

CAS SCIFINDERⁿ

**QUICK
REFERENCE
GUIDE**

CAS

A division of the
American Chemical Society



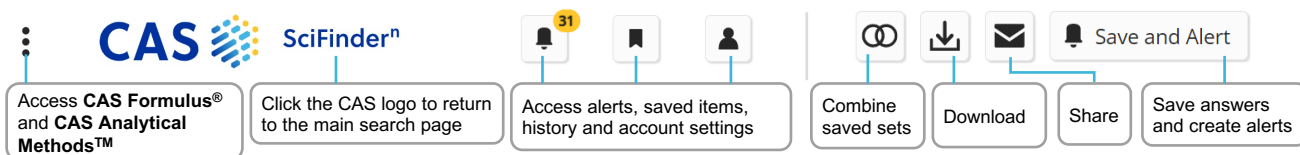
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Solution interface and References search

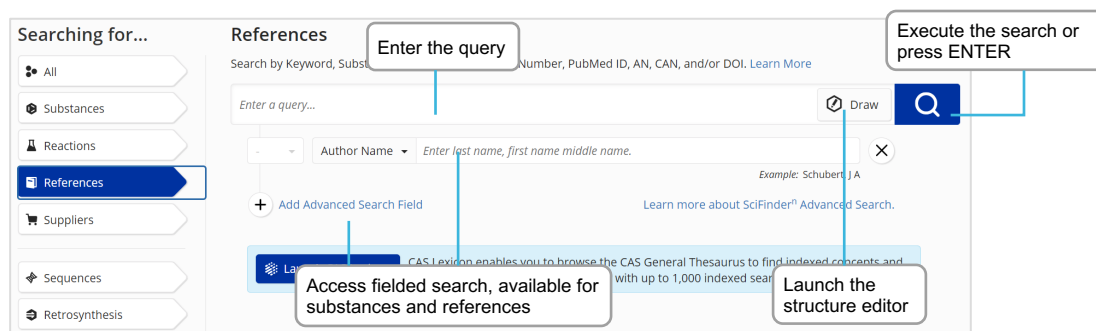
Main interface

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



Search interface

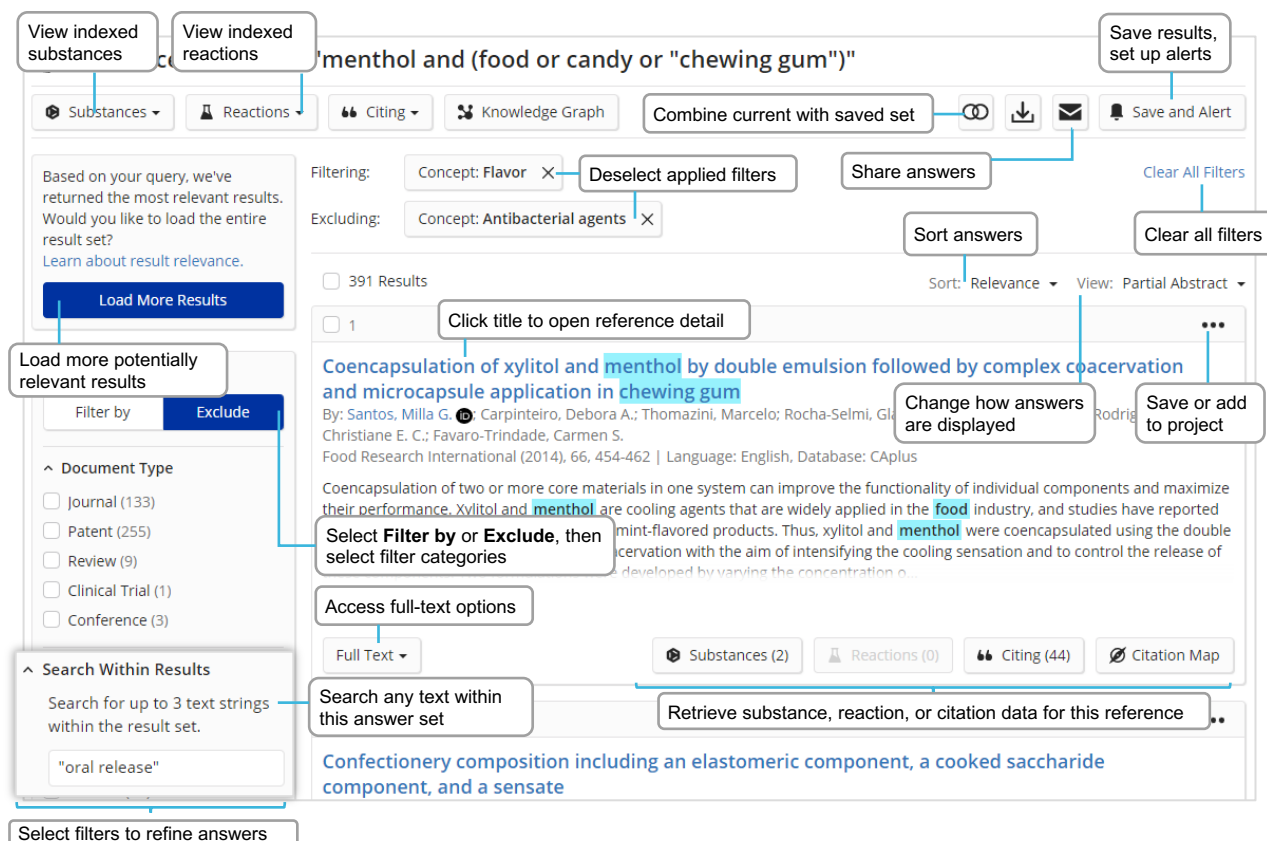
CAS SciFinder[®] features a streamlined search interface.



