

CAS SCIFINDERⁿ

FOR ACADEMIA

QUICK REFERENCE GUIDE

CAS



A division of the
American Chemical Society

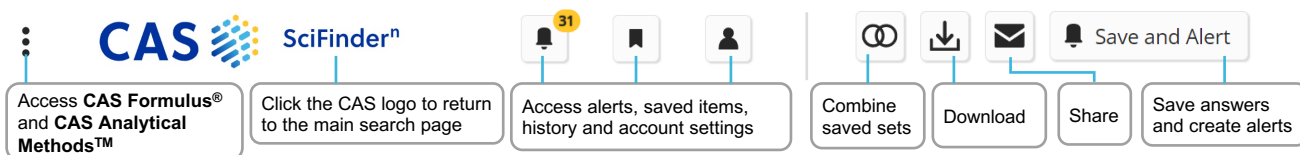
Contents

- 03 Solution Interface
- 03-04 References Search
- 05-06 Substances Search
- 07 Advanced Search
- 08 CAS Roles
- 09-10 Search CAS Sequences
- 11-12 Reactions Search
- 13-16 Retrosynthesis Planner
- 17 Markush and CAS PatentPak[®]
- 18 Supplier Search
- 18 ChemDoodle[®]
- 19 Prior Art Analysis
- 19 Login, Training, and Support

