

CAS SciFinderⁿ Quick Reference Guide

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Interface and Reference Search



SciFinder[®]



Links to CAS solutions: **CAS Formulus[®]** and **CAS Analytical Methods**

Click on the logo to go to the search landing page

Access to alerts, saved items & history and account settings

Combine saved sets

Download

Share

Save answers and create alert

Search Interface

CAS SciFinder[®] features a streamlined search interface.

Searching for...

- All
- Substances
- Reactions
- References**
- Suppliers
- Sequences
- Retrosynthesis

References

Enter the query

Execute the search or press ENTER

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

Enter a query...

Author Name Enter last name, first name middle name. Example: Schubert, A

Draw

Launch CAS Lex

Access fielded search, available for substances and references

Launch the structure editor

Reference Search

The References display features visualizations, dynamic facets and an easy-to-use interface layout

- References are ranked and sorted by relevance
- You may save your searches, send a link, set-up alerts or add to project list
- Filters allow you to focus the answers
- CAS PatentPak shows the location of the indexed substances in the patent full-text

Load further potentially relevant results for comprehensiveness

View indexed substances

View indexed reactions

References search for "menthol and (food or candy or "chewing gum")"

Substances Reactions Citing Knowledge Graph Combine current with saved set Save and Alert

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#)

Load More Results

Filtering: Concept: Flavor X Deselect applied filters Share answers Clear All Filters

Excluding: Concept: Antibacterial agents X

Sort answers Clear all filters

Sort: Relevance View: Partial Abstract

391 Results

1

Click title to open reference detail

Coencapsulation of xylitol and menthol by double emulsion followed by complex coacervation and microcapsule application in chewing gum

By: Santos, Milla G.; Carpinteiro, Debora A.; Thomazini, Marcelo; Rocha-Selmi, Gladys; Christiane E. C.; Favaro-Trindade, Carmen S. Food Research International (2014), 66, 454-462 | Language: English, Database: CAPlus

Coencapsulation of two or more core materials in one system can improve the functionality of individual components and maximize their performance. Xylitol and menthol are cooling agents that are widely applied in the food industry, and studies have reported mint-flavored products. Thus, xylitol and menthol were coencapsulated using the double emulsion with the aim of intensifying the cooling sensation and to control the release of menthol developed by varying the concentration of menthol.

Change how answers are displayed

Save or add to project

Filter Behavior

Filter by Exclude

Document Type

- Journal (133)
- Patent (255)
- Review (9)
- Clinical Trial (1)
- Conference (3)

Search Within Results

Search for up to 3 text strings within the result set.

"oral release"

Select filters to refine answers

Select Filter by or Exclude, then select filter categories

Access full-text options

Full Text

Substances (2) Reactions (0) Citing (44) Citation Map

Search any text within this answer set

Retrieve substance, reaction or citation data for this reference

Confectionery composition including an elastomeric component, a cooked saccharide component, and a sensate

Reference detail and search operators

Fruit juice-containing food products with refreshing and cooling flavors

Publication source information

PATENT

Patent Number
WO2005048743

Publication Date
2005-06-02

Application Number
WO2004JP17524

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

Save

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

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

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

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

Similar References **NEW**

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2005048743	English	A1	PDF PDF+ Viewer	2005-06-02	WO2004JP17524	2004-11-18

Patent Family

Priority Application



Priority Application Number	Application Date
JP2003-389758	
WO2004JP17524	

IPC and indexed subject matter, substance indexing and formulations

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

Boolean Operators Logical operators define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.:

References (flavor **or** odor) **and** menthol **not** cigarette   Draw 

AND Requires both terms to be present within the document



OR Requires either one or both terms to be present
Connect synonyms with OR



NOT Excludes documents from an answer set containing the word(s)
after NOT



Wildcards Wildcards allow for more comprehensive retrieval
Use is allowed in reference, substance and filter searches
Internal and right-hand truncation is available

* Replaces 0 to any number of characters E.g.: polymorph* | immunoglobulin*conjugate*

? Replaces 0 or 1 character E.g.: benzonorboren?