References search 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[®].

Fruit juice-containing food products with refreshing and cooling flavors

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

Citing (6)

Citation Map

View forward and backward citations

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[®]](#).

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.

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

PatentPak Viewer

Get Prior Art Analysis

Full Text

Get prior art for this patent

Get similar references

Get Similar References

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

Similar References **NEW**

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

- 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 X Draw Q

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

Searching for...

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Enter chemical name query

AND Molecular Formula

+ Add Advanced Search Field

Add more advanced search fields

Change advanced search field

Click query structure to edit

Click to draw new structure

Edit Drawing Remove

Search Patent Markush

Check to perform Markush search

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.

Select type of structure match

Structure Match

As Drawn (115)

Substructure (5.9M)

Similarity (1,044)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Start Chemscape Analysis

Filter by Exclude

Reaction Role

Reference Role

Preparation (3M)

Synthetic Preparation (3M)

Uses (2.7M)

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search a (sub)structure within this set of substances

5,986,620 Results

1 90357-06-5

Click CAS Registry Number to open details

149104-88-1

Change sort criterion Sort: Number of Suppliers View: Partial

Change amount of details displayed 80-08-0

Click on structure to open flyout window

Retrieve data related to substance

Get Substance Details

Get Bioactivity Data

Get Reactions (2,395)

Synthesize (9)

Start Retrosynthetic Analysis

Get References (1,330)

Get Suppliers (106)

Open editor with this structure

Download .sdf or .mol. Copy Smiles to Clipboard

CAS RN 149104-88-1

CAS Name [4-(Methylsulfonyl)phenyl]boronic acid

HO-B(OH)2-C6H4-SO2-CH3

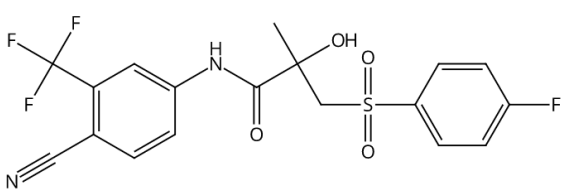
Substance detail and structure editor

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 (4,118) Reactions (227) Suppliers (114) [Download] [Email] [Save]



C₁₈H₁₄F₄N₂O₄S — Molecular formula in hill order

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

Key Physical Properties	Value	Condition
Molecular Weight	430.38	-
Melting Point (Experimental)	190-195 °C (decomp)	-
Boiling Point (Predicted)	650.3±55.0 °C	Pressure: 760.0 Torr
Density (Predicted)	1.41	-

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)
InChI Key: LKJPYSCBVHEWU-UHFFFAOYSA-N

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.

