

CAS SCIFINDERⁿ

**QUICK
REFERENCE
GUIDE**

CAS

A division of the
American Chemical Society



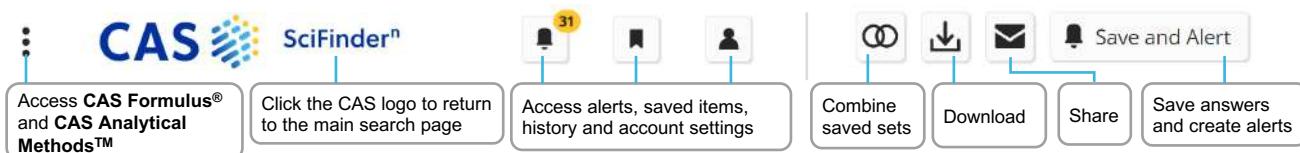
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Solution interface and References search

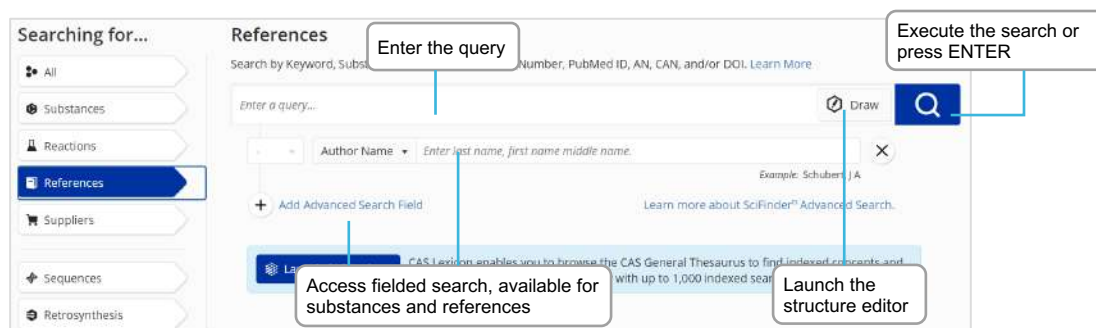
Main interface

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



Search interface

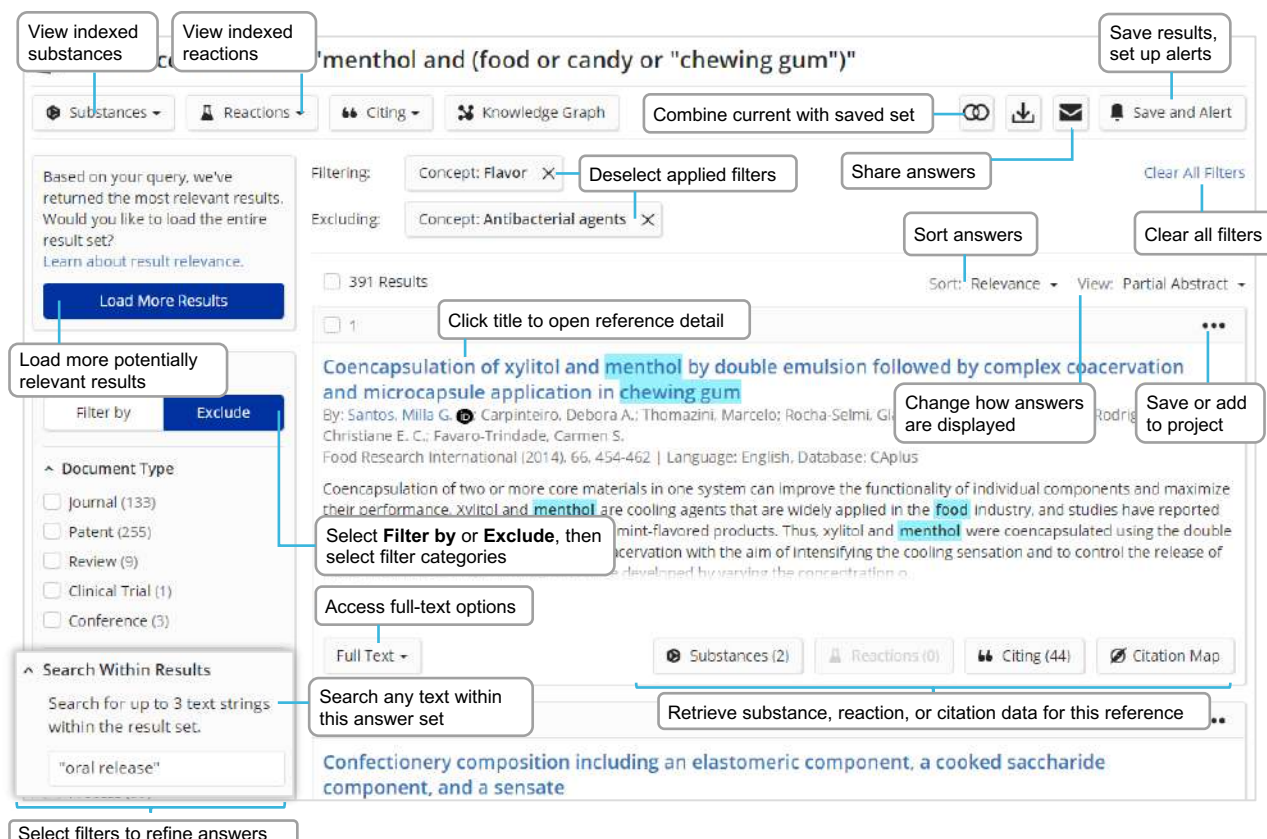
CAS SciFinder[®] features a streamlined search interface.



