

CAS SCIFINDER®

QUICK REFERENCE GUIDE

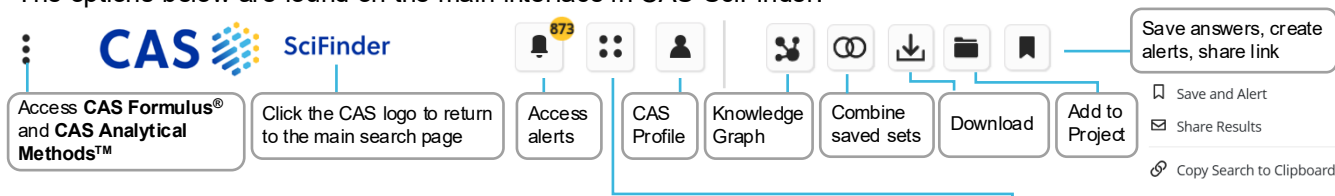
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Solution Interface

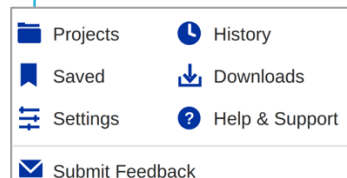
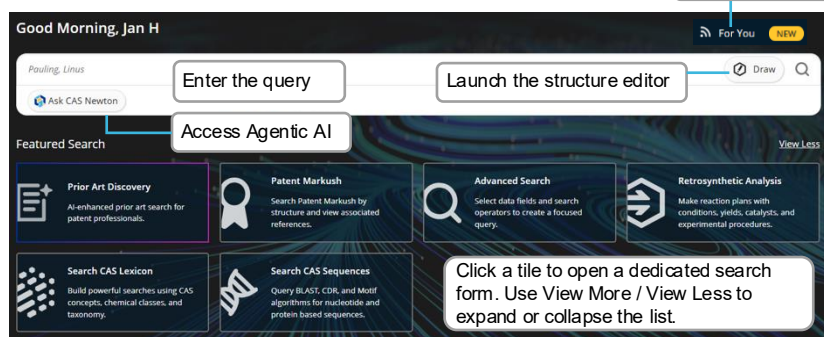
Main interface

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



Search interface

CAS SciFinder features a streamlined search interface.

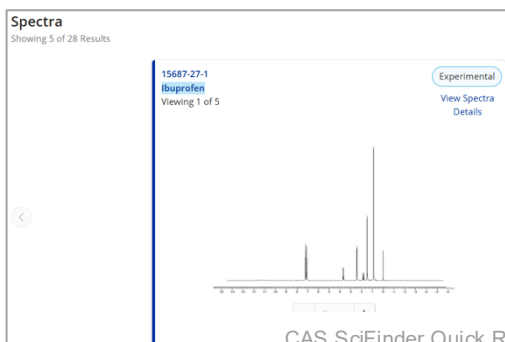
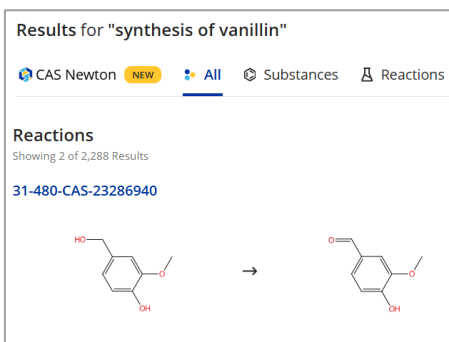
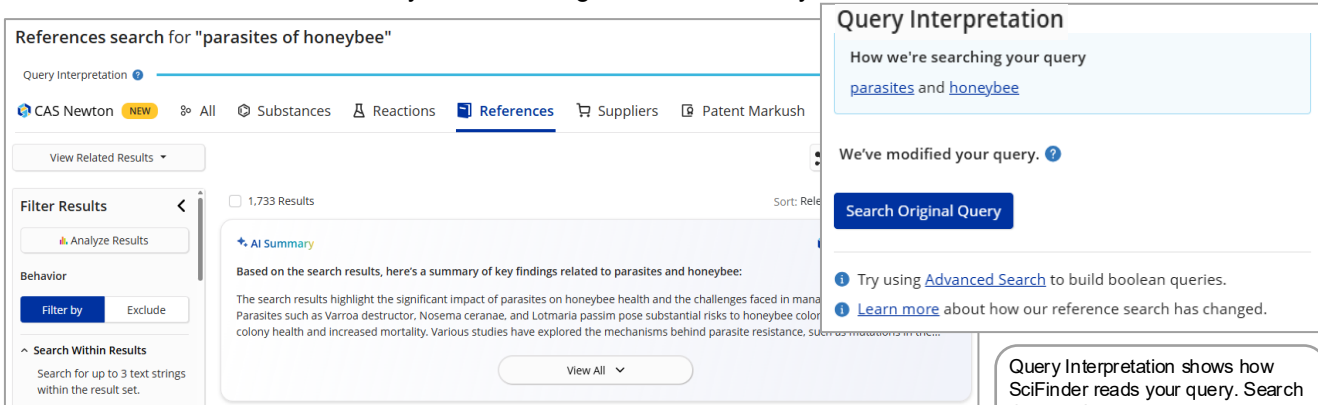