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 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

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

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 | Reaction role

Atom mapping | Lock rings/lock atoms

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)

The screenshot shows the 'References' search section. At the top, it says 'Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)'. Below this is a search bar with a 'General search box' and a 'Draw' button. A 'Change field' button is highlighted with a blue arrow pointing to a dropdown menu currently set to 'Author Name'. The text input field contains 'Enter last name, first name middle name.' and has an 'X' to clear it. Below the search bar, there's a section 'Define operator between search fields' with a '+' button to 'Add Advanced Search Field' and a button to 'Add more specific fields'. An example query 'Schubert, J A' is shown. A link 'Learn more about SciFinder[®] Advanced Search.' is at the bottom right.

Advanced Search examples

Advanced References Search

The screenshot shows a query for 'pollution monitoring' in the 'Chemical Name' field. Below it, an 'Operator to combine search fields' dropdown is set to 'AND'. Another 'Chemical Name' field contains 'polyethylene'. Below that, an 'OR' dropdown is set, followed by another 'Chemical Name' field containing 'polypropylene'.

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

The screenshot shows the search results for 'pollution monitoring' under the 'References' category. There is a blue 'Edit Search' button. A callout box points to the button with the text: 'Click \'Edit Search\' to modify the Advanced Search'.

Advanced Substances Search

The screenshot shows a query for 'steel*' in the 'Chemical Name' field. Below it, an 'AND' dropdown is set, followed by a 'Tensile Strength (Mpa)' field set to '>0'. A note at the bottom says 'Experimental values only.'

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

- Author Name
- Publication Name
- Organization Name
- Title
- Abstract/Keywords
- Concept
- Substances
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Substances Search

- Molecular Formula
- CAS Registry Number/Component Registry Number
- Chemical Name
- Document Identifier
- Patent Identifier
- Experimental Spectra
- 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 structure-based searches.

Example: I am interested in the subject of (marine) pollution, how can I find publications where polypropylene is specifically described as a pollutant?

The search for polypropylene retrieves many references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3,217 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
Polypropylene

278K References | 6,321 Reactions | 20 Suppliers

Substance Role

By Count | Alphanumeric

1 Selected

- ☐ Uses (262K)
- ☐ Technical or Engineered Material Use (186K)
- ☐ Polymer in Formulation (79K)
- ☐ Properties (60K)
- ☐ Process (50K)
- ☐ Biological Use, Unclassified (3,678)
- ☐ Occurrence (3,640)
- ☒ Pollutant (3,217)
- ☐ Miscellaneous (2,437)
- ☐ Biological Study, Unclassified (2,433)

Document Type

Substance Role

- ☐ Uses (262K)
- ☐ Properties (60K)
- ☐ Process (50K)
- ☐ Biological Study (22K)
- ☐ Preparation (19K)
- ☒ Pollutant (3,217)

Language

Pollutant (3,217)

Recycling micro polypropylene in modified hot asphalt mixture

By: Buruliana, Daniela Laura; Georgescu, Puiu Lucian; Carp, Gabriel Bogdan; Ghisman, Viorica

Scientific Reports (2023), 13(1), 3639 | Language: English, Database: CxPlus and MEDLINE

One of the objectives of the circular economy is solving the world's plastic pollution crisis and recycling of materials by ensuring less waste. The motivation of this study was to demonstrate the possibility of recycling two types of wastes with a high risk of pollution, such as plastic based polypropylene and abrasive blasting grit wastes in asphalt roads. The effects of adding together polypropylene based microplastics and grit waste in asphalt mixture for wear layer performance have been shown in this study. The morphol. and elemental composition of the hot asphalt mixture samples before and after freeze-thaw cycle were examined by SEM-EDX and the performance of the modified asphalt mixture was determined with laboratory tests including Marshall stability, flow rate, solid-liquid report, apparent d_w , and water absorption. A hot asphalt mixture suitable for making wear layer in road bitumen, abrasive blasting grit waste and polypropylene based microplastics is also suitable for making asphalt mixtures were added 3 proportions of polypropylene based microplastics such as the mixture performance is shown at the asphalt mixture sample with 0.3% of polypropylene based microplastics are bond with aggregates from mixture well, so the polypropylene-modified hot asphalt mixture can effectively decrease the appearance of cracks during sudden temperature changes.