Terms masked with double quotes will be searched as a precise phrase.

E.g.: "Programmed cell death protein" only finds Programmed cell death protein

Substance name and structure

Name searches

Search with one or more substance names or identifiers

Streptomycin

57-92-1

Streptomycin sulfate

"Streptomycin sulfate" Streptomycin

Sulfoximin*

WO2019234160

Finds Streptomycin record

Finds Streptomycin record, uses CAS Registry Number® as identifier

Finds 3 records: Streptomycin, Streptomycin sulfate and Sulfate

Finds 2 records: Streptomycin sulfate and Streptomycin

Finds all names that start with the stem Sulfoximin

Finds all indexed substances for this patent

Structure searches

Substance searches return results in an intuitive interface. The display highlights most relevant hits, critical property information and high-resolution images

The screenshot displays a chemical search interface with several key components and annotations:

- Search Interface:** A search bar with the placeholder "Enter a query..." and a search button. Below it, a filter menu shows "Substances" selected, with other options like "Reactions", "References", "Suppliers", and "Sequences".
- Advanced Search:** A section for "Substances" with a dropdown for "AND" and "Molecular Formula". A button "Add Advanced Search Field" is annotated with "Add more advanced search fields". A chemical structure of a sulfonamide is shown with the annotation "Click query structure to edit".
- Results List:** A list of search results. The first result is "90357-06-5" with a chemical structure and the annotation "Click CAS Registry Number to open details". The second result is "149104-88-1" with a chemical structure and the annotation "Click on structure to open flyout window". The third result is "80-08-0" with a chemical structure and the annotation "Change amount of details displayed".
- Structure Match Panel:** On the left, a "Structure Match" panel allows filtering by "As Drawn (115)", "Substructure (5.9M)", and "Similarity (1,044)". It also includes "Analyze Structure Precision" and "Chemscape Analysis" options.
- Filter Behavior:** A "Filter Behavior" section with "Filter by" and "Exclude" buttons. Under "Reaction Role", "Reference Role" is selected, with the annotation "Reference Roles show which new information was reported about a substance in the literature".
- Search Within Results:** A "Search Within Results" section with a "Draw" button and the annotation "Search a (sub)structure within this set of substances".
- Structure Detail Panel:** A flyout window for CAS RN 149104-88-1, showing the CAS Name "[4-(Methylsulfonyl)phenyl]boronic acid" and a chemical structure. It includes a "Retrieve data related to substance" section with options like "Get Substance Details", "Get Bioactivity Data", "Get Reactions (2,395)", "Synthesize (9)", "Start Retrosynthetic Analysis", "Get References (1,330)", and "Get Suppliers (106)".
- Structure Editor:** At the bottom right, a panel for editing the structure, with buttons for "Open editor with this structure" and "Download .sdf or .mol. Copy Smiles to Clipboard".

Substance detail and structure editor

Substance detail

Click on the CAS Registry Number to show substance details with structure, molecular formula, properties and further data

CAS Registry Number: 90357-06-5

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

$C_{18}H_{14}F_4N_2O_4S$ 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)	-

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(F)(F)F)NC(=O)C(O)(C)CS(=O)=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
LKJPPYSCBVHEWU-UHFFFAOYSA-N

The chemical identifier list contains SMILES, InChI, systematic, trivial and tradenames. 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-lactotoluidide
Bicalutamide

CAS Draw editor

Define structure and reaction queries with the structure editor

CAS Draw - Import and export structure files

Enter CAS Registry Number, SMILES or InChI to create structure

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

Lasso | Marquee tool objects. Ctrl-click to select or deselect individual objects.