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
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

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

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

Similar References NEW

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

Patent Family

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

Priority Application

Priority Application Number	Application Date
JP2003-369758	
WO2004-JP17524	

IPC and indexed subject matter, substance indexing, and formulations

Get similar references

Get Similar References

IPC Data
Concepts
Substances
Formulations
Cited Documents

Boolean operators

You can use logical operators to create precise text queries.

Use parentheses to group logical expressions, such as related terms using "OR", ex:

References (flavor or odor) and menthol not cigarette X Draw Q

AND Requires both terms to be present within the document

OR Requires either one or both terms to be present (connect synonyms with OR)

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



Wildcards allow for more comprehensive results in reference, substance, and filter searches. Internal and right-hand truncation is possible.

* Replaces 0 to any number of characters ex: polymorph* | immunoglobulin*conjugate*

? Replaces 0 or 1 character ex: benzonorbornen?

Phrases containing double quotes will be searched as a precise phrase.

Ex: a search for "Programmed cell death protein" only finds results that exactly match: "Programmed cell death protein."

Substance name and structure search

Substances search

You can search substances by placing one or more substance names or identifiers into the query box. You can also draw or edit a structure. Below are name search option examples.

Streptomycin

Finds Streptomycin record

57-92-1

Finds Streptomycin record, uses CAS Registry Number® as identifier

Streptomycin sulfate

Finds three records: Streptomycin, Streptomycin sulfate, and Sulfate

"Streptomycin sulfate" Streptomycin

Finds two records: Streptomycin sulfate and Streptomycin

Sulfoximin*

Finds all names that start with the stem Sulfoximin

WO2019234160

Finds all indexed substances for this patent

The screenshot shows the CAS SciFinder search interface. On the left, there is a sidebar with navigation options: All, Substances (selected), Reactions, References, Suppliers, and Sequences. The main search area has a 'Search for...' section with a dropdown menu set to 'Substances'. Below this is a search bar with the placeholder 'Enter a query...' and a button 'Enter chemical name query'. To the right of the search bar is a button 'Click to draw new structure'. Below the search bar, there are options for 'AND' and 'Molecular Formula'. A button 'Add Advanced Search Field' is present, with a callout 'Add more advanced search fields'. Another button 'Change advanced search field' is also shown. On the right side, there is a chemical structure editor with a button 'Click query structure to edit' and a button 'Search Patent Markush'. A callout 'Check to perform Markush search' points to a checkbox. The interface is clean and professional, with a blue and white color scheme.

