

CAS SCIFINDERⁿ

QUICK REFERENCE GUIDE

CAS

A division of the
American Chemical Society



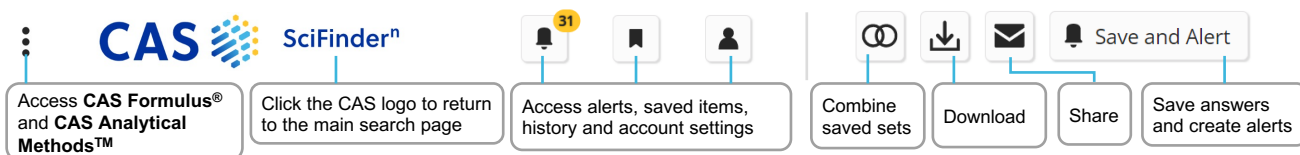
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Solution interface and References search

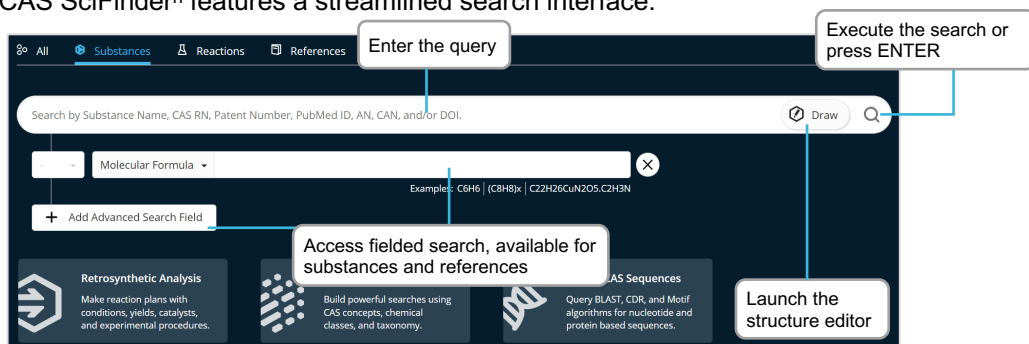
Main interface

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



Search interface

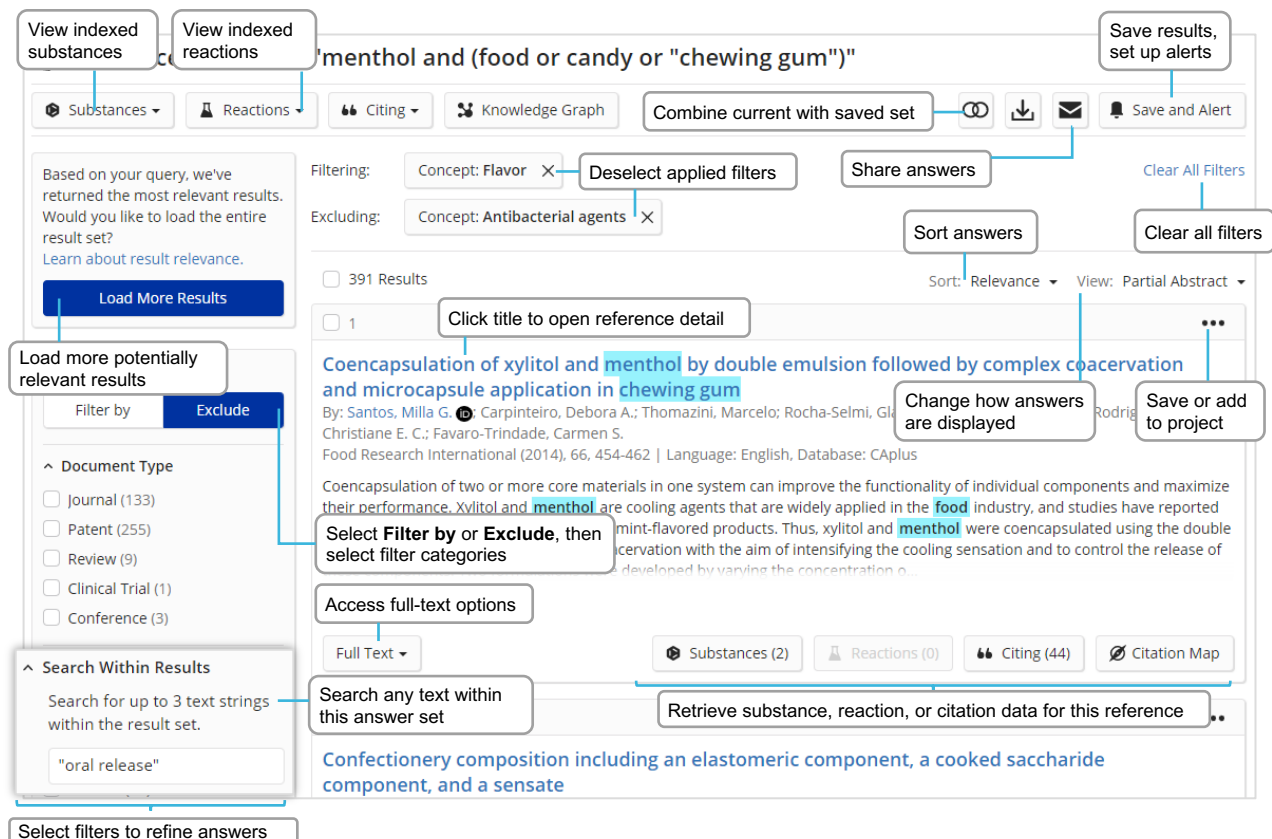
CAS SciFinder[®] features a streamlined search interface.