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. ▲ Triangles indicate further options are available

Draw rings

Resize window

Type element symbol to draw

Molecular Formula: $C_{18}H_{14}F_4N_2O_4S$ (430.38)

Zoom: 90%

OK Cancel

Advanced search query builder

Advanced Search Query Builder

Provides specific reference and substance search fields from CAS SciFinder[®]'s landing page

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

References

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

Enter a query...

Define operator between search fields

Author Name

Example: Schubert, J A

+ Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

Examples

Advanced Reference Search

"pollution monitoring"

AND polyethylene

OR polypropylene

Operator to combine search fields

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

Advanced Substance Search

steel*

AND >0

Experimental values only.

Operator to combine search fields

Query interpretation:
Steel with tensile strength property information

References "pollution monitoring"

Click 'Edit Search' to modify the Advanced Search

Advanced Search Fields

The below advanced search fields and categories are available

Reference

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

Substance

- 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

Roles are linked to the substances and allow you to find focused publications connecting the 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 type of roles that are connected to the substance(s) in the publications.

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 a large number of references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3217 publications that describe polypropylene as a pollutant. Search within or concepts can be used to restrict result to marine pollution.

CAS RN	Chemical Name	Role
9003-53-6	Polystyrene	Pollutant, Occurrence
11898-92-9	1-Propene, homopolymer	Pollutant, Occurrence

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

Sequence searching

Search Options

Three different search modalities exist

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

BLAST similarity search

BLAST allows 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.


Perform a BLAST search

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


The screenshot displays the 'Sequences' search interface. On the left, a sidebar titled 'Searching for...' lists various search categories, with 'References' highlighted. The main area is titled 'Sequences' and includes a search input field containing '> human insulin sequence' and the sequence 'FVNQHLCGSHLVEAYLVCGERGFFYTPKTGIVEQCCTSIICSLYQLENYCN'. Above 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'. Below the input field are three callout boxes: 'Paste sequence into this window', 'Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane', and 'Include NCBI sequences'. On the right side, there are options for 'Sequence Type' (Nucleotide and Protein, with Protein selected), 'Search Within' (Nucleotides and Proteins, with Proteins selected), and a checked option for 'Include NCBI Sequences'. A 'Start Sequence Search' button is at the bottom right. Below the search area is the 'Advanced Sequence Search' section, which includes various parameters: 'Alignment Identity %' (set to -), 'Match with Gaps?' (Yes selected), 'Gap Costs' (Existence 11 Extension 1), 'Query Coverage %' (90), 'Word Size' (3), 'Scoring Matrix' (BLOSUM62), 'BLAST Algorithm' (BLASTp), 'E-Value' (10), and 'Exclude Low Complexity Regions' (No selected). A callout box on the left points to this section, labeled 'Advanced BLAST parameters'.

BLAST result 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%

Results will expire on
May 29, 2023.

> human insulin sequence
FVNQHLCGSHLVEAFLVCGERGFYTPKGTIVEQC
CTSI CSLYQL ENYCN



[View Results](#)

[Edit Search](#)

Complete


View Results

View 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 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

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

View Less v

Alignment Details v References

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

Match

Mismatch

Q 1 FVNQHLCGSH LVEA- YLVCG ERGFFYTPKT ---GIVEQC CTSICSLYQL ENYCN 55

S 1 FVNQHLCGSH LVEAL YLVCG ERGFFYTPKS DDARGIVEQC CTSICSLYQL ENYCN 55

Start of alignment in query and subject sequences

Gap in the query sequence

Matches: 49
Mismatches: 6

Alignment Length:
49+6=55

[References](#)

[Get References for this sequence](#)

Filter Results

Filtering dynamically changes the result set

to

Expectation Value

to

Alignment Length
Query Length

to

Alignment Length
Subject Length

to

Number of Matches
Alignment Length

to

Organisms

Homo sapiens (25)

Mus musculus (25)

Reaction searching

Reaction searches

Reactions queries can be CAS Reaction Numbers, Substance Names, CAS Registry Numbers, document identifiers, or a chemical structure

- Reactions are grouped
 - into schemes with identical reactants and products
 - into transformations
- Reactions are sorted by yield within a scheme

Searching for...

