

**CAS SCIFINDER<sup>n</sup>**

# **QUICK REFERENCE GUIDE**

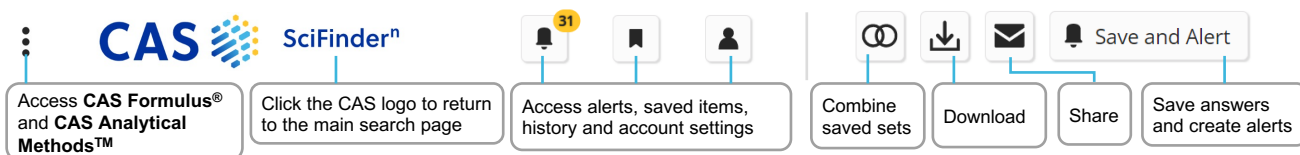
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# Solution interface and References search

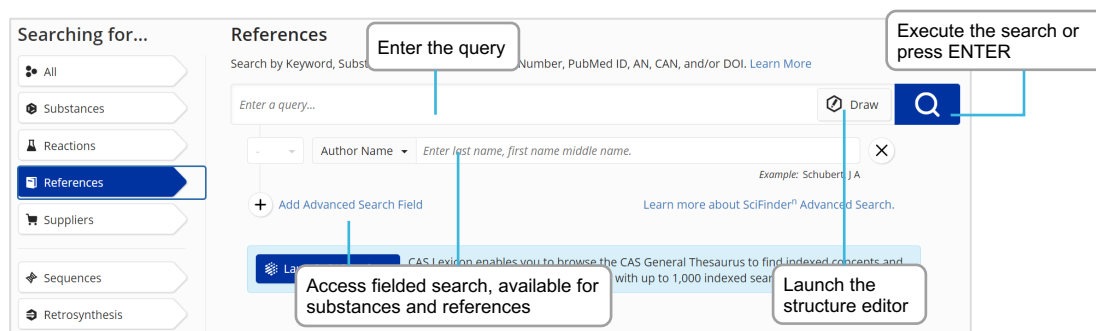
## Main interface

The options below are found on the main interface in CAS SciFinder<sup>®</sup>.



## Search interface

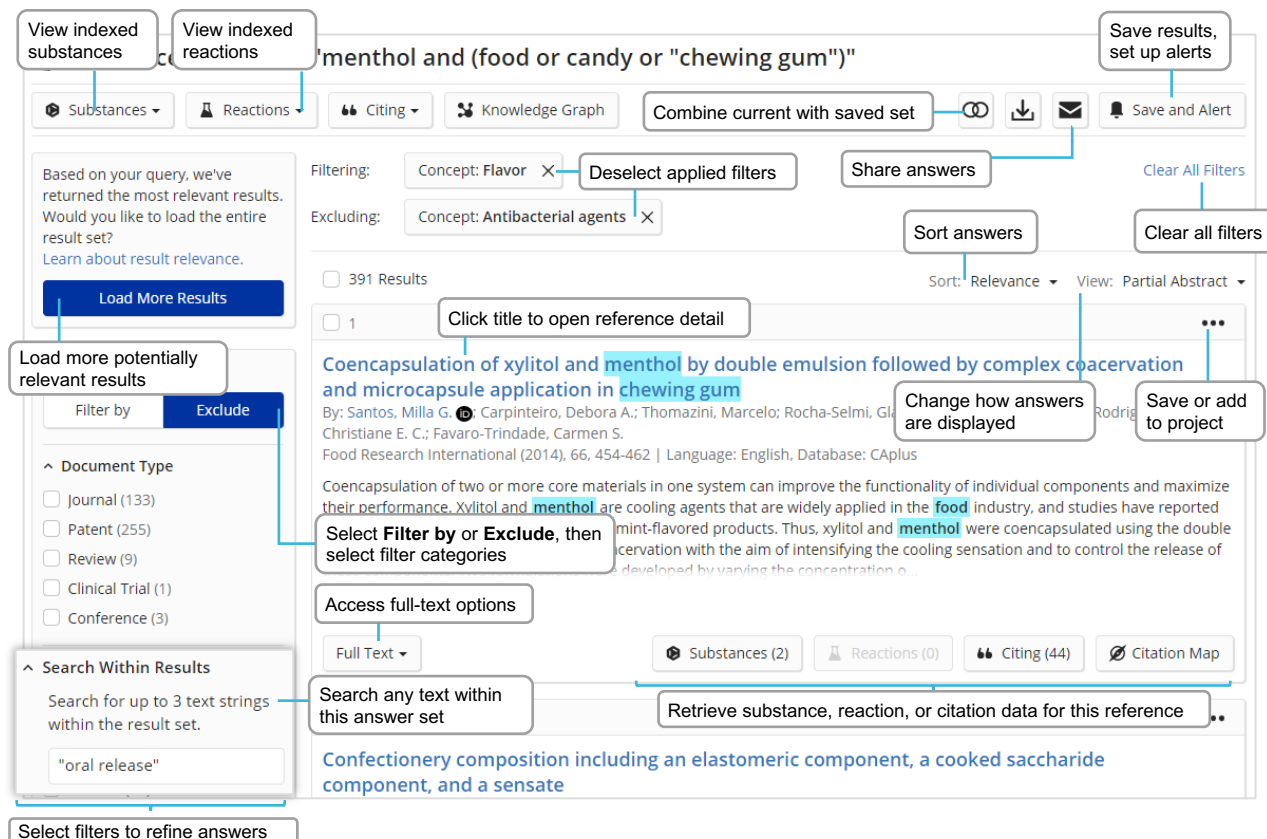
CAS SciFinder<sup>®</sup> features a streamlined search interface.