Solution interface and References search

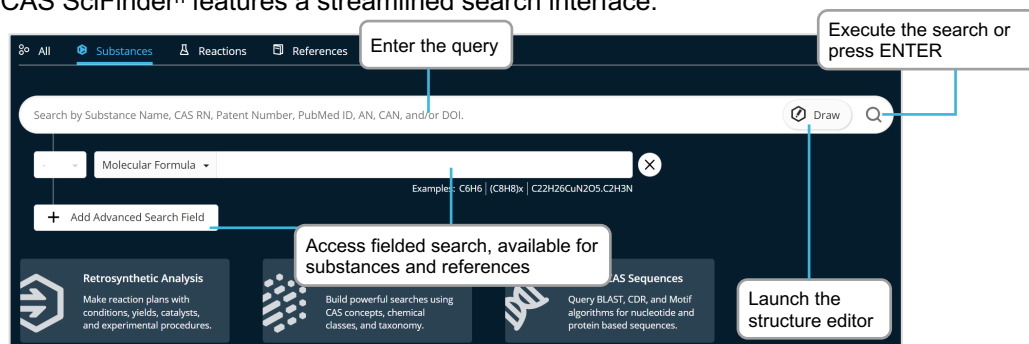
Main interface

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



Search interface

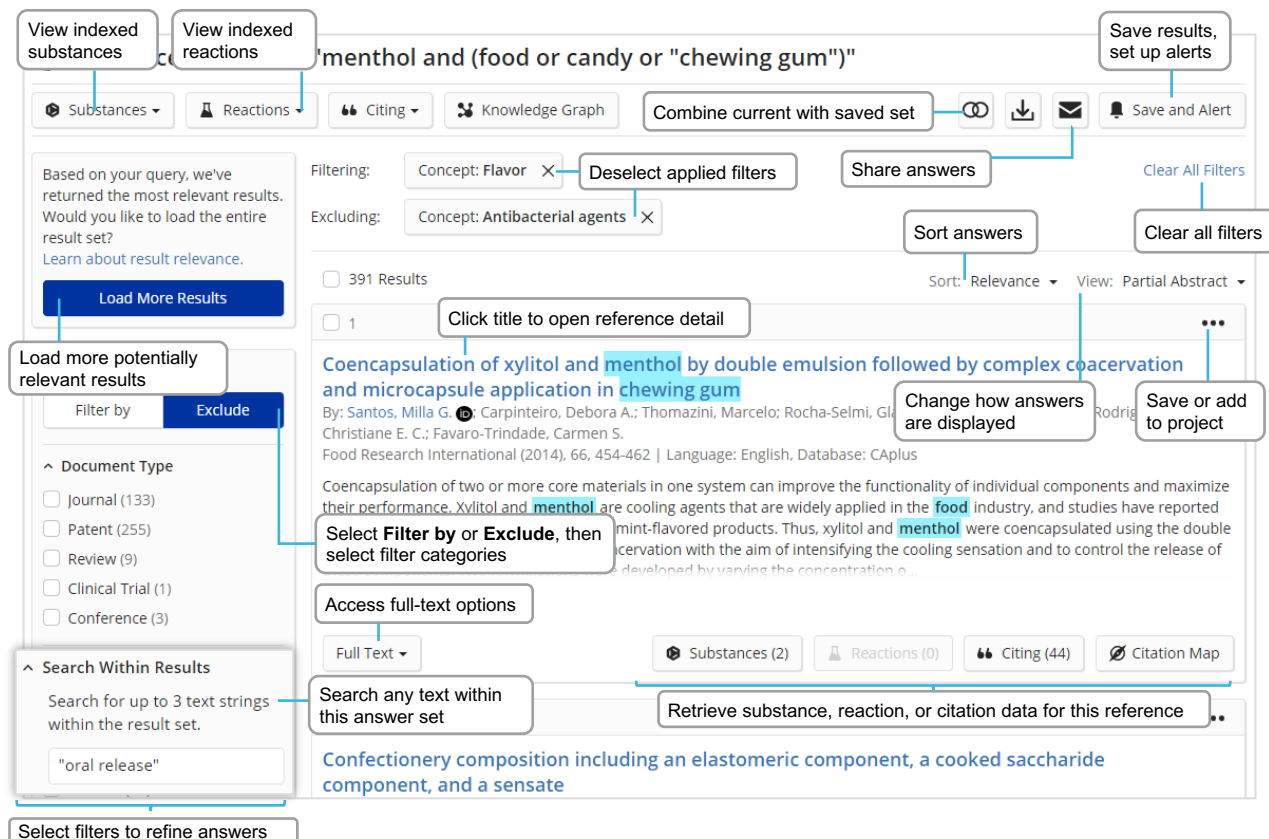
CAS SciFinder[®] features a streamlined search interface.



References search result

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[®].

Publication source information

PATENT

Patent Number
WO2005048743

Publication Date
2005-06-02

Application Number
WO2004-JP17524

Application Date
2004-11-18

Kind Code
A1

Assignee
Takasago International Corporation, Japan

Source
World Intellectual Property Organization

Patent family and priority application information

AN: 2005:470226
CAN: 143:25602
CAplus

Language
English

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-(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 p-menthane-3,8-diol as the cool-tasting component.

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

PatentPak Viewer | Get Prior Art Analysis | Full Text

Similar References **NEW**

PDF displays original patent PDF
PDF+ displays the full text with table of indexed substances
Viewer displays interactive version of annotated full text

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2005048743	English	A1	PDF PDF+ Viewer	2005-06-02		

Priority Application

Priority Application Number	Application Date
JP2003-389758	
WO2004-JP17524	

IPC and indexed subject matter, substance indexing, and formulations

Get similar references

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

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

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 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 sub-options like 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), "Search CAS Sequences" (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences), and "Search Patent Markush" (Check to perform Markush search). A "Click to draw new structure" button is also visible.

Substances search result

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 images.

The screenshot displays search results for "6,055,245 Results". The interface includes a "Select type of structure match" section with options: "As Drawn (116)", "Substructure (6M)", and "Similarity (1,046)". A "Change sort criterion" dropdown is set to "Sort: Number of Suppliers" and "View: Partial". A "Change amount of details displayed" dropdown is set to "80-08-0". The results list includes entries like "90357-06-5" (Biclutamide, $C_{14}H_{14}F_4N_2O_4S$), "149104-88-1" (4-(Methylsulfonyl)phenylboronic acid, $C_7H_9BO_4S$), and "80-08-0" (Dapsone, $C_{12}H_{12}N_2O_2S$). A detailed view for "149104-88-1" is shown, including CAS Name, CAS RN, and a list of actions: "Get Substance Details", "Get Bioactivity Data", "Get Reactions (2,426)", "Synthesize (9)", "Start Retrosynthetic Analysis", "Get References (1,361)", and "Get Suppliers (113)". Annotations include: "Click CAS Registry Number to open details", "Click on structure to open flyout window", "Retrieve data related to substance", "Open editor with this structure", and "Download .sdf or .mol. Copy Smiles to Clipboard". Other annotations include "Analyze structure precision", "Start Chemscape Analysis", "Search a (sub)structure within this set of substances", and "Reference Roles show which new information was reported about a substance in the literature".