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 menthoxyalkanol (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

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

Get similar references

Get Similar References

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

×

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

The screenshot shows the top navigation bar with tabs for All, Substances, Reactions, References, and Suppliers. Below this is a search bar with the text "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and a button "Enter chemical name query". To the right of the search bar is a button "Click to draw new structure" and a button "Edit". Below the search bar are three main search options: "Add Advanced Search Field", "Search CAS Lexicon", and "Search CAS Sequences". The "Add Advanced Search Field" option includes a button "Add advanced search fields" and a description "Make reaction plans with conditions, yields, catalysts, and experimental procedures." The "Search CAS Lexicon" option includes a button "Search CAS Lexicon" and a description "Build powerful searches using CAS concepts, chemical classes, and taxonomy." The "Search CAS Sequences" option includes a button "Search CAS Sequences" and a description "Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences." There is also a button "Click query structure to edit" and a button "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.

The screenshot shows the search results interface. On the left, there are filters for "Structure Match" (As Drawn (116), Substructure (6M), Similarity (1,046)), "Analyze Structure Precision", "Chemscape Analysis", "Filter Behavior", and "Search Within Results". The main area displays a list of search results. The first result is "90357-06-5" with a chemical structure and the name "Biclutamide". The second result is "149104-88-1" with a chemical structure and the name "[4-(Methylsulfonyl)phenyl]boronic acid". The third result is "80-08-0" with a chemical structure and the name "Dapsone". Each result shows the number of references, reactions, and suppliers. On the right, there is a detailed view of the substance "149104-88-1". It shows the CAS RN, CAS Name, 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)". There is also a button "Retrieve data related to substance". At the bottom right, there is a button "Open editor with this structure" and a button "Download .sdf or .mol. Copy Smiles to Clipboard".

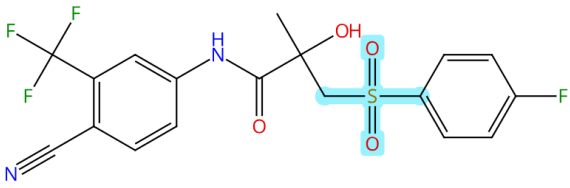
Substance detail and structure editor

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) [Download] [Email] [Save]



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

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	Press: 760 Torr
Density (Predicted)		

Key properties

Other Names

Experimental Properties

Experimental Spectra

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

Canonical SMILES
N#CC1=CC=C(C=C1C(F)(F)F)NC(=O)C(C)(O)CS(=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

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-trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-methyl-m-lactoluidide
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%

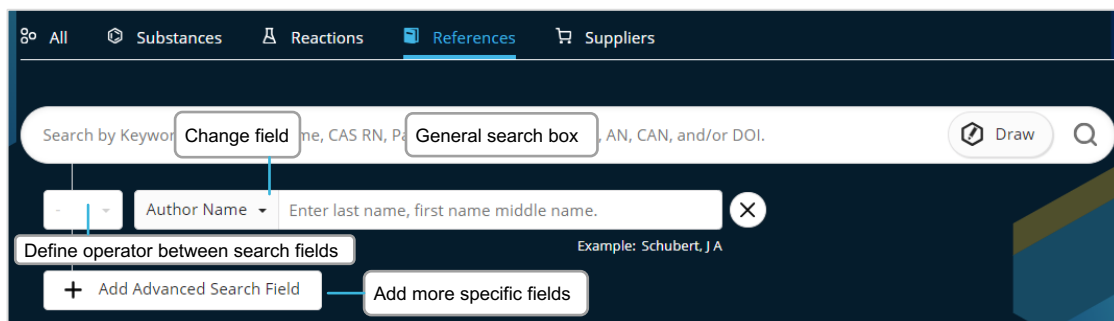
OK Cancel

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[®].