Full Text ▾

Substances (2) | Reactions (0) | Citing (0) | Citation Map

Microplastics in marine environment review of methods for identification and quantification

By: Hidalgo-Ruz, Valeria; Gutow, Lars; Thompson, Richard C.; Thiel, Martin

Environmental Science & Technology (2012), 46(6), 3060-3075 | Language: English, Database: CxPlus 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: d. 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 d.) 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 m²" 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-5 mm, which are retained by a 500 μ m sieve; 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 (2,083) | Citation Map

Substances

9003-53-4

CAS RN | Chemical Name | Role

Every publication in this set of 3,217 references discusses polypropylene in the context of a pollutant

Sequences search

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 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.

The screenshot displays the 'Sequences' search module in CAS SciFinder. On the left, a sidebar titled 'Searching for...' contains navigation links: All, Substances, Reactions, References (highlighted), Suppliers, Sequences, and Retrosynthesis. The main area is titled 'Sequences' and includes a text input field for a protein or nucleotide string, with a link to 'Learn more about Sequence Search'. Below the input field are tabs for 'BLAST', 'CDR', and 'Motif', with 'BLAST' selected. To the right of the tabs are buttons for 'Upload Sequence' and 'Clear Search'. A 'Sequence Search options' button is also present. The input field contains the text: '> human insulin sequence' followed by the amino acid sequence 'FVNQHLCGSHLVEAYLVCGERGFFYTPKTGIVEQCCTSIICSLYQLENYCN'. Two callout boxes point to the input field: 'Paste sequence into this window' and 'Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane'. On the right side, there are settings for 'Sequence Type' (Nucleotide or Protein, with Protein selected), 'Search Within' (Nucleotides or Proteins, with Proteins selected), and a checked option for 'Include NCBI Sequences'. A 'Start Sequence Search' button is at the bottom right. A callout box points to this button with the text 'Include NCBI sequences'. The bottom section, titled 'Advanced Sequence Search', contains various parameters: 'Alignment Identity %' (set to -), 'Match with Gaps?' (Yes selected), 'Gap Costs' (Existence 11 Extension 1), 'Query Coverage %' (set to 90), 'Word Size' (set to 3), 'Scoring Matrix' (BLOSUM62), 'BLAST Algorithm' (BLASTp), 'E-Value' (set to 10), and 'Exclude Low Complexity Regions' (No selected). A callout box points to this entire section with the text '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.

April 28, 2023

☐ Sequences
5:00 PM

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

> human insulin sequence
FVNQHLCGSHLVEAYLVCGERGFFYTPKTGIVEQC
CTSI CSLYQL ENYCN

View Results

Edit Search

Complete

Results will expire on
May 29, 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 '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

View Less

Subject and links to NCBI and substance information in CAS SciFinder[®]

Reference previews

References

Get References for this sequence

Alignment Details

Alignment

Subject

References

Match

Mismatch

+ Mismatch: Query aa aligned to functional equivalent subject aa

Start of alignment in query and subject sequences

Gap in the query sequence

BLAST Score: 201

E-Value: 5.12823e-26

Q

1

FVNQHLCGSH LVEA YLVCG ERGFFYTPKT

-----GIVEQC CTSICSLYQL ENYCN

55

S

1

FVNQHLCGSH LVEA YLVCG ERGFFYTPK S

DDARGIVEQC CTSICSLYQL ENYCN

55

Filter results

Filtering dynamically changes your result set.

^ E-Value

0 to 10⁶

^ 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

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.

The screenshot shows the 'Reactions' search section of the CAS SciFinder interface. On the left, a sidebar titled 'Searching for...' contains buttons for 'All', 'Substances', 'Reactions' (highlighted), 'References', 'Suppliers', 'Sequences', and 'Retrosynthesis'. The main area is titled 'Reactions' and includes a search bar with the placeholder 'Enter a query...'. Below the search bar is a 'Select reactions' button. To the right of the search bar, there is a 'Click on reaction query to edit' button and a small chemical structure diagram with 'Edit Drawing' and 'Remove' buttons.