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 CAS SciFinder search results interface. On the left, there is a sidebar with navigation options: Structure Match (selected), As Drawn (115), Substructure (5.9M), Similarity (1,044), Analyze Structure Precision, Chemscape Analysis, and Filter Behavior. The main results area shows a list of substances with their CAS numbers and chemical structures. Callouts point to various features: 'Select type of structure match' points to the 'Structure Match' dropdown; 'Click CAS Registry Number to open details' points to the CAS number '90357-06-5'; 'Change sort criterion' points to the 'Sort: Number of Suppliers' dropdown; 'Change amount of details displayed' points to the 'View: Partial' dropdown; 'Analyze structure precision' points to the 'Analyze Structure Precision' button; 'Click on structure to open flyout window' points to the chemical structure of 4-(Methylsulfonyl)phenylboronic acid; 'Retrieve data related to substance' points to the 'Get Substance Details' button; 'Open editor with this structure' points to the 'Edit Structure' button; 'Download .sdf or .mol. Copy Smiles to Clipboard' points to the download buttons; 'Reference Roles show which new information was reported about a substance in the literature' points to the 'Reference Roles' section; and 'Search a (sub)structure within this set of substances' points to the 'Draw' button. The interface is intuitive and provides a wealth of information for each substance.

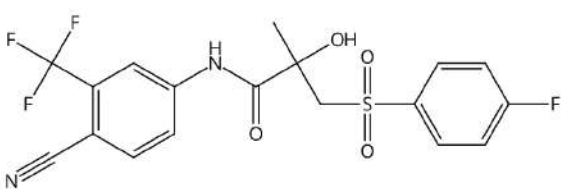
Substance detail and structure editor

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)



$C_{18}H_{14}F_4N_2O_4S$ 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)	-
Boiling Point (Predicted)		
Density (Predicted)		

Other Names

Experimental Properties

Experimental Spectra

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

Key properties

Canonical SMILES
N#CC1=CC=C(C(=C1C(F)(F)F)NC(=O)C(C)C(S(=O)(=O)C2=CC=C(C(F)=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

9 Other Names for this Substance

N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide (ACI)
Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (±)- (ZCI)
(±)-4'-Cyano-α,α,α-trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-methyl-m-lactoluidide
Bicalutamide

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

CAS Draw editor

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

CAS Draw

Import and export structure files

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

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

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

Lasso | Marquee tool

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

Draw atoms and bonds | Eraser

Hetero atom and H isotope selection

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Add attachment point to fragment | Select from templates

Add positive charge | Add negative charge

Repeating groups | Carbon chain tool

Define variable point of attachment at ring | Reaction role

Atom mapping | Lock rings/lock atoms

Bond mapping | Draw reaction arrow

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw

Zoom: 90%

OK Cancel

Advanced Search

Performing an Advanced Search

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

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

The screenshot shows the 'References' search section. At the top, it says 'Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)'. Below this is a search bar with a 'General search box' and a 'Draw' button. A 'Change field' button is also present. The main search area has a dropdown menu set to 'Author Name' with a text input field containing 'Enter last name, first name middle name.' and a clear button (X). Below the search bar, there is a section for 'Define operator between search fields' with a '+ Add Advanced Search Field' button and an 'Add more specific fields' button. A link 'Learn more about SciFinder[®] Advanced Search.' is also visible.

Advanced Search examples

Advanced References Search

The screenshot shows a query for 'pollution monitoring' in quotes. Below it, there is a section for 'Operator to combine search fields' with a dropdown menu set to 'AND'. The search fields are 'Chemical Name' and 'polyethylene'. Below this, there is another section with a dropdown menu set to 'OR' and search fields 'Chemical Name' and 'polypropylene'.

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

Advanced Substances Search

The screenshot shows a query for 'steel*' in quotes. Below it, there is a section for 'Operator to combine search fields' with a dropdown menu set to 'AND'. The search fields are 'Tensile Strength (Mpa)' and '>0'. Below this, there is a note 'Experimental values only.'

