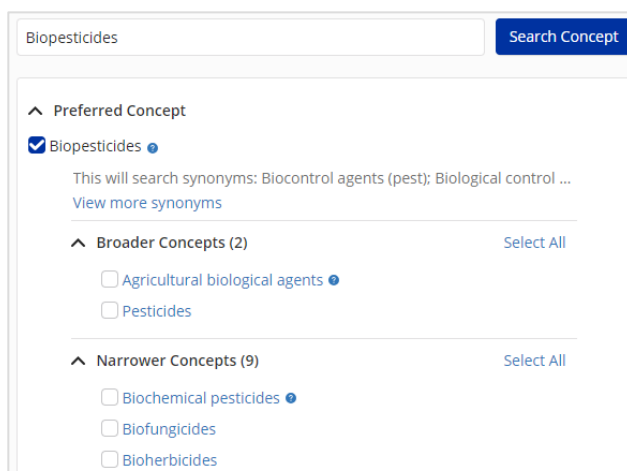
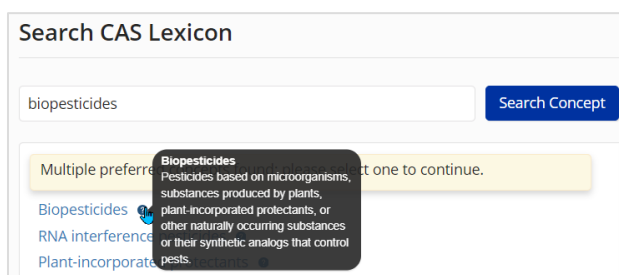
The CAS Lexicon is an ideal tool to understand CAS concept hierarchies, identify scientific expressions, gather relevant keyword synonyms for query building, or perform narrow and focused Lexicon searches.

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.

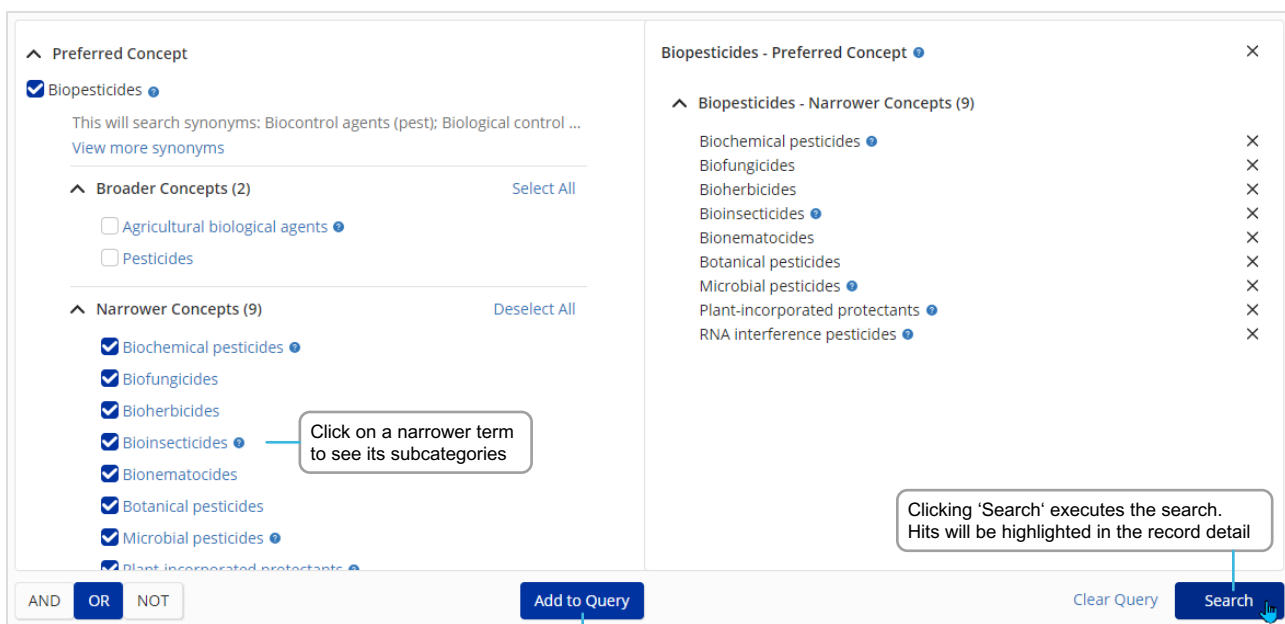
Access and navigation



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

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.