SearchSense

Query interpretation built into CAS SciFinder, starts automatically with every query.

Follow-up questions or chat-type conversations are not supported in the general search box.

- Uses open language models to convert questions into CAS SciFinder search logic, e.g., adds logical operators, removes irrelevant terms, resolves names to CAS Registry Numbers®
- Shows the matching answer directly, e.g.:
 - synthesis of vanillin → reactions producing vanillin
 - boiling point of ethyl acetate → experimental BP for ethyl acetate
 - proton spectrum of ibuprofen → ¹H NMR spectrum of ibuprofen
- Reference searches additionally return an AI-generated summary of the most relevant hits



Query Interpretation shows how SciFinder reads your query. Search Original Query runs your input unchanged. Underlined terms link to the CAS Lexicon.

References Search

References search results

Performing a References search provides you with access to a full result set in an easy-to-use interface where:

- An AI Summary of the most relevant hits is shown at the top (for non-filtered, relevance-sorted result sets)
- References are sorted by relevance by default 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.

2,487 Results Sort: Relevance View: Full Abstract

AI Summary Powered by CAS Newton

Based on the search results, here's a summary of key findings related to menthol and candy or chewing gums:

The search results highlight various aspects of menthol in candy and chewing gums, including its role in flavor enhancement, cooling sensation, and health benefits. Menthol is commonly used in chewing gum and candy to provide a cooling sensation and enhance flavor. Studies have shown that menthol can improve the aroma release and flavor intensity of these products. Additionally, menthol has been incorporated into various oral care compositions to provide a cooling effect and soothe the mouth. Some research has explored the use of menthol in combination with other compounds, such as xylitol, to enhance the cooling sensation and control the release of these components.

Key Findings:

- Flavor Enhancement and Cooling Sensation:**
 - Coencapsulation of xylitol and menthol in chewing gum can intensify the cooling effect and control the release of these components. (11)
- Health Benefits:**
 - A menthol chewing gum was found to reduce the intensity and discomfort of preoperative thirst in surgical patients. (12)
 - A Chinese medicinal chewing gum containing mint and menthol has been developed to remove bad breath, protect teeth, and prevent tooth decay. (19)
- Composition and Formulations:**
 - A method for preparing a composition with a mint aroma that substitutes for natural mint oil or dementholized mint oil has been proposed. (2)

References search for "menthol in candy or chewing gums"

Query Interpretation

CAS Newton **NEW** All Substances Reactions **References** Suppliers Patent Markush

View Related Results View related substances, reactions and citations

Filter Results Analyze Results

Behavior Filter by Exclude

Search Within Results Search for up to 3 text strings within the result set. Enter a query... "oral release"

Document Type ☐ Journal (38) ☐ Patent (221) ☐ Review (3) ☐ Clinical Trial (1) ☐ Conference (3)

Filtering: Concept: Flavor Deselect applied filters Clear All Filters

Excluding: Concept: Antibacterial agents Sort answers Change how answers are displayed

☐ 262 Results Sort: Relevance View: Full Abstract

Neo-menthyl derivatives as flavor materials Click title to open reference detail

Assignee: Symrise G.m.b.H. & Co. K.-G. See preview of status of patent family members