Substance detail and structure editor

Substance detail

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

References (4,222) Reactions (228) Suppliers (117)

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: 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)

Experimental Properties: InChI Key LKJPYSCBVHEWU-UHFFFAOYSA-N

Experimental Spectra: 9 Other Names for this Substance

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

CAS Draw editor

You can further 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...

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

Lasso | Marquee tool

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 | Reaction role

Atom mapping | Lock rings/lock atoms

Bond mapping | Draw reaction arrow

Learn about keyboard shortcuts to e.g., easily draw hetero atoms

Hetero atom and H isotope selection

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw

Zoom: 90%

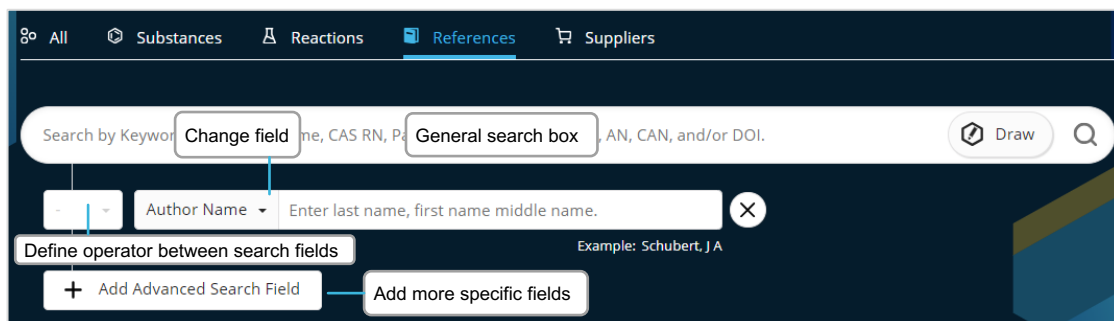
OK Cancel

Advanced Search

Performing an Advanced Search

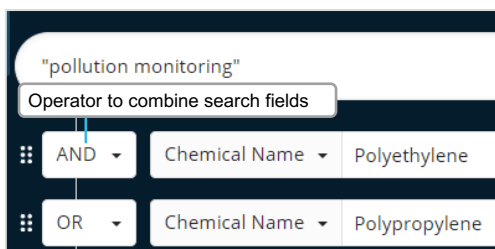
You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinder[®].

- 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)



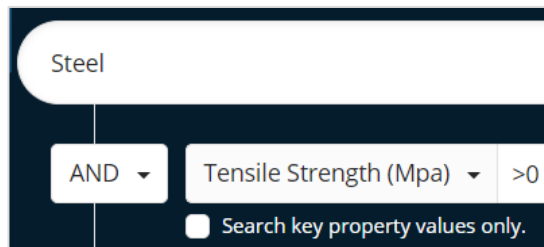
Advanced Search examples

Advanced References Search

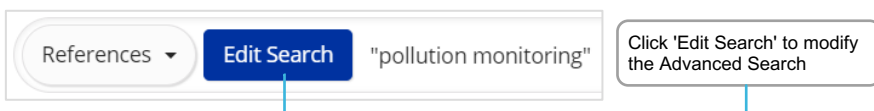


Query interpretation:
"pollution monitoring" and (polyethylene or polypropylene)

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. They relate to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in a plant (Natural Product Occurrence).

Roles in substance results

From a search on substance(s), the roles filter will indicate the 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

0 Selected

- 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 result sets whenever you have retrieved hits in the substance indexing segment of the records, i.e., by retrieving substance names or performing a crossover after 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

Language

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: (i) 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 λ) 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 μ m items which are retained by a 500 μ m sieve/net, and (ii) 1-500 μ m, 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

Search CAS Sequences

Search options

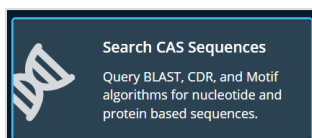
You can search sequences using three different modalities:

- 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.
- Recognize 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.