- All
- Substances
- Reactions** Select reactions
- References
- Suppliers
- Sequences
- Retrosynthesis

Reactions

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

Enter a query... Edit Q

Click on reaction query to edit

Edit Drawing Remove

View by structure match

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

Reactions search for drawn structure

References

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)

[View All](#)

Reaction Mapping

26,932 Results

Group: By Scheme Sort: Yield View: Expanded

Scheme 1 (2 Reactions) Steps: 1 Yield: 100%

Click on structure to view substance information

Absolute stereochemistry shown, Rotation (+)

Suppliers (48) View suppliers Suppliers (387)

Click on reaction query to edit

Yield for displayed reactions

View reaction details

View reaction reference

Access annotated patent full-text

Filter reaction results

31-614-CAS-27240963 Steps: 1 Yield: 100%
1.1 Reagents: [Triethylamine](#), [Diphenylphosphoryl 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, WO2002024705 A1
2002-03-28
[PatentPak](#) Full Text

31-614-CAS-27633989 Steps: 1 Yield: 100%
1.1 Reagents: [Triethylamine](#), [Diphenylphosphoryl azide](#)
Solvents: [Toluene](#); 40 - 50 °C; 1 h, 110 °C; 110 °C → 70 °C
1.2 70 °C; overnight, 70 °C → 85 °C
[Experimental Protocols](#)

Preparation of N-(isoxazoloquinolinyl)cyclohexyl)carbox amides and analogs as MRP1 inhibitors
By: Bonjouklian, Rosanne; et al
World Intellectual Property Organization, WO2001046199 A1
2001-06-28
[PatentPak](#) Access annotated patent full-text

Reaction details

Reaction details

Details incl. 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 et al.
View All
Organic Process Development (2016), 20(5), 965-969

View Source Full Text

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

View all authors

Step 1

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (-)

Suppliers (48)

Suppliers (133)

Supplier (1)

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

View alternatives Alternative Steps (5)

Experimental Protocols

Synthetic Methods View detailed procedures

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

Reactants 1-Ethyl(1R,3S)-1,3-cyclohexanedicarboxylate
Benzyl alcohol

Reagents Triethylamine
Diphenylphosphoryl azide

Solvents Toluene

Procedure 1. Add diphenylphosphoryl azide (DPPA) (166 mL, 769 mmol) and triethylamine (107 mL, 769 mmol) to (1S, 3R)-3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).

Characterization Data View characterization data

Ethyl (1R,3S)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate

Proton NMR Spectrum	(300 MHz, CDCl ₃) δ7.48-7.30 (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

Launch plan generation

There are two main options to launch CAS SciFinderⁿ's Retrosynthesis Planner

- 1 Draw structure in the Retrosynthesis editor from the landing page, substance can be novel
- 2 Open structure flyout window and start Retrosynthetic Analysis

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: $C_{13}H_{12}F_3N_3O_5$ (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)

2 Start Retrosynthetic Analysis

Get References (1)

Get Suppliers (0)

Edit Structure Reset

Plan options

Edit plan options to...

- increase the synthetic depth
- protect bonds through the entire synthetic route
- define bonds to be broken in the first disconnection
- change the starting material cost limit
- create a predictive plan with more meaningful alternatives, e.g. for poly- or heterocyclic molecules

Change 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.