Select reactions

Good Afternoon, Ilja

All Substances Reactions References Suppliers

Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.

Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Search CAS Lexicon
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Click on reaction query to edit
algorithms for nucleotide and protein based sequences.

Edit Drawing Remove

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.

Reactions search for drawn structure

Change grouping to 'By Document' or 'By Transformation'

References

View by structure match

Structure Match

As Drawn (0)

Substructure (20K)

Similarity (18)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (428)

80-89% (263)

70-79% (295)

50-69% (379)

30-49% (207)

View All

Number of Steps

1 (2,455)

20,459 Results

Click on structure to view substance information

Group: By Scheme Sort: Yield View: Expanded

Save, alert, and share options

Send to CAS Draw

Yield for displayed reactions

Steps: 1 Yield: 100%

Absolute stereochemistry shown, Rotation (+)

Suppliers (48) View suppliers

Suppliers (484)

Filter reaction results

View reaction details

View reaction reference

Access annotated patent full text

Get similar reactions

Get Similar Reactions

Set Reaction Similarity

Broad (107,942) Reaction centers only

Medium (21,764) Reaction centers plus adjacent atoms and bonds

Narrow (4,822) Reaction centers plus extended atoms and bonds

Get Reactions Cancel

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 authors](#)

View All [View Source](#) [Full Text](#)

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

Reaction

Absolute stereochemistry shown, Rotation (+) [Stage 2] Absolute stereochemistry shown, Rotation (-)
Suppliers (48) Suppliers (149) Suppliers (2)

Step 1

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

[View alternatives](#) [Alternative Steps \(5\)](#)

Experimental Protocols

Synthetic Methods [View detailed procedures](#)

Products [Ethyl \(1R,3S\)-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 ₃) 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] ⁺ calculated for C ₁₇ H ₂₄ NO ₄ 306.1700, found 306.1700
State	sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations [Overview of transformations](#)
1. Schmidt Reaction

Reaction Notes [Further important notes](#)
scalable

Retrosynthesis planner

Launching the tool

There are two primary ways to launch the '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, a text input field for 'Enter a CAS Registry Number, SMILES, or InChI', and a 'Start Retrosynthetic Analysis' button. To the right, a substance flyout window is open for CAS RN 2408121-76-4, displaying the CAS Name and a list of actions: 'Get Substance Details', 'Get Bioactivity Data', 'Get Reactions (1)', 'Synthesize (1)', 'Start Retrosynthetic Analysis', 'Get References (1)', and 'Get Suppliers (0)'. The 'Synthesize (1)' button is highlighted with a blue '2' and a red arrow. The chemical structure is shown in a 3D ball-and-stick model.

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.](#)

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

Chemical Structure: Cc1ccc(NC(=O)C2=CC=CC=C2)cc1 (with callouts: **First bond to be broken** and **Protected bonds**)

Callouts:

- 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
- Change upper cost limit for starting materials (USD/mol or USD/g)
- First bond to be broken
- Protected bonds
- 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 Excluded Options

View plan steps

Show experimental steps

Switch predicted steps on/off

Blue lines mark experimental steps

Green dotted lines indicate predicted steps

Adjust scoring options

Review and select alternative disconnections

Powered by ChemPlanner*

Feedback

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
View All
Average Yield: 59%
Evidence (23)
Alternative Steps (34)
[Experimental Protocols](#) 1