United States, US20090311401 A1 2009-12-17 | Language: English, Database: CPlus

Patent Status: Alive Family Members: EP EP US CN CN

primarily to the use of particular ureas, thioureas, carbamates, based on the neomenthyl structure and corresponding mixtures with one another or with further compounds as flavor materials or flavor material mixtures for producing, imparting, modifying and/or enhancing savory flavor notes. The invention furthermore relates to particular compositions, preparations and semifinished products which comprise the said compounds, as imparting, modifying and/or enhancing particular flavor impressions, to the compounds themselves and to corresponding mixtures

Access full-text options PatentPak Full Text 78 56 1

Retrieve substance, reaction, or citation data for this reference

Analyze Results Top Document Types Patent Journal C R

Patent Offices

Callouts:

- Save, share and alerts
- Add to Project
- Download answers
- Combine current with saved set
- Open related Knowledge Graph
- Analyze results. Click X to collapse panel.
- Select Filter by or Exclude, then select filter categories
- Search any text within this answer set
- Access full-text options
- Select filters to refine answers

Reference Detail and Search Operators

Reference detail

Access full details for each reference found in CAS SciFinder.

Neo-menthyl derivatives as flavor materials

78 56 1 Citation Map View forward and backward citations

In This Patent

- Claims
- Classifications
- CAS Concepts
- Markush Structures
- Substances
- Reactions
- Formulations

Assignee: Symrise G.m.b.H. & Co. K.-G.
Inventors: Ley, Jakob Peter; Oertling, Heiko; Backes, Michael; Vossing, Tobias

The present invention relates primarily to the use of particular ureas, thioureas, carbamates, thiocarbamates and guanidines based on the neomenthyl structure and corresponding mixtures with one another or with further compounds as flavor materials or flavor material mixtures for producing, imparting, modifying and/or enhancing savory flavor notes. The invention furthermore relates to particular compositions, preparations and semifinished products which comprise the said compounds, as well as methods for producing, imparting, modifying and/or enhancing particular flavor impressions. Lastly, the invention also relates to the compounds themselves and to corresponding mixtures

Set citation alert

Table of contents provides a quick overview and navigation to content

Keywords: neomenthyl derivative flavoring savory flavor food

PatentPak Get Prior Art Analysis Full Text View in CAS Formulus

View bibliographic details

Get prior art for this patent View related formulation details

Publication Information Patent

Patent family, application and priority application information

Patent	Language	Full Text	Publication Date	Application Number	Application Date	Patent Status	Status Date
US20090311401 A1	English	PatentPak PDF	2009-12-17	US2009-12482210	2009-06-10	Alive	2020-11-21
EP2135516 A1	German		2009-12-23	EP2009-162075	2009-06-05	Indeterminate	2020-11-06
EP2135516 B1	German	PatentPak PDF	2012-08-15	EP2009-162075	2009-06-05	Indeterminate	2020-11-06
US8852664 B2	English	PatentPak PDF	2014-10-07	US2009-12482210	2009-06-10	Alive	2020-11-21
CN101611857 A	Chinese		2009-12-30	CN2009-10148323	2009-06-15	Alive	2020-11-21
CN101611857 B	Chinese	PatentPak PDF	2013-09-25	CN2009-10148323	2009-06-15	Alive	2020-11-21

PatentPak PDF displays annotated OCR'd full-text. Basic Patent (top in the list) shows locations of indexed substances.

Logical operators

You can use logical operators to create precise text queries.

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

CAS SciFinder (flavor or odor) and menthol not cigarette

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 in reference searching ex: benzonorbomen?

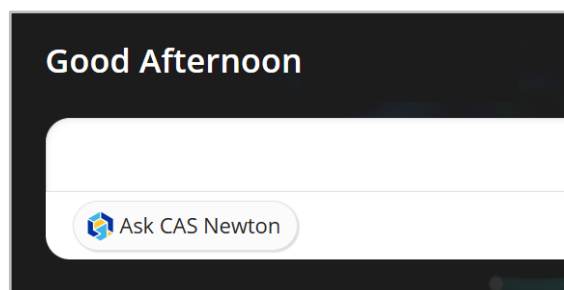
Phrases containing double quotes will be searched as a precise phrase. Ex: a search for "Programmed cell death" only finds results that exactly match 'Programmed cell death'.

