

CAS SCIFINDERⁿ

FOR ACADEMIA

QUICK REFERENCE GUIDE

CAS



A division of the
American Chemical Society

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Solution interface and References search

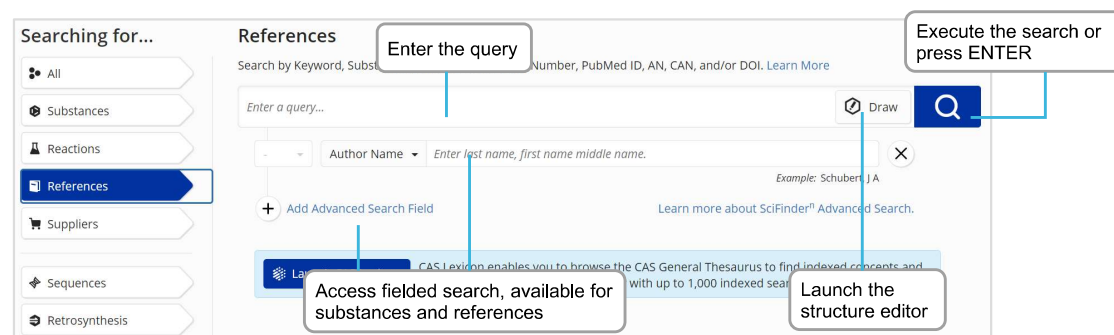
Main interface

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



Search interface

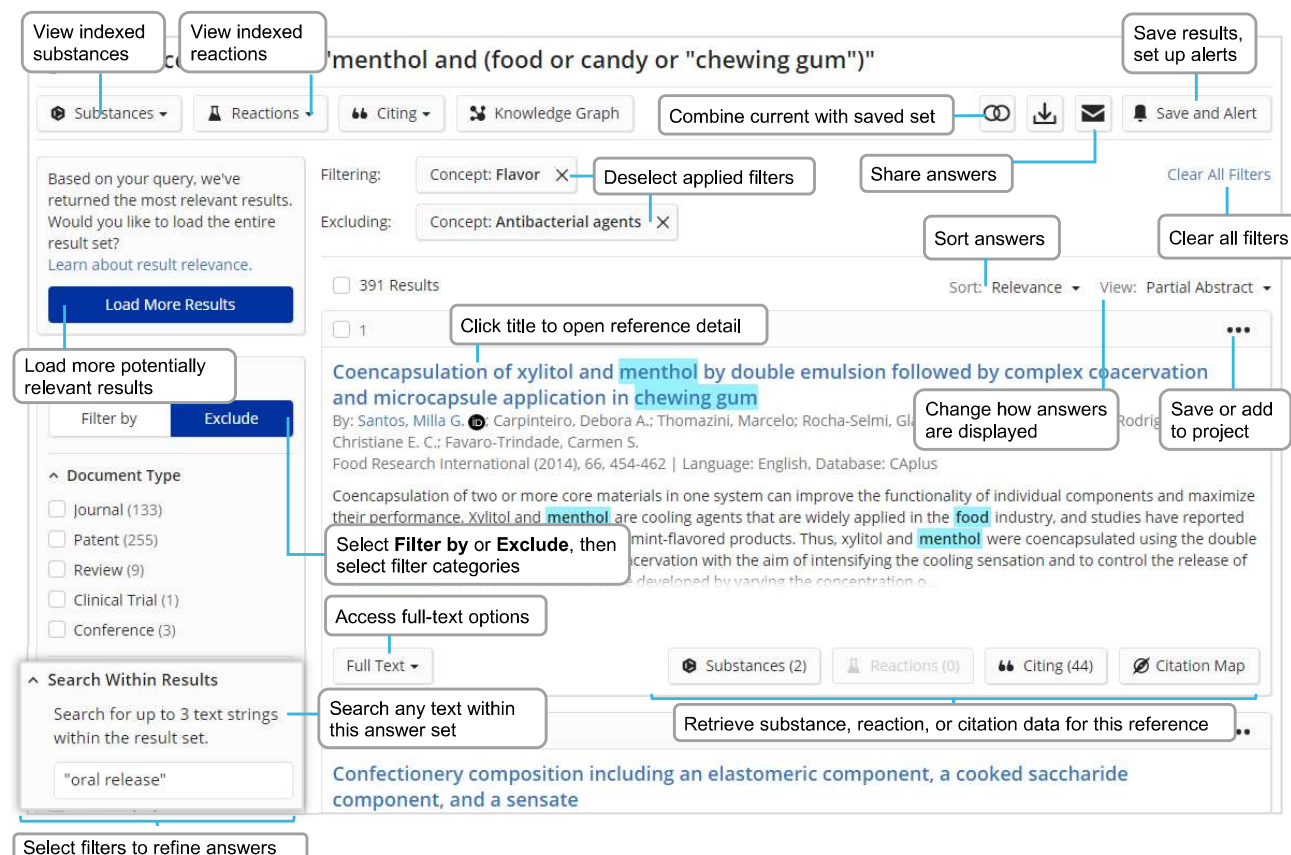
CAS SciFinder[®] features a streamlined search interface.