BLAST CDR Motif Sequence Search options Clear Search

> human insulin sequence
fvnqhlcghlveaylvcgergfftypktgiveqccsicslyqlenycn

Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane

Upload Sequence (.fasta or .txt)

Sequence Type:
Nucleotide Protein

Search Within:
 Nucleotides Proteins

Include NCBI Sequences

Search Sequences

Advanced Sequence Search Adjust Parameters for Short Sequences | Reset All

Alignment Identity % Match with Gaps? Yes No Gap Costs Existence 11 Extension 1

Query Coverage % Word Size Scoring Matrix BLOSUM62

BLAST Algorithm E-Value Exclude Low Complexity Regions Yes No

Advanced BLAST parameters

BLAST results analysis

Access results

Sequence search results appear in the Recent Search History and general Search History (🕒 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%

Results will expire on
Oct 31, 2023.

> human insulin sequence
fvnqhlcgshlveaylvcgergffytptktgiveqcctsiclslyqlenycn

View Results

Edit Search

Complete

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 '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

92 Alignment Identity: 89.09%

Query 1 50 Query Length

Subject 1 55 Subject Length

Matches: 49
Mismatches: 6

Alignment Length: 49+6=55

Alignment Details | Subject and links to NCBI and substance information in CAS SciFinder[®] | Reference previews

Alignment | Subject | References

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

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

Q 1 FVNQHLCGSH LVEA-YLVG ERGFFYTPKT - - - - - GIVEQC CTSICLSYQL ENYCN 55

S 1 FVNQHLCGSH LVEALYVG ERGFFYTPKS DDARGIVEQC CTSICLSYQL ENYCN 55

Start of alignment in query and subject sequences | Gap in the query sequence

Get References for this sequence

Filter results

Filtering dynamically changes your result set.

Expectation Value to

Alignment Length to Query Length

Alignment Length to Subject Length

Number of Matches to Alignment Length

Sequence Length to

Organisms

Homo sapiens (25)

Mus musculus (25)

Reactions search

Performing a Reactions search

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

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

Reactions search results are grouped into schemes with identical reactants and products or into transformations. A robust panel of filters, including yield and steps, enables 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 (2,142)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (429)

80-89% (261)

70-79% (290)

50-69% (372)

30-49% (206)

View All

Number of Steps

1 (2,368)

2 (2,135)

20,022 Results

Click on structure to view substance information

Group: By Scheme Sort: Yield View: Expanded

Send to CAS Draw

Steps: 1 Yield: 100%

Yield for displayed reactions

Absolute stereochemistry shown. Rotation (+)

Suppliers (48) View suppliers

Suppliers (604)

Filter reaction results

View reaction details

View reaction reference

Access annotated patent full-text

31-614-CAS-27240963 Steps: 1 Yield: 100%

1.1 Reagents: TriethylamineDiphenylphosphoryl azide

Solvents: Toluene

1.2 -

Experimental Protocols

Stereoselective process for preparing isoxazolo-quinoline-substituted cyclohexyl derivatives

By: Barnett, Charles Jackson; et al
World Intellectual Property Organization, WO2002-03-28

PatentPak Full Text

31-614-CAS-27633989 Steps: 1 Yield: 100%

1.1 Reagents: TriethylamineDiphenylphosphoryl azide

Solvents: Toluene; 40 - 50 °C; 1 h, 110 °C; 110 °C → 70 °C

1.2 70 °C; overnight, 70 °C → 85 °C

Preparation of N-(isoxazoloquinolinylcyclohexyl)carbox amides and analogs as MRP1 inhibitors

By: Bonjouklian, Rosanne; et al
World Intellectual Property Organization, WO2001046199 A1
2001-06-28

Get similar reactions

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.

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

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 [Organic Process Development](#) (2016), 20(5), 965-969
[View Source](#) [Full Text](#)

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

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
[View detailed procedures](#)

Products [Ethyl \(1*R*,3*S*\)-3-\[\(benzyloxycarbonyl\)amino\]cyclohexanecarboxylate](#), Yield: 85%

Reactants [1-Ethyl \(1*R*,3*S*\)-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 (1*S*, 3*R*)-3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).