Agentic AI CAS NewtonSM

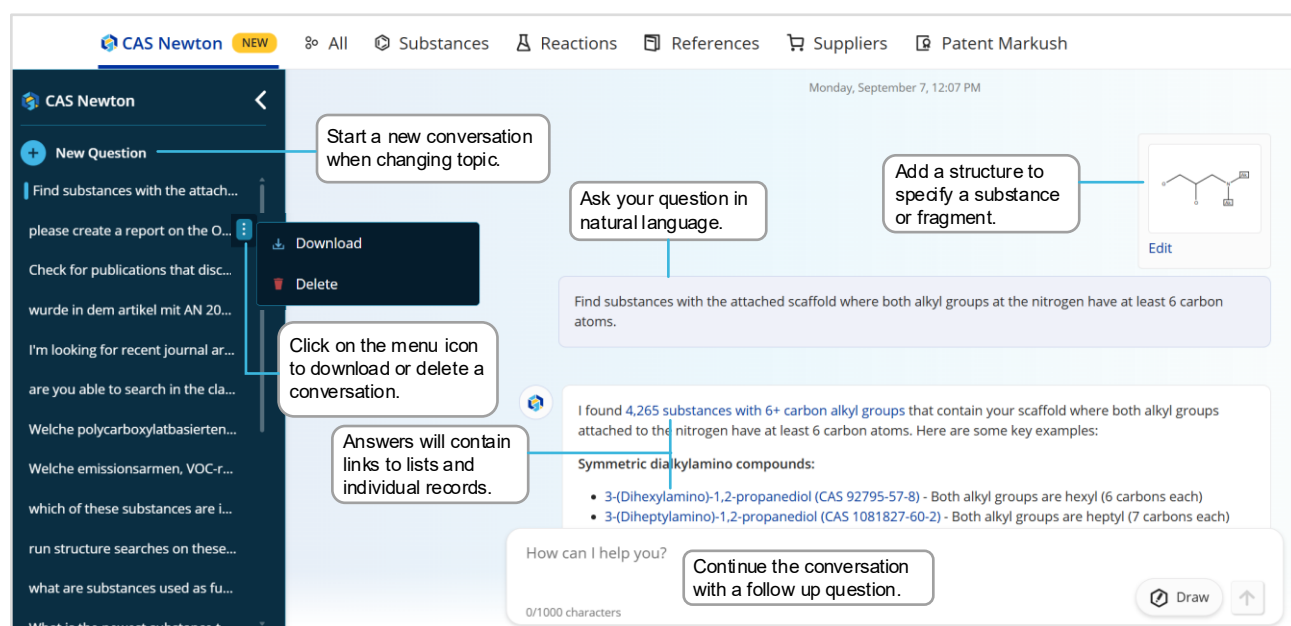
Agentic AI access to CAS content

Access CAS Newton from the landing page.

Ask a question in plain language and **CAS Newton** searches the CAS Content CollectionTM to build a cited answer. CAS Newton plans and runs multiple search steps on its own, tackling complex questions. It also analyzes the results automatically.



- Ask questions in any language. CAS Newton will respond in the same language.
- Search across the CAS Content Collection, including patents and scientific publications.
- Every answer includes source citations, allowing you to verify the underlying documents.
- AI-generated content may contain inaccuracies. Always verify information against the cited sources.



What you can ask CAS Newton

You can ask Newton anything covered by CAS SciFinder's content.

- **Trends:** Summarize recent advances in solid-state battery electrolytes.
- **Reactions and synthesis:** What are recent or alternative routes to make a compound?
- **Competitor activity:** Which organizations are filing patents in a given technology area?
- **Complex tasks:** Create a table of characterized natural products comprising a pyrrolizidine fragment that were flagged with the natural occurrence in publications discussing the fungus *Aspergillus flavus*.
- **Structure search beyond the editor:** Find substances with the attached scaffold where both alkyl groups at the nitrogen have at least six carbon atoms.
- **Follow-up questions:** Refine or ask a follow-up in the same conversation, just like chatting

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

57-92-1

Streptomycin sulfate

Sulfoximin*

WO2019234160

Finds Streptomycin record, and Streptomycin in Notes

Finds Streptomycin record, uses CAS Registry Number as the identifier

Finds three records: Streptomycin sulfate, and Streptomycin sulfate in Note

Finds all names that start with the stem Sulfoximin

Finds firstly this patent and in Tab Substances: all indexed substances for this patent

Click to draw new structure

Enter text query

Ask CAS Newton

Perform advanced search in specified fields

Advanced Search
Select data fields and search operators to create a focused query.