Query interpretation:
Steel with tensile strength property
information

The screenshot shows the 'References' dropdown menu and the 'Edit Search' button. A callout box points to the 'Edit Search' button with the text '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

CC(C)C

(C₃H₆)_n

Polypropylene

278K References | 6,321 Reactions | 20 Suppliers

Document Type

Substance Role

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

View All

Language

Publication Year

Available at My Institution

Full Text

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

Recycling micro polypropylene in modified hot asphalt mixture

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

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

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

Full Text

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

Microplastics in marine environment: review of methods for identification and quantification

By: Rodriguez-Ruiz, Valeria; Suarez-Lana, Thomas; Richard, C.; Tress, Marlene

Environmental Science & Technology (2012), 46(1), 300-301 | Language: English, Database: Cxplus and MEDLINE

The review of 48 studies compares the methodologies used for the identification and quantification of microplastics from the marine environment. Three main sampling strategies were identified: selective, volumetric, 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: 1. 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 criteria. Chem. and phys. characteristics (e.g., specific density) 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. Grits commonly used for abundance estimates are "items per m²" for sediment and "no. 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: 10-500 µm (5 mm), which are retained by a 500 µm sieve, and 0.1-500 µm, or "nanoplasts" that are retained on filters. We recommend that future programs of monitoring continue to investigate these size fractions, but we suggest standardized sampling procedures which allow the spatiotemporal comparison of microplastic abundance across marine environments.

Full Text

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

Substances

Substances (0)

Substances (0)

Chemical Name

Role

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

Sequences search

Search options

You can search sequences using three different modalities:

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

BLAST similarity search

BLAST allows you to search for similar nucleotide and amino acid sequences. Alignment results are shown in an intuitive graphical layout with easy-to-use precision filtering for identity and coverage percentages. Reference results are linked to the sequence hits.

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

The screenshot displays the 'Sequences' search module in CAS SciFinder. On the left, a sidebar titled 'Searching for...' lists various search categories, with 'References' highlighted. The main area is titled 'Sequences' and includes a text input field for a protein or nucleotide string, with an example: '> human insulin sequence' followed by the amino acid sequence 'FVNQHLCGSHLVEAYLVCGERGFFYTPKGTGIVEQCCTSIICSLYQLENYCN'. Below the input field are two callout boxes: 'Paste sequence into this window' and 'Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane'. To the right of the input field are buttons for 'BLAST', 'CDR', 'Motif', 'Sequence Search options', 'Upload Sequence', and 'Clear Search'. Further right, a 'Sequence Type' section has 'Nucleotide' and 'Protein' buttons, with 'Protein' selected. Below this is a 'Search Within' section with radio buttons for 'Nucleotides' and 'Proteins' (selected), and a checked checkbox for 'Include NCBI Sequences'. A 'Start Sequence Search' button is at the bottom right. A callout box points to this button with the text 'Include NCBI sequences'. At the bottom, an 'Advanced Sequence Search' section is expanded, showing various parameters: 'Alignment Identity %' (set to -), 'Match with Gaps?' (radio buttons for 'Yes' and 'No', with 'Yes' selected), 'Gap Costs' (set to 'Existence 11 Extension 1'), 'Query Coverage %' (set to 90), 'Word Size' (set to 3), 'Scoring Matrix' (set to 'BLOSUM62'), 'BLAST Algorithm' (set to 'BLASTp'), 'E-Value' (set to 10), and 'Exclude Low Complexity Regions' (radio buttons for 'Yes' and 'No', with 'No' selected). A callout box points to this section with the text 'Advanced BLAST parameters'.

BLAST results analysis

Access results

Sequence search results appear in the Recent Search History and general Search History (🕒 History). Click 'View Results' to view sequence answers.

April 28, 2023

Sequences

5:00 PM

Sequence Type: Protein

Search Within: Proteins

NCBI Included: Yes

BLAST Algorithm: BLASTp

Alignment Identity: -

Query Coverage: 90%

> human insulin sequence

FVNQHLCGSHLVEA...LVCGERGFFYTPKTGIVEQC

CTICSLSLYQL ENYCN

View Results

Edit Search

Complete

Results will expire on May 29, 2023.

View results

When viewing BLAST sequence similarity results:

- Alignments are sorted by Sequence Identity.
- Simplified graphical overview shows alignment quality.
- Mismatches are indicated by red lines.
- Detailed alignments can be viewed in 'Alignment' tab.
- Subject details and patent previews are available in separate tabs.
- Click References to retrieve related references.
- XLSX result download is available.