## 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<sup>®</sup>.

**Fruit juice-containing food products with refreshing and cooling flavors**

Publication source information

**PATENT**

Patent Number  
WO2005048743

Publication Date  
2005-06-02

Application Number  
WO2004-JP17524

Application Date  
2004-11-18

Kind Code  
A1

Assignee  
Takasago International Corporation, Japan

Source  
World Intellectual Property Organization

Patent family and priority application information

AN: 2005:470226  
CAN: 143:25602  
CAplus

Language  
English

Citing (6)

Citation Map

View forward and backward citations

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

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

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

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

PatentPak Viewer Get Prior Art Analysis Full Text

Get prior art for this patent

Get similar references

Get Similar References

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

Similar References **NEW**

Patent Family

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

Priority Application

Priority Application Number	Application Date
JP2003-389758	
WO2004-JP17524	

IPC and indexed subject matter, substance indexing, and formulations

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

## Boolean operators

You can use logical operators to create precise text queries.

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

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

**AND** Requires both terms to be present within the document

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

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



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

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

? Replaces 0 or 1 character ex: benzonorbornen?

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

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



# Substance name and structure search

## Substances search

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

**Streptomycin**

Finds Streptomycin record

**57-92-1**

Finds Streptomycin record, uses CAS Registry Number® as identifier

**Streptomycin sulfate**

Finds three records: Streptomycin, Streptomycin sulfate, and Sulfate

**"Streptomycin sulfate" Streptomycin**

Finds two records: Streptomycin sulfate and Streptomycin

**Sulfoximin\***

Finds all names that start with the stem Sulfoximin

**WO2019234160**

Finds all indexed substances for this patent

Searching for...

Substances

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

Enter a query... Enter chemical name query

AND Molecular Formula

+ Add Advanced Search Field

Add more advanced search fields

Change advanced search field

Click query structure to edit

Click to draw new structure

Edit Drawing Remove

Search Patent Markush

Check to perform Markush search

## Substances search result

Substances search results are displayed in an intuitive interface where you will see the most relevant results for your search, including critical property information and high-resolution images.

Select type of structure match

Structure Match

As Drawn (115)

Substructure (5.9M)

Similarity (1,044)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Start Chemscape Analysis

Filter by Exclude

Reaction Role

Reference Role

Preparation (3M)

Synthetic Preparation (3M)

Uses (2.7M)

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search a (sub)structure within this set of substances

5,986,620 Results

1

90357-06-5

Click CAS Registry Number to open details

149104-88-1

Change sort criterion

Sort: Number of Suppliers View: Partial

Change amount of details displayed

80-08-0

Click on structure to open flyout window

Retrieve data related to substance

Get Substance Details

Get Bioactivity Data

Get Reactions (2,395)

Synthesize (9)

Start Retrosynthetic Analysis

Get References (1,330)

Get Suppliers (106)