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

Click query structure to edit

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 structure images.

CAS Newton NEW All Substances Reactions References Suppliers Patent Markush

View Related Results

Change amount of details displayed

Visualization of filters

Filter Results

Select type of structure match

Structure Match

As Drawn (126)

Substructure (6,5M)

Similarity (15)

Analyze Structure Precision

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Reaction Role

Product (884K)

Change sort criterion

Sort: CAS RN: Ascending View: Partial

Click CAS Registry Number to open details

Analyze structure precision

Click on structure to open flyout window

Reaction Roles indicate the role a substance plays in the preparation.

Open editor with this structure

Download .png, .cxr, .sdf, or .mol. Copy SMILES to Clipboard

Retrieve data related to substance

- Get Substance Details
- Get Life Science Data
- Get Reactions (616)
- Synthesize (379)
- Start Retrosynthetic Analysis
- Get References (657)
- Get Suppliers (72)
- View in CAS BioFinder

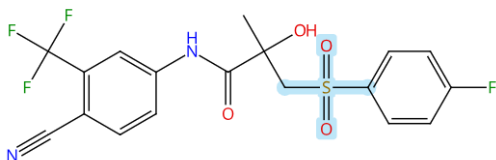
Substance Detail and Structure Editor

Substance detail

When you click a CAS Registry Number for one of your Substances search results, substance details including structure, molecular formula, properties, spectra and GHS data are displayed.

CAS Registry Number: 90357-06-5

4,922 250 122 View in CAS BioFinder



C₁₈H₁₄F₄N₂O₄S

Molecular formula in hill order

Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI, ACI)



GHS Hazard pictograms, full list available in substance record

Systematic name

Properties

Molecular Weight

Melting Point (Experimental)

Boiling Point (Predicted)

Value

430.38

190 °C

650.308±55.00 °C

Condition

-

-

Press: 760.00 Torr

Key properties

Experimental Properties | Spectra

Other Names and Identifiers

Experimental Properties

Experimental Spectra

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

Patents Containing Substance in Claims

List of patents where substance is reported in claims

Treatment regimen using PSMA-binding radioligands in combination with androgen receptor pathway inhibitors

Patent Number: WO2026159621

Publication Date: 2026-07-30

Pharmaceutical composition comprising polysubstituted benzene ring compound, and use method therefor

Patent Number: WO2026145506

Publication Date: 2026-07-09

Pharmaceutical composition comprising CGP60474 exhibits anticancer activity against brain cancer

Patent Number: KR2026096036

Publication Date: 2026-06-24

View All Patents

Canonical SMILES

NC(=O)C(C)(O)C(=O)C1=CC=C(C(F)(F)F)C(=O)C1=CC=C(C(F)(F)F)C#N

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

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

CAS Draw structure editor

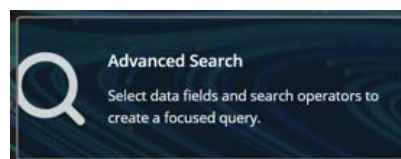
You can define structure and reaction queries using the CAS Draw structure editor.

The screenshot shows the CAS Draw structure editor interface. At the top, there's a search bar with a dropdown menu set to 'CAS Draw'. Below it, a 'Select Search Type' section includes tabs for 'Substances', 'References', 'Reactions', 'Suppliers', 'Patent Markush', and 'All'. A 'Choose Search Type' button is also present. The main workspace displays a chemical structure of a complex molecule. To the left, a toolbar contains various drawing tools: '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 | Lock rings', 'Lock atoms | Rotate/Flip fragment', 'Reaction role | Atom mapping', and 'Bond mapping | Draw reaction arrow'. To the right, a panel shows 'Enter a Systematic Name, CAS Registry Number, SMILES, or InChI to create structure'. Below this, there's a 'Learn about keyboard shortcuts to e.g., easily draw hetero atoms' link. Further down, a 'C, hetero atom and H isotope selection' panel is visible. At the bottom, there's a 'Draw rings' panel with various ring shapes and a 'Resize window' button. The interface also includes a 'Zoom: 100%' slider and 'Cancel' and 'OK' buttons.