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[®].

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

Database information

AN: 2005:470226
CAN: 143:25602
CAplus

Language
English

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

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

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

IPC and indexed subject matter, substance indexing, and formulations

Similar References **NEW**

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

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 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:

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: benzonorboren?

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 to draw new structure

Edit

Click query structure to edit

Learn more about Sci

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

Analyze structure precision

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

Create Chemscape Analysis

Filter Behavior

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)

Synthesis (9)

Start Retrosynthetic Analysis

Get References (1,330)

Get Suppliers (106)

Open editor with this structure

Download .sdf or .mol. Copy Smiles to Clipboard

16K 4,932 102

CAS RN 149104-88-1

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

HO-B-C6H4-SO2-CH3

Open editor with this structure

Download .sdf or .mol. Copy Smiles to Clipboard

Edit Structure - Reset +

References 4,118 Reactions 227 Suppliers 114

References 851 Reactions 34 Suppliers 98

19542-67-7

Reference Roles show which new information was reported about a substance in the literature

C10H9NO2S (2E)-3-[[4-(Methylphenyl)sulfonyl]-2-propenenitrile

1,330 2,395 106

CAS SciFinder® Quick Reference Guide Academic | 5

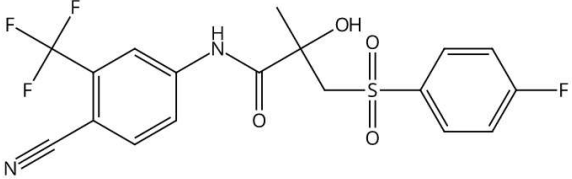
Substance detail and structure editor

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]



$C_{18}H_{14}F_4N_2O_4S$ — Molecular formula in hill order

Propanamide, M-[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)	650.3-650.8 °C	Pressure: 760 Torr
Density (Predicted)	1	-

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: LKJPYSVBVHEWU-UHFFFAOYSA-N

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

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

Key properties

CAS Draw editor

You can further define structure and reaction queries using the CAS Draw structure editor.

CAS Draw — Import and export structure files

Enter CAS Registry Number, SMILES, or InChI to create structure

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

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

Lasso | Marquee tool

Draw atoms and bonds | Eraser

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Add attachment point to fragment | Select from templates