Open editor with this structure

Download .sdf or .mol. Copy Smiles to Clipboard

CAS RN 149104-88-1

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

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

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

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

851 References 34 Reactions 98 Suppliers

19542-67-7

16K 4,932 102

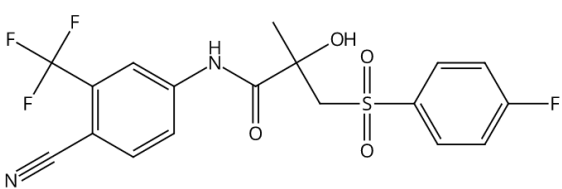
# Substance detail and structure editor

## 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)	650.3±55.0 °C	Pressure: 760 Torr
Density (Predicted)	1.45 g/cm <sup>3</sup>	-

Other Names

Experimental Properties

Experimental Spectra

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

Key properties

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

Canonical SMILES  
N#CC1=CC=C(C=C1C(F)(F)F)NC(=O)C(C)(O)CS(=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*-lactotoluidide  
Bicalutamide

## CAS Draw editor

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

CAS Draw

Import and export structure files

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

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

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

Lasso | Marquee tool

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

Hetero atom and H isotope selection

Draw atoms and bonds | Eraser

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Add attachment point to fragment | Select from templates

Add positive charge | Add negative charge

Repeating groups | Carbon chain tool

Define variable point of attachment at ring | Reaction role

Atom mapping | Lock rings/lock atoms

Bond mapping | Draw reaction arrow

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw

Zoom: 90%

OK Cancel

# Advanced Search

## Performing an Advanced Search

You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinder<sup>®</sup>.

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

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

## Advanced Search examples

### Advanced References Search

The screenshot shows a query for 'pollution monitoring' in quotes. Below it, there's a section 'Operator to combine search fields' with a dropdown set to 'AND'. To the right, there are two search fields: 'Chemical Name' with the value 'polyethylene' and 'Chemical Name' with the value 'polypropylene'. Below this, there's another 'OR' operator dropdown and the same two search fields.

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

The screenshot shows a 'References' dropdown menu, a blue 'Edit Search' button, and the query text '"pollution monitoring"'. A callout box points to the 'Edit Search' button with the text 'Click \'Edit Search\' to modify the Advanced Search'.

### Advanced Substances Search

The screenshot shows a query for 'steel\*' in the main search box. Below it, there's a section 'Operator to combine search fields' with a dropdown set to 'AND'. To the right, there are two search fields: 'Tensile Strength (Mpa)' with the value '>0' and 'Experimental values only.' below it.

Query interpretation:  
Steel with tensile strength property information

## Available Advanced Search fields

You can utilize many search fields and categories as part of an Advanced Search query, including:

### References Search

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

### Substances Search

- Molecular Formula
- CAS Registry Number/Component Registry Number
- Chemical Name
- Document Identifier
- Patent Identifier
- Experimental Spectra
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

# CAS Roles

## CAS Roles overview

Roles are linked to substances, allowing you to find focused publications connecting a substance of interest to its specific role within the scope of the publication.

- Super roles are broad categories and comprise all related specific roles. Examples are Analytical Study, Preparation, or Occurrence.
- Specific roles are more precise. They relate to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in a plant (Natural Product Occurrence).

## Roles in substance results

From a search on substance(s), the roles filter will indicate the types of roles that are connected to the substance(s) in the publications.

Reference Role

By Count | **Alphanumeric**

Example of 'reference roles' appearing in a substance answer set

Number of substance(s) in the answer set with that role

0 Selected

- ☐ Adverse Effect (15)
- ☐ Agricultural Use (29)
- ☐ Analyte (17)
- ☐ Diagnostic Use (3)
- ☐ Food or Feed Use (120)
- ☐ Formation, Non-preparative
- ☐ Pharmacological Activity (10)
- ☐ Physical, Engineering, or Chemical Process (888)

## Roles in reference results

Roles will appear as a filter in reference result sets whenever you have retrieved hits in the substance indexing segment of the records, i.e., by retrieving substance names or performing a crossover after structure-based searches.

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

The search for polypropylene retrieves many references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3,217 publications that describe polypropylene as a pollutant. The Search Within function or concepts can be used to restrict results to marine pollution.