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.

The screenshot displays the 'Reactions search for drawn structure' results page. The top section shows '26,932 Results' and options to 'Change grouping to 'By Document' or 'By Transformation'', 'Group: By Scheme', 'Sort: Yield', and 'View: Expanded'. A chemical structure of a substituted cyclohexyl derivative is shown with a callout 'Click on structure to view substance information'. Below the structure, there are buttons for 'Suppliers (48)' and 'View suppliers'. The results are listed in a table with columns for 'Steps', 'Yield', and 'Reaction Details'. Two results are shown: one for 'Stereoselective process for preparing isoxazoloquinoline-substituted cyclohexyl derivatives' and another for 'Preparation of N-(isoxazoloquinolinylcyclohexyl)carbox amides and analogs as MRP1 inhibitors'. Callouts point to 'View reaction details', 'View reaction reference', and 'Access annotated patent full-text'. On the left, a sidebar titled 'Filter reaction results' includes 'Structure Match' (As Drawn (0), Substructure (26K), Similarity (2,082)), 'Filter Behavior' (Filter by, Exclude), 'Search Within Results', 'Yield', 'Number of Steps', 'Non-Participating Functional Groups' (Carboxylic ester (151), Halide (143), Ether (125), Ketone (103), Carbamate (98)), and 'Reaction Mapping'.

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.

Reaction Overview

Steps: 1 Yield: 85%

Reaction reference

JOURNAL

Development of a Scalable Synthesis of an Azaindoly-Pyrimidine Inhibitor of Influenza Virus Replication

By: Liang, Jiang [View All](#)

Organic Process Development (2016), 20(5), 965-969

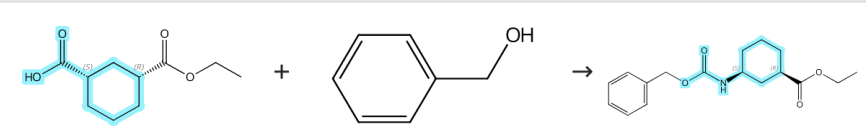
[View Source](#) [Full Text](#)

Company/Organization

Vertex Pharmaceuticals Incorporated

Boston, Massachusetts 02210

United States



Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (-)

[Suppliers \(48\)](#)

[Suppliers \(133\)](#)

[Supplier \(1\)](#)

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, CDCl₃) 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 C₁₇H₂₄NO₄ 306.1700, found 306.1700

State

sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations

1. Schmidt Reaction

[Overview of transformations](#)

Reaction Notes

scalable

[Further important notes](#)

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.

Searching for... Retrosynthesis

Draw or import a structure to perform a retrosynthetic analysis. Learn more about Retrosynthesis searching.

Enter a CAS Registry Numbers, SMILES,

Draw or change atoms or bonds.

Molecular Formula: $C_{13}H_{11}F_3N_2O_2S$ (355.34)

Zoom: 100%

1 Start Retrosynthetic Analysis

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 Download

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.

Change the number of disconnections in the plan

Break bond in first disconnection

Protect bond in entire plan

Clear selections

Retrosynthesis Plan Options for drawn structure

Powered by ChemPlanner[®]

Select Synthetic Depth [Learn more.](#)

1
2
3
4

Set Rules Supporting Predicted Reactions [Learn more.](#)

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

Select uncommon or rare rules supported by fewer literature examples

Set Starting Materials Cost Limit [Learn more.](#)

1000 USD/mol

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

Break and Protect Bonds

Break Bond Protect Bond Clear All Bond Selections

First bond to be broken

Protected bonds

Create Retrosynthesis Plan

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 a bit longer.