Advanced Search

Specifying search terms by field

You can perform specific References and Substances searches using the **Advanced Search** tile on the landing page of 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

Advanced Search examples

Identify publications that discuss monitoring of polypropylene pollution. Limit to organizations that include the word 'marine'.

Query interpretation:

*pollution AND monitoring AND
SUBSTANCE: polypropylene AND
ORGANIZATION: marine*

Get all substances that are derivatives of cellulose with a specifically defined carboxylic acid.

Query interpretation:

FUNCTIONAL GROUP IN THE STRUCTURE:
*Carboxylic acid AND COMPONENT
REGISTRY NUMBER: 9004-34-6 (Cellulose)*

Edit an Advanced Search

Modify a query from the result view via the search bar or from the Search History.

When to use Advanced Search fields

Advanced Search is useful to add specificity to the search query, especially when not interpreted properly in the general search. Some typical examples are given below.

- **Author:** The name of the author is also a regular English word
- **Organization:** Company name not identified as organization but searched as keyword
- **Concept:** If a keyword should only be searched in the concepts and not in title and abstract
- **Component CAS Registry Number:** Essential for comprehensive search of modified substances without structure, e.g., Cellulose or Lignin.
- **Bioactivity and Property Data:** For precise combinations of multiple values. Essential if you want to define if predicted values should be included.

Analytical Methods and Formulations

CAS Analytical Methods™

CAS Analytical Methods enables you to search, review, and compare validated analytical procedures, including HPLC, GC, and spectroscopy methods, for specific compounds and applications, sourced from scientific journals and patents.

The screenshot displays the CAS Analytical Methods interface. On the left, a sidebar titled 'Filter By' includes categories like Analyte, Matrix, Method Category, Technique, Validation, and Year. The main search bar at the top prompts 'Search for keywords, matrices or analyte.' Below the search bar, there are two main sections: 'Explore Methods' and 'Advanced Search'. The 'Explore Methods' section shows 488 results, sorted by Relevance, grouped by Method. The first result is 'Analysis of Iron in Soils by Inductively coupled plasma atomic emission spectrometry' by Zhou, Yanfei; Liu, Xiaoning; Wang, Jun. The result details include the analyte (Iron), matrix (Soils), and other materials (Reagent: Nitric acid; Hydrofluoric acid; Material: 0.150 mm sieve). A callout box points to the 'Filter by analyte, matrix, etc.' section. Another callout box points to the 'Compare' button, with a note 'Compare different methods'.

Search for keywords, matrices or analyte.

Explore Methods
Search methods using criteria like method categories and subcategories.

Advanced Search
Search methods using criteria like keywords, analytes, matrices and more.

Advanced search in specific fields

Explore methods by category (environmental, water, food analysis, etc)

488 Results

Sort: Relevance Group: By Method

1

Analysis of Iron in Soils by Inductively coupled plasma atomic emission spectrometry

By: Zhou, Yanfei; Liu, Xiaoning; Wang, Jun
Characterization of **microplastics** and the association of heavy metals with **microplastics** in suburban soil of central China
Science of the Total Environment (2019), 694, -, Elsevier B.V.

Analyte Iron
Matrix Soils
Other Materials Reagent: Nitric acid; Hydrofluoric acid
Material: 0.150 mm sieve
Soil Analysis; Element Detection
Acid digestion; Inductively coupled plasma atomic emission spectrometry
Inductively coupled plasma-optical emission spectrometer

Equipment Used

View Abstract Full Text View in CAS SciFinder

Filter by analyte, matrix, etc.

Compare

Compare different methods

CAS Formulus®

Search published formulations by ingredient, industry, application, or physical form to uncover formulation components, preparation methods, and regulatory information that accelerate product development.

The screenshot displays the CAS Formulus interface. On the left, a sidebar titled 'Filter Behavior' includes categories like Industry, Regulatory Information, Experimental Properties, Commercial Availability, and Toxicity/Ecological Toxicity. The main search bar at the top prompts 'Search by Ingredient Name, CAS Registry Number, or Function'. Below the search bar, there are two main sections: 'Formulation Designer' and 'Advanced Search'. The 'Formulation Designer' section shows 2 results, sorted by Relevance, grouped by Method. The first result is 'Ezetimibe' with CAS RN: 163222-33-1. The result details include the chemical structure, molecular weight (409.43), melting point (164-166 °C), and commonly used applications (Cholesterol absorption inhibitors; Anticholesteremic agents; Hypolipemic agents; Cardiovascular agents; Antiarteriosclerotics...). A callout box points to the 'Filter by Industry, Regulatory info, etc.' section. Another callout box points to the 'Advanced search in specific fields' section.