Substances ▾ polypropylene

9003-07-0

C3H6  
**Polypropylene**

278K References | 6,321 Reactions | 20 Suppliers

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

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

One of the objectives of the circular economy is solving the world's plastic pollution crisis and recycling of materials by ensuring less waste. The motivation of this study was to demonstrate the possibility of recycling two types of wastes with a high risk of pollution, such as plastic based polypropylene and abrasive blasting grit wastes in asphalt roads. The effects of adding together polypropylene based microplastics and grit waste in asphalt mixture for wear layer performance have been shown in this study. The morphol. and elemental composition of the hot asphalt mixture samples before and after freeze-thaw cycle were examined by SEM-EDX and the performance of the modified asphalt mixture was determined with laboratory tests including Marshall stability, flow rate, solid-liquid report, apparent d<sub>10</sub>, 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 shown. The results of the study show that the hot asphalt mixtures were added 3 proportions of polypropylene based microplastics such as the mixture performance is shown at the asphalt mixture sample with 0.3% of polypropylene based microplastics are bond with aggregates from mixture well, so the polypropylene-modified hot asphalt mixture can effectively decrease the appearance of cracks during sudden temperature changes.

Full Text ▾

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

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)

Microplastics in marine environment review of methods for identification and quantification

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

Environmental Science & Technology (2012), 46(6), 3060-3075 | Language: English, Database: CxPlus and MEDLINE

This review of 68 studies compares the methodologies used for the identification and quantification of microplastics from the marine environment. Three main sampling strategies were identified: selective, volume-reduced, and bulk sampling. Most sediment samples came from sandy beaches at the high tide line, and most seawater samples were taken at the sea surface using neuston nets. Four steps were distinguished during sample processing: d. separation, filtration, sieving, and visual sorting of microplastics. Visual sorting was one of the most commonly used methods for the identification of microplastics using type, shape, degradation stage, and color as criteria. Chem. and phys. characteristics (e.g., specific d) were also used. The most reliable method to identify the chem. composition of microplastics is by IR spectroscopy. Most studies reported that plastic fragments were polyethylene and polypropylene polymers. Units commonly used for abundance estimates are "items per m<sup>2</sup>" for sediment and sea surface studies and "items per m<sup>3</sup>" 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; and (ii) 1-500 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

9003-53-4

CAS RN | Chemical Name | Role

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

# Reactions search

## Performing a Reactions search

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

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'. The main area is titled 'Reactions' and includes a search bar with the placeholder 'Enter a query...'. Below the search bar is a 'Select reactions' button. To the right of the search bar is an 'Edit' button and a search icon. A callout box points to the search bar with the text 'Click on reaction query to edit'. Another callout box points to a chemical structure in the search results with the text 'Click on reaction query to edit'. Below the structure are 'Edit Drawing' and 'Remove' buttons.

## Reactions search results

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

The screenshot shows the 'Reactions search for drawn structure' results page. The top section includes a title bar with a funnel icon and the text 'Reactions search for drawn structure'. Below the title bar is a 'Change grouping to 'By Document' or 'By Transformation'' button. The main area displays search results for 'Structure Match'. The left sidebar contains filters for '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'. The main results area shows 'Scheme 1 (2 Reactions)' with a chemical structure of a carboxylic acid derivative. Below the structure are buttons for 'Suppliers (48)' and 'View suppliers'. The results are grouped by 'Scheme' and sorted by 'Yield'. The first result is '31-614-CAS-27240963' with 'Steps: 1' and 'Yield: 100%'. It includes reagents 'Triethylamine, Diphenylphosphoryl azide' and solvents 'Toluene'. A callout box points to the structure with the text 'Click on structure to view substance information'. Another callout box points to the yield with the text 'Yield for displayed reactions'. A third callout box points to the reaction details with the text 'View reaction details'. A fourth callout box points to the reaction reference with the text 'View reaction reference'. A fifth callout box points to the patent full-text with the text 'Access annotated patent full-text'. The results are displayed in a table with columns for 'CAS Number', 'Steps', 'Yield', 'Reaction Details', and 'Reaction Reference'.



# Reaction details

## Reviewing Reaction details

The details of a reaction provide you with access to information including solvents, catalysts, reagents, conditions, and experimental protocols extracted from the publication and its supplement.