Characterization Data [View characterization data](#)

^ **Ethyl (1*R*,3*S*)-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 retrosynthesis tool within CAS SciFinder[®]:

1. Draw or import a structure into the Retrosynthesis window accessed by selecting the Retrosynthesis option on the main page. The substance can be novel.
2. Choose the Start Retrosynthetic Analysis option found on the substance flyout window.

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. Draw

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.

Search CAS Sequences
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

Retrosynthetic Analysis
Draw or import a structure.
Click and drag to select objects. Ctrl-click to select or deselect individual objects.

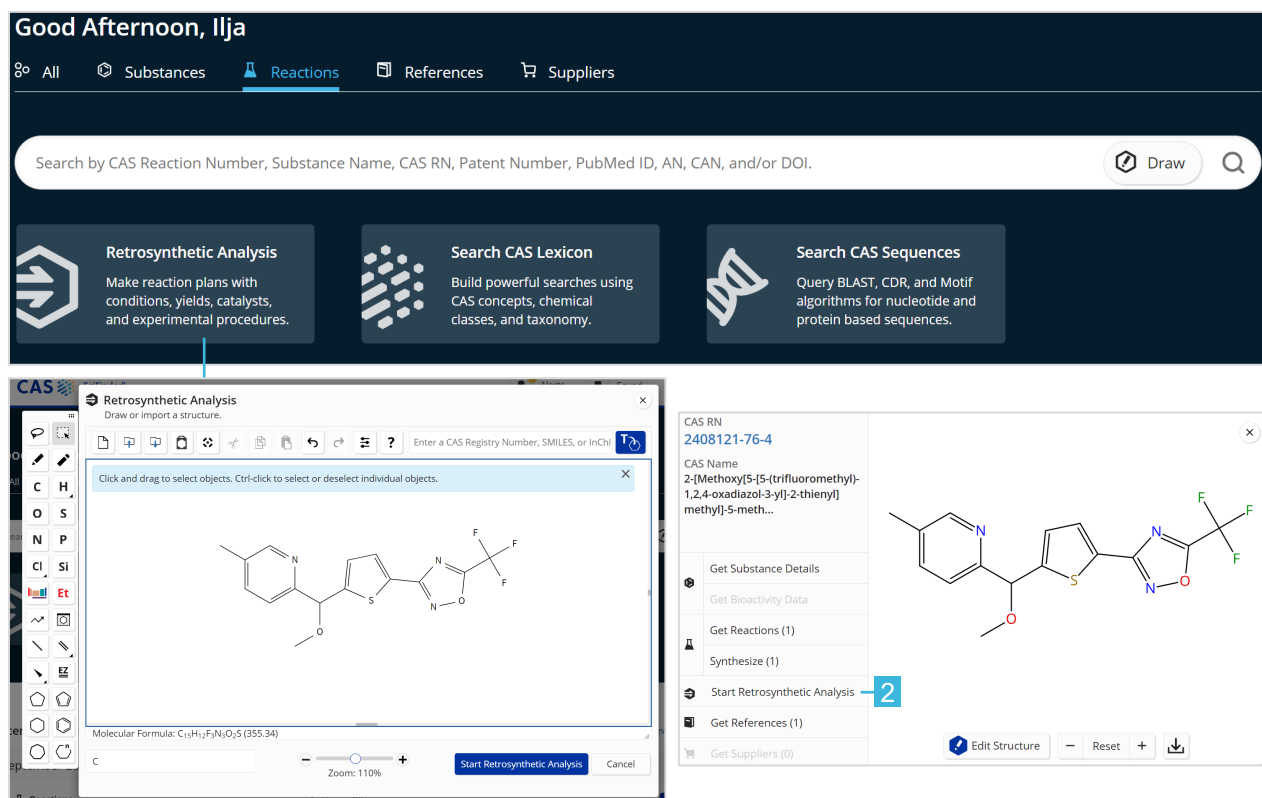
Molecular Formula: C₁₅H₁₇F₃N₃O₂S (355,34)

Start Retrosynthetic Analysis Cancel

CAS RN
2408121-76-4
CAS Name
2-[Methoxy[5-[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-2-thienyl]methyl]-5-meth...