The interface displays a retrosynthesis plan for a drawn structure. Key features include:

- Overview Tab:** Shows Plan Information (Estimated Yield: 22%, Overall Price: \$108.55, Commercially Available: D, E, F, G, H, I, J), Plan Options (Synthetic Depth: 3, Predicted Rules: Common, Break & Protect Bonds: Yes, Starting Material Cost Limit: \$1,000.00/mol), and Scoring Profiles (Complexity Reduction, Convergence, Evidence, Cost).
- Steps Tab:** Displays the retrosynthetic plan with nodes A through H. Purple lines mark experimental steps, and green dotted lines indicate predicted steps.
- Retrosynthesis Step Key:** Explains the color coding for experimental and predicted steps.
- Adjust scoring options:** Sliders for Complexity Reduction, Convergence, Evidence, and Cost.
- Exclude steps or substances:** A button to exclude specific steps or substances.
- Switch predicted steps on/off:** A toggle switch to toggle the visibility of predicted steps.
- View Excluded Options:** A button to view excluded options.
- Download, Share, and Save your plan:** Buttons for downloading, sharing, and saving the plan.
- Review and select alternative disconnections:** A button to review and select alternative disconnections.

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.

The interface displays alternative steps and evidence reactions. Key features include:

- Overview Tab:** Shows step-specific evidence and alternate steps below or select the node between steps on the plan.
- Steps Tab:** Displays the retrosynthetic plan with nodes A through H. Purple lines mark experimental steps, and green dotted lines indicate predicted steps.
- Filter by:** A section to filter by Alternative Step Type (Predicted (49), Non-Selective (49)) and Stereochemistry (Non-Selective (49)).
- Grouped similar reactions:** A section to view grouped similar reactions, including a link to View 4 similar Alternatives and a link to View Evidence (1,580).
- Reactions from Retrosynthesis Plan Evidence:** A section to view evidence reactions for a predicted disconnection of precursor C. It includes a list of references and a detailed reaction scheme showing the synthesis of a compound from a precursor.
- Evidence reactions for (predicted) disconnection of precursor C:** A section to view evidence reactions for a predicted disconnection of precursor C.

Retrosynthesis scoring options

Scoring options

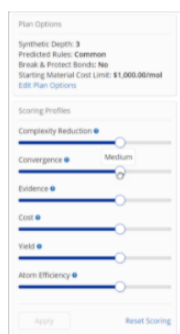
For plans with predicted steps, you may increase or decrease the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

- 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.



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.



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

References

Patent Markush Match

As Drawn (96)

Substructure (119)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (55)

United States (25)

European Patent Organization (8)

China (3)

United Kingdom (2)

View All

Markush search type

96 Results

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)

CAS PatentPak

PAGE 21 / 22

DOWNLOAD PDF PDF+

Download PDF including list of marked-up substances and annotations

Key Substances in Patent

CAS RN 33454-82-9

CAS Name Lithium trifluoromethanesulfonate

Components: 2

Component RN: 1493-13-6

Get Substance Details

Get Bioactivity Data

Get Reactions (2,406)

Synthesize (101)

Start Retrosynthetic Analysis

Get References (8,854)

Get Suppliers (88)

Link to related information

Highlighted key substance is marked

Link to location of substance in patent

Key substances identified in the patent are annotated

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

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)

Sort options: Sort: Relevance

Relevance
Supplier: A to Z
Supplier: Z to A
Ships Within
Purity

Supplier: 1

Oakwood Chemical
United States
Last Updated: 1 Mar 2023

Substance: 7664-93-9
Sulfuric Acid, ACS Grade

Purity: 95-98%

Purchasing Det: Order From Sup
100 ml, USD 25
1 L, USD 40.00
2.5 L, USD 80.00

Link to detail

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 Mar 2023

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 tablets and mobile devices.

Select Center Flip fragment Cut | Copy | Paste

ChemDoodle

Model with CAS Registry Number

Clear | Eraser

Labeling

Undo | Redo

Templates

Open | Save

Zoom

Draw bonds

Draw rings

Add charges

Chain tool

Repeating groups

Variable point of attachment

Lock atoms/chains/rings

Make reaction

Reaction mapping

Break/form bonds

OK Cancel

ChemDoodle®

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, an isocyanate compound, an agent, at least one isothiazolone biocide, and a binder.

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

PatentPak Viewer Get Prior Art Analysis Full Text

References

8:57 AM

Prior Art Analysis (198)

[Aqueous dendritic amine coatings containing dendritic poly\(amido\)amine \(PAMAM\)](#)

View Results

Complete

View Results from the search history

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