Add positive charge | Add negative charge

Repeating groups | Carbon chain tool

Define variable point of attachment at ring | Reaction role

Atom mapping | Lock rings/lock atoms

Bond mapping | Draw reaction arrow

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

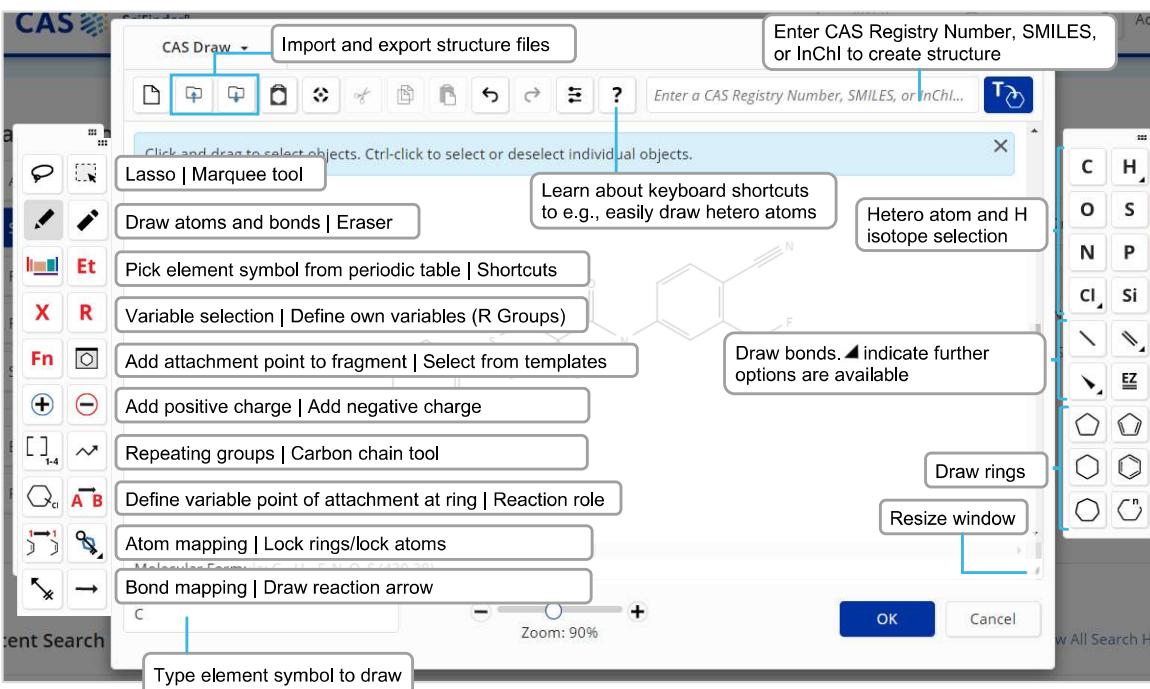
Hetero atom and H isotope selection

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw



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)

References

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

Enter a query... Change field General search box Draw

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

Define operator between search fields

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

Advanced Search examples

Advanced References Search

"pollution monitoring"

Operator to combine search fields

AND Chemical Name polyethylene

OR Chemical Name polypropylene

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

Advanced Substances Search

steel*

AND Tensile Strength (Mpa) >0

Experimental values only.

Query interpretation:
Steel with tensile strength property information

References Edit Search "pollution monitoring"

Click 'Edit Search' to modify the Advanced Search

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)x
Polypropylene

278K References | 6,321 Reactions | 20 Suppliers

Document Type

Substance Role

- Uses (262K)
- Properties (60K)
- Process (50K)
- Biological Study (22K)
- Preparation (19K)

View All

Language

Publication Year

Available at My Institution

Recycling micro polypropylene in modified hot asphalt mixture
By: Burulana, Daniela Laura; Georgescu, Puiu Lucian; Carp, Gabriel Bogdan; Ghisman, Vioricia
Scientific Reports (2023), 13(1), 3639 | Language: English, Database: CAPlus 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., 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...
...hlt mixtures were added 3 proportions of polypropylene-based microplastics such e mixture performance is shown at the asphalt mixture sample with 0.3% of -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

After clicking "View All", more specific roles can be selected

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)

View All

Language

Publication Year

1974 to 2023

No Min to No Max Apply

Microplastics in marine environment review of methods for identification and quantification
By: Hidalgo-Ruz, Valeria; Gustow, Lars; Thompson, Richard C.; Thiel, Martin
Environmental Science & Technology (2013), 46(6), 3060-3075 | Language: English, Database: CAPlus 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 m³" for sediment and sea surface studies and "Items per m³" for water column studies. Mesh size of sieves and filters used during sampling or sample processing influence abundance estimates. Most studies reported two main size ranges of microplastics: (I) 500 µm-5 mm, which are retained by a 500 µm sieve/net, and (II) <500 µm, or fractions thereof that are retained on filters. We recommend that future programs of monitoring continue to distinguish these size fractions, but we suggest standardized sampling procedures which allow the spatiotemporal comparison of microplastic abundance across marine environments.