Sequences search for your query

References

Get references for all sequences

92

Alignment Identity: 89.09%

Query

1

50

Query Length

Subject

1

55

Subject Length

Matches: 49

Mismatches: 6

Alignment Length: 49+6=55

View Less

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

Reference previews

Alignment Details

Alignment

Subject

References

Match

Mismatch

+ Mismatch: Query aa aligned to functional equivalent subject aa

Get References for this sequence

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.

The screenshot shows the 'Reactions' search interface. On the left, a sidebar titled 'Searching for...' contains buttons for 'All', 'Substances', 'Reactions' (highlighted), 'References', 'Suppliers', 'Sequences', and 'Retrosynthesis'. A callout 'Select reactions' points to the 'Reactions' button. The main area is titled 'Reactions' and includes a search bar with the placeholder 'Enter a query...'. A callout 'Click on reaction query to edit' points to a reaction scheme icon in the search results. Below the search bar, there are buttons for 'Edit Drawing' and '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.

The screenshot displays the 'Reactions search for drawn structure' results page. The top section shows '26,932 Results' and a 'Group: By Scheme' dropdown. A callout 'Change grouping to 'By Document' or 'By Transformation'' points to the 'Group' dropdown. The main results area shows 'Scheme 1 (2 Reactions)' with a chemical reaction scheme. A callout 'Click on structure to view substance information' points to a reactant structure. Another callout 'Yield for displayed reactions' points to the 'Yield: 100%' text. Below the reaction scheme, there are buttons for 'Suppliers (48)' and 'Suppliers (387)', with a callout 'View suppliers' pointing to the 'Suppliers (48)' button. The left sidebar contains a 'Filter reaction results' section with 'Structure Match' (As Drawn (0), Substructure (26K), Similarity (2,082)), 'Filter Behavior' (Filter by, Exclude), 'Search Within Results', 'Yield', 'Number of Steps', 'Non-Participating Functional Groups' (Carboxylic ester (151), Halide (143), Ether (125), Ketone (103), Carbamate (98)), and 'Reaction Mapping'. A callout 'View by structure match' points to the 'Substructure (26K)' button. The right sidebar shows 'View reaction details' and 'View reaction reference' buttons. A callout 'Access annotated patent full-text' points to the 'PatentPak' button.

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, Jilang et al.

View All

Organic Process Development (2016), 20(5), 955-969

View Source

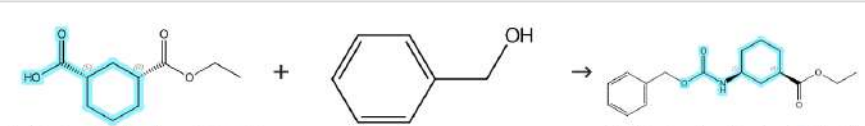
Full Text

Company/Organization

Vertex Pharmaceuticals Incorporated

Boston, Massachusetts 02210

United States



Absolute stereochemistry shown, Rotation (+)

Suppliers (48)

Absolute stereochemistry shown, Rotation (-)

Suppliers (133)

Supplier (1)

Step 1

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

View alternatives

Alternative Steps (5)

Experimental Protocols

Synthetic Methods

View detailed procedures

Products

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

Reactants

[1-Ethyl \(1R,3S\)-1,3-cyclohexanedicarboxylate](#)

[Benzyl alcohol](#)

Reagents

[Triethylamine](#)

[Diphenylphosphoryl azide](#)

Solvents

[Toluene](#)

Procedure

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

Characterization Data

View characterization data

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

Proton NMR Spectrum (300 MHz, CDCl₃) δ 7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, J = 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t, J = 11.8 Hz, 1H), 2.28 (d, J = 12.6 Hz, 1H), 2.10-1.79 (m, 3H), 1.50-1.19 (m, 6H), 1.19-1.00 (m, 1H).

Optical Rotatory Power = -33.3° (c = 1 in DCM).

HRMS (ESI) [M + H]⁺ calculated for C₁₇H₂₄NO₄ 306.1700, found 306.1700

State sticky solid

CAS Method Number 3-451-CAS-15598720

Transformations

1. Schmidt Reaction

Overview of transformations

Reaction Notes

scalable

Further important notes

Retrosynthesis planner

Launching the tool

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

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

Selecting plan options

You can edit plan options to:

- Increase the synthetic depth.
- Protect bonds through the entire synthetic route.
- Define bonds to be broken in the first disconnection.
- Change the starting material cost limit.
- Create a predictive plan with more meaningful alternatives, (such as poly- or heterocyclic molecules).