**Reaction Overview**

Steps: 1 Yield: 85%

**Reaction reference**

JOURNAL

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

By: Liang, Jiang [View all authors](#)

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

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (-)

[Suppliers \(48\)](#) [Suppliers \(133\)](#) [Supplier \(1\)](#)

**Step 1**

Stage	Reagents	Catalysts	Solvents	Conditions
1	<a href="#">Triethylamine</a> <a href="#">Diphenylphosphoryl azide</a>	-	<a href="#">Toluene</a>	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<sub>3</sub>) 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]<sup>+</sup> calculated for C<sub>17</sub>H<sub>24</sub>NO<sub>4</sub> 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<sup>®</sup>:

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

Searching for... Retrosynthesis

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

Enter a CAS Registry Numbers, SMILES,

Draw or change atoms or bonds.

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

Zoom: 100%

Start Retrosynthetic Analysis

CAS RN: 2408121-76-4

CAS Name: 2-[Methoxy[5-[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-2-thienyl]methyl]-5-meth...

Get Substance Details

Get Bioactivity Data

Get Reactions (1)

Synthesize (1)

Start Retrosynthetic Analysis

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<sup>®</sup>

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

**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**

- Complexity Reduction
- Convergence
- Evidence
- Cost

**Adjust scoring options**

**Retrosynthesis Step Key**

- Experimental Steps (Purple line)
- Predicted Steps (Green dotted line)

**Exclude steps or substances**

**View Excluded Options**

**Download, Share, and Save your plan**

**Review and select alternative disconnections**

## Alternative steps

Get an overview of all experimental and predicted disconnections along with the evidence reactions displayed as a reaction answer set. You can access these evidence reactions from either the (1) link in the steps overview or (2) alternative reaction scheme.

**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**

**1** 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%

31-614-CAS-24629063

1.1 Reagents: Triethylamine, hydroxylamine

Solvents: Dimethylformamide, Tetrahydrofuran

1.2 0.5 h, reflux

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

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), 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.

Plan Options

Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: No  
Starting Material Cost Limit: \$1,000.00/mol  
Edit Plan Options

Scoring Profiles

Complexity Reduction: [Slider]

Convergence: [Slider] Medium

Evidence: [Slider]

Cost: [Slider]

Yield: [Slider]

Atom Efficiency: [Slider]

Apply Reset Scoring

### Complexity Reduction

Reduces the complexity of a step's reactants compared to its product.

**In retrosynthesis plans, you typically want high complexity reduction.**

### Convergence

Determines how "branched" the plan is; **you typically want the plan to be as branched as possible (high convergence)**, rather than linear.

For a given step, the more precursors there are, and the closer their relative sizes are, the more it's considered convergent.

**Increasing Convergence displays steps/alternatives with more reactants.**

### Evidence

Ranks plan steps/alternatives based on the number of evidence examples supporting the particular reaction type.

**More evidence examples for a step means that the reaction type has more applications and is more versatile in terms of conditions and substrates**, and hence predictions made based on it are probably more reliable.

**Increasing Evidence displays steps/alternatives with more supporting examples.**

### Cost

Weights the expenses of the reactions by ranking starting materials based on the lowest price found amongst catalogs.

### Yield

Applies to the yield of each step in the plan, which contributes to the yield of the target molecule.

**Increasing the Yield displays a higher yield target molecule and steps/alternatives.**

### Atom Efficiency

Reduces reactant parts not included in a plan step's product.

**Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.**

Clicking the **Apply** button redraws the retrosynthesis plan with the revised scoring profiles; clicking **Reset Scoring** restores the "Medium" default.

Apply Reset Scoring

# Markush search and CAS PatentPak

## Markush search

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

The screenshot shows the CAS SciFinder Patent Markush search interface. At the top, there's a search bar with "Enter a query..." and a "Search" button. Below the search bar, the "Patent Markush search for drawn structure" section is active. A chemical structure is shown in the center, with a "Markush search type" label pointing to it. To the left, there's a "Patent Markush Match" section with a "References" dropdown and a "Filter Behavior" section. The "Filter Behavior" section has a "Filter by" button and an "Exclude" button. Below that, the "Patent Office" section lists various organizations like "World Intellectual Property Organization (55)", "United States (25)", "European Patent Organization (8)", "China (3)", and "United Kingdom (2)". A "Markush search option" label points to the "Search Patent Markush" checkbox. A "Link to a specific patent reference" label points to the "Patent claim 1" section. A "Markush location" label points to the "PatentPak" dropdown menu. A "Link to CAS PatentPak Viewer" label points to the "Full Text" dropdown menu. A "Link to related information" label points to the "Heterocycle derivatives and methods of use" section. A "Filter by patent authority" label points to the "Patent Office" section. A "Markush hit structure" label points to the chemical structure in the center.