Full Text ▾

Substances (3) | Reactions (0) | Citing (2,083) | Citation Map

Substances

9003-53-6

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 interface. On the left is a navigation sidebar with categories like 'Substances', 'Reactions', 'References', 'Suppliers', 'Sequences', and 'Retrosynthesis'. The main area is titled 'Sequences' and includes a search input field with the example sequence: '> human insulin sequence' followed by 'FVNQHLCGSHLVEAFLVKGERGFFYPKTKTIVEQCCTSIICSLYQLENYCN'. There are tabs for 'BLAST', 'CDR', and 'Motif', and buttons for 'Upload Sequence' and 'Clear Search'. A callout box labeled 'Sequence Search options' points to the 'BLAST' tab. Below the search input is an 'Advanced Sequence Search' section with various parameters: 'Alignment Identity %' (set to -), 'Match with Gaps?' (radio buttons for Yes/No), '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' (radio buttons for Yes/No). A callout box labeled 'Advanced BLAST parameters' points to this section. On the right side, there are options for 'Sequence Type' (Nucleotide/Protein) and 'Search Within' (Nucleotides/Proteins). A callout box labeled 'Include NCBI sequences' points to the 'Include NCBI Sequences' checkbox, which is checked. A 'Start Sequence Search' button is also visible.

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
CTSICSLYQLENYCN

[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](#)

[Alignment Details](#) [Alignment](#) [Subject](#) [References](#)

[Get References for this sequence](#)

+ Mismatch: Query aa aligned to functional equivalent subject aa

Match Mismatch

E-Value: 5.12823e-26

Q 1 FVNQHLCGSH LVEA YLVCGERGFFYTPKT -----GIVEQC CTSICSLYQL ENYCN 55

S 1 FVNQHLCGSH LVEA YLVCGERGFFYTPK **DDAR**GIVEQC CTSICSLYQL ENYCN 55

Start of alignment in query and subject sequences

Gap in the query sequence

Filter results

Filtering dynamically changes your result set.

E-Value

0 to 10⁶

Expectation Value

Query Coverage %

0 to 100

Alignment Length
Query Length

Subject Coverage %

0 to 100

Alignment Length
Subject Length

Alignment Identity %

0 to 100

Number of Matches
Alignment Length

Sequence Length

26 to 9521

Organisms

Homo sapiens (25)

Mus musculus (25)

Reactions search

Performing a Reactions search

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

Searching for...

- All
- Substances
- 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...

Select reactions

Click on reaction query to edit

Edit Drawing Remove

Reactions search results

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

Reactions search for drawn structure

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

References

View by structure match

Structure Match

- As Drawn (0)
- Substructure (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

Yield for displayed reactions

Suppliers (48) View suppliers Suppliers (387)

View reaction details

View reaction reference

Access annotated patent full-text

Filter reaction results

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, et al.
View All [View all authors](#)

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

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

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

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

Reactants [1-Ethyl \(1*R*,3*S*\)-1,3-cyclohexanedicarboxylate](#)
[Benzyl alcohol](#)

Reagents [Triethylamine](#)
[Diphenylphosphoryl azide](#)

Solvents [Toluene](#)

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

Characterization Data [View characterization data](#)

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

Proton NMR Spectrum	(300 MHz, CDCl ₃) δ 7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, <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° (c = 1 in DCM).
HRMS	(ESI) [M + H] ⁺ calculated for C ₁₇ H ₂₄ NO ₄ 306.1700, found 306.1700
State	sticky solid

CAS Method Number 3-451-CAS-15598720

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

Reaction Notes [Further important notes](#)
scalable

Retrosynthesis planner

Launching the tool

There are two primary ways to launch the retrosynthesis tool within CAS SciFinder[®]:

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

Searching for... Retrosynthesis

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

Enter a CAS Registry Number, SMILES, or InChI

Draw or change atoms or bonds.

Molecular Formula: C₁₇H₁₂F₃N₂O₂S (355.34)

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

Get References (1)

Get Suppliers (0)

Edit Structure Reset

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.