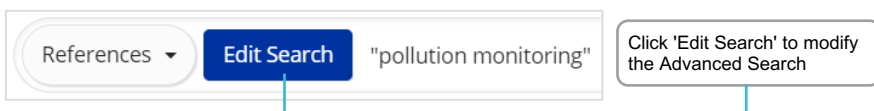
- Operators are processed in this order: **OR, AND, NOT**
- Operators are not available for a search using a single advanced search field
- Wildcards are allowed, e.g., peek*
- Use up to 50 Advanced Search Fields (49 if also using the main search field)



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: CAPIUS

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

Microplastics in marine environment review of methods for identification and quantification

By: Hidalgo-Ruz, Valeria; Gutwirth, Lars; Thompson, Richard C.; Threlkeld, Martin
Environmental Science & Technology (2012), 46(6), 3060-3075 | Language: English, Database: CAPIUS 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 δ) 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-rins, 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

Substances

Substances (3)

CAS RN | Chemical Name | Role

9003-07-0

C3H6
Polypropylene

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

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.

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.

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.

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, Jianglin et al.
[View All](#) [View all authors](#)
 Organic Process
 Development (2016), 20(5), 965-969
[View Source](#) Full Text

Absolute stereochemistry shown, Rotation (+) [Stage 2] Absolute stereochemistry shown, Rotation (-)
 Suppliers (48) Suppliers (149) 85% Suppliers (2)

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

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

View alternatives Alternative Steps (5)

Experimental Protocols

Synthetic Methods

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) 6.74-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, <i>J</i> = 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t, <i>J</i> = 11.8 Hz, 1H), 2.28 (d, <i>J</i> = 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° (<i>c</i> = 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.

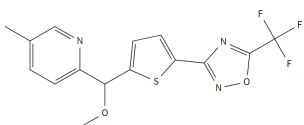
**Search CAS Lexicon**
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

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

Retrosynthetic Analysis
Draw or import a structure.

Enter a CAS Registry Number, SMILES, or InChI 🔍

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



Molecular Formula: C₁₅H₁₂F₃N₃O₂S (355.34)

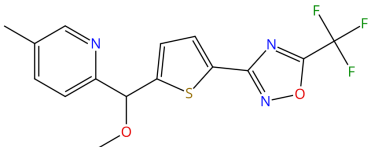
Zoom: 110% Start Retrosynthetic Analysis Cancel

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 Download



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.

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

Break and Protect Bonds [Learn more.](#)

[Clear All Bond Selections](#)

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

☐ Email me when my plan is complete

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

First bond to be broken

Protected bonds

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

Exclude steps or substances

Download, Share, and Save your plan

View plan steps

Edit plan options

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

Max Yield 79%

Avg. Yield 59%

Max Yield 83%

Avg. Yield 50%

Max Yield 47%

Reset +

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

1.1 Reagents: Butyllithium

Average Yield: 47%
Evidence (16)
Alternative Steps

1.1 Reagents: Potassium *tert*-butoxide
Solvents: Tetrahydrofuran
View All
Experimental Protocols (1)

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

Predicted Step Only
No reaction summary
Experimental Protocols

1.1 Solvents: Carbon tetrachloride

Maximum Yield: 79%
Evidence (1)
Alternative Steps (11)

Maximum Yield: 83%
Evidence (1)
Alternative Steps (14)

Filter by

Alternative Step Type

Predicted (48)

Stereochemistry

Non-Selective (48)

5 of 15

Predicted Step

Grouped similar reactions

Select View 8 similar Alternatives 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

Evidence reactions for (predicted) disconnection of precursor C

31-614-CAS-29434160

Steps: 1

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

Suppliers (49)

Suppliers (51)

Suppliers (61)

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

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

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. At the top, there's a search bar with 'Enter a query...' and a 'Substances' dropdown. Below the search bar, there's a 'Patent Markush search for drawn structure' section. On the left, there's a 'Patent Markush Match' section with a 'References' dropdown and a 'Filter Behavior' section. The main area displays a chemical structure with Markush search type annotations. On the right, there's a 'Markush search option' section with a 'Search Patent Markush' checkbox. Below the structure, there's a 'Patent claim 1' section with a 'PatentPak' dropdown and a 'Full Text' dropdown. A 'Link to a specific patent reference' is also present. The bottom section shows 'Heterocycle derivatives and methods of use' with a 'By: Peterson, John W.; Gessell, Lee, Deborah L.; Saini, Shamsher S.' citation.

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. At the top, there's a search bar with 'Enter a query...' and a 'Substances' dropdown. Below the search bar, there's a 'PatentPak' section. On the left, there's a 'Key Substances in Patent' section with a 'Download PDF' dropdown. The main area displays a chemical structure with key substances marked. On the right, there's a 'Download PDF including list of marked-up substances and annotations' section. Below the structure, there's a 'Link to related information' section. The bottom section shows 'Highlighted key substance is marked' and 'Link to location of substance in patent'. The bottom right section shows '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 (selected) 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)

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 Details: Order From Supplier
100 ml, USD 25.00
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 Aug 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, 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

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