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)

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)

1st bond to be broken

Protected bonds

Generate plan

Retrosynthesis plan and alternative steps

Open plan

The Experimental Plan is available within a few seconds, the calculation of the Predictive Retrosynthesis Plan will take a bit longer

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Overview Steps Predicted Results **ON** Switch predicted steps on/off

Exclude steps or substances

View Excluded Options

Download, Share and Save your plan

Plan Information

View plan steps

View plan information

Estimated Yield: 22%
Overall Price: \$108.55
(USD per 100 grams)

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
Edit Plan Options

Edit plan options

Scoring Profiles Adjust Scoring Options

Complexity Reduction

Convergence

Evidence

Cost

Purple lines mark experimental steps,

Green dotted lines indicate predicted steps

Review and select alternative disconnections

Alternative steps

Provide an overview of all experimental and predicted disconnections
Evidence reactions are displayed as a reaction answer set

- Access Evidence Reactions from the ① link in the steps overview or ② the alternative reaction scheme

Overview Steps

View step specific evidence and alternate steps below or select the node between steps on the plan.

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

B → D + E
Average Yield: 59%
Evidence (23)
Alternative Steps (34)

C → F + G
Average Yield: 59%
① Evidence (1,580)
Alternative Steps (49)

D → H + I
Maximum Yield: 79%
Evidence (1)
Alternative Steps (11)

Filter by

Alternative Step Type

Predicted (49)

Stereochemistry

Non-Selective (49)

Grouped similar reactions

View 4 similar Alternatives

View Evidence (1,580)

Average Yield: 59%

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Mapping Data Available (727)

Reaction Scale

Milligram (130)

Gram (20)

No Scale Provided (577)

Experimental Protocols

Synthetic Methods (286)

Experimental Procedure (467)

Filtering: Experimental Protocols: 2 Selected

727 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction)

Steps: 1 Yield: 72%

HO-C(=O)-C6H4-CN + F-C(=O)-O-C(=O)-F → F-C(=O)-O-C(=O)-F + HO-C(=O)-C6H4-CN

Suppliers (81) Suppliers (77) Suppliers (65)

31-614-CAS-24629063 Steps: 1 Yield: 72%
1.1 Reagents: Triethylamine, Hydroxylamine
Solvents: Dimethylformamide, Tetrahydrofuran; 2 h, reflux
1.2 0.5 h, reflux

Synthesis, Antifungal Activity, DFT Study and Molecular Dynamics Simulation of Novel 4-(1,2,4-Oxadiazol-3-yl)-N-(4-phenoxyphenyl)benzamide Derivatives
By: Yang, Zihui et al
Chemistry & Biodiversity (2021), 18(12), e2100651

Evidence reactions for (predicted) disconnection of precursor C

Scoring Options

Scoring Options

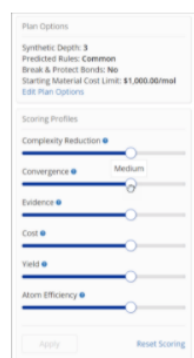
For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

- 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

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

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.



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Supplier Searching and ChemDoodle®

Suppliers searching

Suppliers searching allows for direct access to 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 Product List United States Last Updated: 1 Mar 2023	<input checked="" type="checkbox"/> 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 Product List United States Last Updated: 1 Mar 2023			
<input type="checkbox"/> 3 Oakwood Chemical Product List 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)

Purity: ≥99% (2), 95-98% (106)

Preferred Supplier: Oakwood Chemical

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: 1 Mar 2023; Last Updated: 1 Mar 2023; Order From Supplier

Substance Information: CAS Registry Number: 7664-93-9; CAS Name: Sulfuric acid

OS(=O)(=O)O

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Select, Clear | Eraser, Labeling, 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

Model with CAS Registry Number

Undo | Redo, Templates, Open | Save, Zoom

OK, Cancel

Prior Art Analysis

Prior Art Analysis

Upon viewing a patent Reference Detail page, an option to Get Prior Art Analysis is available. Results appear in the search history.

- AI-based relevance prediction
- Based on a single patent document as the starting point
- Analysis of CAS concepts, indexed substances, IPC codes and additional full-text
- Generates list of relevance-ranked previously known documents, comprising patents 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 agent, at least one isothiazolone biocide, and a binder.

Keywords: aqueous dendritic amine coating, PAMAM, 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 \(PAMAM\)](#)

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