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)

Email me when my plan is complete

Create Retrosynthesis Plan

Generate plan

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

Powered by ChemPlanner®

Overview Steps Predicted Results ON Switch predicted steps on/off View Excluded Options Save

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

Scoring Profiles Adjust scoring options

Complexity Reduction
Convergence
Evidence
Cost

Retrosynthesis Step Key

Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

Experimental Steps
Predicted Steps

View plan steps
View plan information
Edit plan options
Adjust scoring options
Switch predicted steps on/off
Purple lines mark experimental steps
Green dotted lines indicate predicted steps
Review and select alternative disconnections
Download, Share, and Save your plan

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.

Overview Steps

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

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

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

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

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

Filter by

Alternative Step Type
 Predicted (49)

Stereochemistry
 Non-Selective (49)

Grouped similar reactions

1 of 15
View 4 similar Alternatives **2** 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%

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

31-614-CAS-24629063 Steps: 1 Yield: 72%
1.1 Reagents: Triethylamine, Hydroxylamine
Solutions: 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

Full Text

Evidence reactions for (predicted) disconnection of precursor C

Retrosynthesis scoring options

Scoring options

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

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

Scoring profiles

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

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



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.



Markush search and CAS PatentPak

Markush search

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

The screenshot shows the CAS SciFinder interface for a Markush search. The search bar at the top contains the text "Enter a query...". Below the search bar, there is a drawing tool with a "Search Patent Markush" checkbox. The results panel on the left shows "Patent Markush Match" with "As Drawn (96)" selected. The main area displays a chemical structure with Markush groups (G1-G4) and a patent reference: "Preparation of deuterated dihydrofuranones for the treatment of irritation symptoms of joint degeneration, as well as of acute pain, and dysmenorrhea". Callouts point to various features: "Markush search option" (checkbox), "Markush search type" (dropdown), "Assembled Markush hit structure" (chemical structure), "Filter by patent authority" (checkboxes for WIPO, US, etc.), "Markush location" (dropdown), and "Link to a specific patent reference" (text).

CAS PatentPak

There are three CAS PatentPak options for viewing a patent PDF:

- **PDF:** Full-text patent PDF only; text-searchable PDF
- **PDF+:** Full-text patent PDF with marked-up Key Substances; text-searchable PDF
- **Viewer:** Patent PDF with linked markups of Key Substances (see below)

The screenshot shows the CAS PatentPak interface for viewing a patent PDF. The interface includes a search bar, a drawing tool, and a results panel. Callouts highlight various features: "Download PDF including list of marked-up substances and annotations" (dropdown), "Download PDF" (button), "Link to related information" (text), "Highlighted key substance is marked" (text), "Marks key substance curated by CAS scientists" (text), and "Link to location of substance in patent" (text). The main area displays a patent PDF with marked-up key substances and annotations.

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

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)

389 Results

Supplier	Substance	Purity	Purchasing Det
1	7664-93-9	95-98%	Order From Sup
Oakwood Chemical	Sulfuric Acid, ACS Grade		100 ml, USD 25.00 1 L, USD 40.00 2.5 L, USD 80.00

Sort options: Relevance, Supplier: A to Z, Supplier: Z to A, Ships Within, Purity

Recency of information: Last Updated: 1 Mar 2023

Link to detail

Oakwood Chemical Product List

Preferred Supplier

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

Email: sales@oakwoodchemical.com

Phone: 1-800-467-3386

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

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

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

Stock Status: Maintained in stock

Pricing Information: Last Updated 1 Mar 2023

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

ChemDoodle®

OK, Cancel

Prior Art Analysis

Reviewing Prior Art

When viewing a patent Reference Detail page, an option to "Get Prior Art Analysis" is available. Results will also appear in the search history. This functionality:

- Provides an AI-based relevance prediction.
- Is based on a single patent document as the starting point.
- Includes analysis of CAS concepts, indexed substances, IPC codes, and additional full-text.
- Generates a list of relevance-ranked previously known documents, comprising patent and non-patent literature.

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

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

PATENT

Patent Number: [WO2017135893](#)

Publication Date: 2017-08-10

Application Number

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

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

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

PatentPak Viewer Get Prior Art Analysis Full Text

References

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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