Get Substance Details
Get Bioactivity Data
Get Reactions (1)
Synthesize (1)
Start Retrosynthetic Analysis 2
Get References (1)
Get Suppliers (0)

Edit Structure Reset



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, (such as poly- or heterocyclic molecules).

Once you have completed your option selections, choose 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](#)

Chemical Structure: COc1ccc(NC(=O)C2=CC=CS2)cc1C(=O)N3C=CC(=O)N3C(F)(F)F

Annotations:

- Change the number of disconnections in the plan (points to Synthetic Depth)
- Break bond in first disconnection (points to Break Bond button)
- Protect bond in entire plan (points to Protect Bond button)
- Clear selections (points to Clear All Bond Selections)
- Select uncommon or rare rules supported by fewer literature examples (points to Uncommon/Rare rules)
- Change upper cost limit for starting materials (USD/mol or USD/g) (points to Cost Limit input)
- First bond to be broken (points to the bond between the pyridine ring and the carbonyl group)
- Protected bonds (points to the C-F bonds in the trifluoromethyl group)
- Generate plan (points to the Create Retrosynthesis Plan button)

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 a bit 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
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
Experimental Protocols

D ⇒ H + I Predicted Step Only
No reaction summary
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

Grouped similar reactions

Select View 8 similar Alternatives 2 View Evidence (55) Average Yield: 63%

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

1.1 Solvents: Dichloromethane; rt
1.2 Reagents: Triethylamine; rt: 18 h, rt

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.
- Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor in step selection or alternative ranking.

Scoring profiles

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

Each scoring profile may be set to **Off** (extreme left), **Low**, **Medium**, or **High** (extreme right); the default setting for each profile is "Medium," as shown below. Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor step selection or alternative ranking.

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

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.

Apply Reset Scoring

Supplier search and ChemDoodle®

Suppliers search

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

Suppliers for 7664-93-9

389 Results

Sort options: Sort: Relevance

Supplier	Substance	Purity	Purchasing Det
<input type="checkbox"/> 1 Oakwood Chemical United States Last Updated: 1 Mar 2023	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
<input type="checkbox"/> 2 Oakwood Chemical United States Last Updated: 1 Mar 2023			
<input type="checkbox"/> 3 Oakwood Chemical United States Last Updated: 1 Mar 2023			

Filter Behavior: Filter by Exclude

Preferred Suppliers:
 Preferred (51)
 No Preference (338)

Supplier:
 Hayashi Pure Chemical Products Catalog (109)
 KANTO CHEMICAL (41)
 FUJIFILM Wako Chemicals Europe GmbH Product List (37)
 FUJIFILM Wako Chemicals U.S.A. Corporation Product List (37)
 FUJIFILM Wako Pure Chemical Corporation Product List (37)
[View All](#)

Purity:
 ≥99% (2)
 95-98% (106)
 90-94% (9)

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: 080325

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 Aug 2023

Order From Supplier

Substance Information

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

Chemical structure: OS(=O)(=O)O

ChemDoodle

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

ChemDoodle

Model with CAS Registry Number

Clear | Eraser

Labeling

Undo | Redo

Templates

Open | Save

Zoom

ChemDoodle®

OK Cancel

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 functionality:

- 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.

Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)

Substances (13) Reactions (0) Citing (1) Citation Map

PATENT

Patent Number: **WO2017135893**

Publication Date: 2017-08-10

Application Number

By: Wang, Shaofeng; Li, Hairong; Seow, Swee How

The present invention relates to a water-based emulsion coating composition, e.g. paint composition, comprising a hyper-branched or dendritic poly(amido)amine, a surfactant, a solvent, a pigment, a thickener, a crosslinking agent, at least one isothiazolone biocide, and a binder.

Keywords: aqueous dendritic coating, dendritic poly(amido)amine

PatentPak Viewer Get Prior Art Analysis Full Text

References 1:52 PM

Prior Art Analysis (195)

Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)

View Results

Complete

View Results from the search history

Login, training, and support

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www.cas.org/cas-past-webinars

CAS SciFinderⁿ training topics: www.cas.org/support/training/scifinder-n

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