Once you have completed your option selections, choose the Create Retrosynthesis Plan button.

Retrosynthesis plan 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

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

- Experimental Steps (purple line)
- Predicted Steps (green dotted line)

View plan steps

View plan information

Edit plan options

Adjust scoring options

Exclude steps or substances

Purple lines mark experimental steps

Green dotted lines indicate predicted steps

Download, Share, and Save your plan

Review and select alternative disconnections

Reset

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 → 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%
- Evidence (1,580)
- Alternative Steps (49) **1**

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

1 of 15

Predicted Step

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)

Suppliers (81)

Suppliers (77)

Suppliers (63)

31-614-CAS-24629063

Steps: 1 Yield: 72%

1.1 Reagents: Triethylamine, Hydroquinone

1.2 0.5 M, 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, Zhiwei et al

Chemistry & Biodiversity (2021), 18(12), e2190651

Full Text

Evidence reactions for (predicted) disconnection of precursor C

Retrosynthesis scoring options

Scoring options

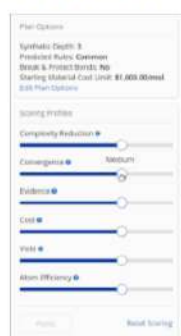
For plans with predicted steps, you may increase or decrease the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

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

Scoring profiles

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

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



Plan Options

Synthetic Route: 3
Predicted Rules: Common
Reagents & Protect Groups: No
Starting Material Cost Limit: \$1,000.00/mol
Salt Percentages

Scoring Profiles

Complexity Reduction: Medium

Convergence: Medium

Evidence: Medium

Cost: Medium

Yield: Medium

Atom Efficiency: Medium

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 displays the CAS SciFinder interface for a Patent Markush search. The top navigation bar includes the CAS logo, SciFinder, and a search bar. The main content area is titled "Patent Markush search for drawn structure". On the left, there are filters for "Patent Markush Match" (As Drawn (96), Substructure (119)), "Filter Behavior" (Filter by, Exclude), and "Patent Office" (World Intellectual Property Organization (55), United States (25), European Patent Organization (8), China (3), United Kingdom (2)). The central area shows the "Assembled Markush hit structure" with a chemical structure diagram. To the right, the "Patent claim 1" is displayed, along with a "PatentPak" dropdown menu and a "Full Text" dropdown. A "Markush search option" is highlighted in the top right, and a "Link to a specific patent reference" is shown below the patent claim. A "Markush location" is indicated on the chemical structure, and a "Link to CAS PatentPak Viewer" is provided at the bottom.

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 displays the CAS PatentPak interface for viewing a patent PDF. The top navigation bar includes the CAS logo, PatentPak, and a search bar. The main content area is titled "Key Substances in Patent". On the left, there are filters for "CAS RN" (33454-82-9, 90076-65-6, 1473-24-8) and "Analyst Markup Locations" (Page 21). The central area shows the patent PDF with marked-up key substances. A "Download PDF" button is highlighted, and a "Link to related information" is shown below the patent PDF. A "Highlighted key substance is marked" is indicated on the patent PDF. A "Marks key substance curated by CAS scientists" is shown at the bottom. The bottom left corner contains the text "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

Stock Status: Maintained in stock

Pricing Information: 1 Mar 2023

Order From Supplier

Substance Information:

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

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

ChemDoodle

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

ChemDoodle interface showing various tools and options:

Top bar: Select, Center, Flip fragment, Cut | Copy | Paste

ChemDoodle dropdown menu

Clear | Eraser, Undo | Redo, Templates, Open | Save, Zoom

Model with CAS Registry Number

Left sidebar tools:

- 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

Chemical structure: CC(=O)OC1=CC=C(C=C1)C(F)(F)F

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, 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

Login, training, and support

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www.cas.org/cas-past-webinars

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Support contact

Email help@cas.org to reach a CAS Customer Center representative.

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