C → F + G 1.1 Reagents: Diisopropylethylamine
Ammonium chloride
O-(7-Azabenzotriazol-1-yl)-N,N,N,N-tetramethyluronium hexafluoro phosphate
Solvents: Dimethylformamide; 2 d, rt
View All
Average Yield: 50%
Evidence (38)
Alternative Steps (48)
[Experimental Protocols](#)

D → H + I Predicted Step Only
No reaction summary
View All
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)
[Experimental Protocols](#)

Filter by

Alternative Step Type
 Predicted (48)

Stereochemistry
 Non-Selective (48)

5 of 15

Select View 8 similar Alternatives 2 View Evidence 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,
WO2010080864 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.

Plan Information
Estimated Yield: 76%
Overall Price: \$599.28
(USD per 100 grams)

Scoring Profiles

Complexity Reduction ●

Convergence ● Medium

Evidence ●

Cost ●

Yield ●

Atom Efficiency ●

Apply Reset Scoring

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

Weights 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.

Apply Reset Scoring

Markush search and CAS PatentPak

Markush search

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

The screenshot shows the CAS SciFinder interface for a Markush search. At the top, there's a search bar and a drawing tool. The main area displays the search results for a drawn structure, including a chemical structure with Markush locations (G1-G4) and a list of patent references. Callouts highlight the 'Markush search option', 'Markush location', 'Link to a specific patent reference', 'Assembled Markush hit structure', and 'Filter by patent authority'.

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)

The screenshot shows the CAS PatentPak interface for viewing a patent PDF. The interface includes a search bar, a list of key substances, and a detailed view of a key substance with its chemical structure and related information. Callouts highlight the 'Download PDF including list of marked-up substances and annotations', 'Marks key substance curated by CAS scientists', 'Link to related information', 'Highlighted key substance is marked', and 'Link to location of substance in patent'.

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 view for the first result.

Suppliers search for "7664-93-9"

Filter Behavior: Filter by (selected), Exclude

490 Results

Sort options: Sort: Relevance

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 1 L, USD 40.00 2.5 L, USD 80.00
2 Link to detail			
3			

Oakwood Chemical Product List

Preferred Supplier

Web: <https://www.oakwoodchemical.com>

Email: 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: 1 Mar 2024

Last Updated: 1 Mar 2024

Order From Supplier

Substance Information

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

OS(=O)(=O)O

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 chemical structure editor interface. It features a toolbar with various drawing and editing tools, a central workspace with a chemical structure, and a sidebar with additional tools.

ChemDoodle

Model with CAS Registry Number

Clear | Eraser

Labeling

Undo | Redo

Templates

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

Zoom

Open | Save

CC(F)(F)C1=CC=C(C=C1)NC(=O)CC2=CC=C(C=C2)S(=O)(=O)C3=CC=C(C=C3)F

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 for a patent reference titled "Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)". The interface includes a header with document statistics (13 citations, 0 authors, 1 like, 1 notification) and a "Citation Map" button. Below the header, the "In this Reference" section lists links for "IPC Data", "CAS Concepts", and "Substances". The main text area shows the patent abstract and keywords, with a callout box pointing to the "Get Prior Art Analysis" button. Below the main text, there are buttons for "PatentPak Viewer", "Get Prior Art Analysis", and "Full Text". A "References" section at the bottom shows "Prior Art Analysis (195)" with a "View Results" button and a "Complete" status. A "View Results from the search history" button is also present.

Login, feedback, training, and support

Login details

Log in at 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:

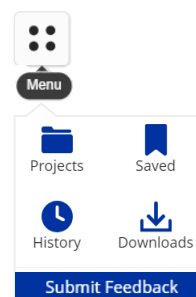
www.cas.org/cas-webinars

Recorded events and webinars:

www.cas.org/cas-past-webinars

CAS SciFinder training topics:

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



Support contact

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

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