## CAS PatentPak

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

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

The screenshot shows the CAS PatentPak interface. At the top, there's a "PAGE" section with "21" and a "ZOOM" section with "722". Below that, there's a "DOWNLOAD" section with "PDF" and "PDF+" buttons. A "Download PDF including list of marked-up substances and annotations" label points to the "PDF+" button. On the left, there's a "Key Substances in Patent" section. It lists "CAS RN 33454-82-9" with a chemical structure of "Lithium trifluoromethanesulfonate" and "CAS RN 90076-65-6" with a chemical structure of "Lithium bis(trifluoromethanesulfonyl)imide". A "Link to location of substance in patent" label points to the "Page 21" link. In the center, there's a "Download PDF" button. A "Link to related information" label points to the "Get Substance Details" button. On the right, there's a "Highlighted key substance is marked" label pointing to a chemical structure of "Lithium trifluoromethanesulfonate". At the bottom, there's a "Marks key substance curated by CAS scientists" label pointing to a chemical structure of "Lithium bis(trifluoromethanesulfonyl)imide". A "Key substances identified in the patent are annotated" label points to the "Key Substances in Patent" section.



# Supplier search and ChemDoodle®

## Suppliers search

Using Suppliers search allows you to directly access chemical catalog information based on chemical structure, names, or other identifiers.

**Suppliers for 7664-93-9**

389 Results

Filter Behavior: Filter by Exclude

Preferred Suppliers:

- ☐ Preferred (51)
- ☐ No Preference (338)

Supplier:

- ☐ Hayashi Pure Chemical Products Catalog (109)
- ☐ KANTO CHEMICAL (41)
- ☐ FUJIFILM Wako Chemicals Europe GmbH Product List (37)
- ☐ FUJIFILM Wako Chemicals U.S.A. Corporation Product List (37)
- ☐ FUJIFILM Wako Pure Chemical Corporation Product List (37)

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

Preferred/non-preferred supplier tagging

Reactivity of information

Link to detail

**Oakwood Chemical Product List**

Preferred Supplier

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

Email: [sales@oakwoodchemical.com](mailto:sales@oakwoodchemical.com)

Phone: 1-800-467-3386

Item Details

Chemical Name: Sulfuric Acid, ACS Grade

Order Number: 080325

Purity: 98%

Quantity, Price: 100 ml, USD 25.00  
1 L, USD 40.00  
2.5 L, USD 80.00

Bulk Available

Stock Status: Maintained in stock

Pricing Information: Last Updated: 1 Mar 2023

Order From Supplier

Substance Information

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

OS(=O)(=O)O

## ChemDoodle

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

Select Center Flip fragment Cut | Copy | Paste

ChemDoodle

Model with CAS Registry Number

Clear | Eraser

Labeling

Undo | Redo

Templates

Open | Save

Zoom

Draw bonds

Draw rings

Add charges

Chain tool

Repeating groups

Variable point of attachment

Lock atoms/chains/rings

Make reaction

Reaction mapping

Break/form bonds

OK Cancel

N#Cc1ccc(cc1)C(=O)N(C)C(=O)C2=CC=CC=C2S(=O)(=O)C3=CC=CC=C3F

# Prior Art Analysis

## Reviewing Prior Art

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

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

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

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

**PATENT**

Patent Number: **WO2017135893**

Publication Date: 2017-08-10

Application Number:

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

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

### Login details

Log in at [scifinder-n.cas.org](https://scifinder-n.cas.org)

Use your existing CAS SciFinder<sup>®</sup> username and password.

### Feedback button

Provide direct feedback to CAS from within the CAS SciFinder<sup>®</sup> solution.



Feedback

### Training

Upcoming events and webinars:

[www.cas.org/cas-webinars](https://www.cas.org/cas-webinars)

Recorded events and webinars:

[www.cas.org/cas-past-webinars](https://www.cas.org/cas-past-webinars)

CAS SciFinder<sup>®</sup> training topics: [www.cas.org/support/training/scifinder-n](https://www.cas.org/support/training/scifinder-n)

### Support contact

Email [help@cas.org](mailto:help@cas.org) to reach a CAS Customer Center representative.

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