Search by Ingredient Name, CAS Registry Number, or Function

Formulation Designer
Design custom formulation templates based on selections and ingredients

Advanced Search
Search Formulations using criteria like ingredients, targets, and more.

Advanced search in specific fields

Design formulation by choosing industry, purpose, physical form and main ingredients

2 Results

1

CAS RN: 163222-33-1
View Details

Ezetimibe

Key Physical Properties	Value	Condition
Molecular Weight	409.43	-
Melting Point (Experimental)	164-166 °C	-

Commonly Used As: Cholesterol absorption inhibitors; Anticholesteremic agents; Hypolipemic agents; Cardiovascular agents; Antiarteriosclerotics...

Commonly Formulated With | Regulatory Information | Experimental Properties

Filter by Industry, Regulatory info, etc.

Get Formulations Get Suppliers Add to Formulation Designer

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, relating to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in an organism (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**

0 Selected

☐ Adverse Effect (15)

☐ Diagnostic Use (3)

☐ Pharmacological Activity (10)

☐ Agricultural Use (29)

☐ Food or Feed Use (120)

☐ Physical, Engineering, or Chemical Process (888)

☐ Analyte (17)

☐ Formation, Non-preparative

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

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

Roles in reference results

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

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

The search for polypropylene retrieves many references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 7,890 publications that describe polypropylene as a pollutant. The Search Within function or concepts can be used to restrict results to marine pollution.

polypropylene

9003-07-0

(C₃H₆)_x
Polypropylene

379K 9.946 83

Filter by Exclude

379,115 Results

Sort: Relevance View: Partial Abstract

1

Assessing the Efficacy of Pyrolysis-Gas Chromatography-Mass Spectrometry for Nanoplastic and Microplastic Analysis in Human Blood

By: Rauert, Cassandra; Charlton, Nathan; Bagley, Angus; Dunlop, Sarah A.; Symeonides, Christos; Thomas, Kevin V.

Environmental Science & Technology (2025), 59(4), 1984-1994 | Language: English; Database: Capius and MEDLINE

Humans are constantly exposed to micro- and nanosized plastics (MNPs); however, there is still limited understanding of their fate within the body, partially due to limitations with current analytical techniques. The current study assessed the appropriateness of pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS) analysis for the quantification of a range of polymers in human blood. An extraction protocol that reduced matrix interferences (false positives) of polyethylene (PE) and polyvinyl chloride (PVC) was developed and validated. Extraction recoveries ranged 7-100%, although surface-modified and

View More

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

Substance Role

By Count | Alphanumeric

1 Selected

☐ Properties (67K)

☐ Process (62K)

☒ Pollutant (7,850)

☐ Reactant or Reagent (7,274)

☐ Reactant (7,039)

Filter Results

Analyze Results

Behavior

Filter by Exclude

7,850 Results

Sort: Relevance

1

Microplastic contamination in some popular seafood fish species from the northern Bay of Bengal and possible consumer risk assessment

By: Jahal, Helima Tuz; Islam, Rakib Ul Md; Sultana, Salma; Banik, Partho; Naeem, Mohammed; Akai, Takashi; Yu, Jimmy; Hosain, Md. Golam; Food Control (2025), 171, 111114 | Language: English; Database: Capius

Microplastics (MPs) are a growing environmental concern in marine ecosystems, marine life and human health, though their specific health impacts remain unclear. MP contamination in three popular seafood fish, analyzing organ specific distribution with body weight and feeding habits. It further calculated human health exposure established models. Samples of gill, gastrointestinal tract (GIT), and muscle tissue from *Lutjanus rhomboides* and *Brachydanus brachyotus* collected from the northern Bay of Bengal.

View More

Full Text 3 0 21

2

Microplastics in human skeletal tissues: Presence, distribution, and implications

By: Yang, Qiaoyi; Peng, Ye; Wu, Xiaodong; Cao, Xiaorui; Zhang, Peng; Zhang, Yongfeng; Gao, Peipei; Fu, Yunfang; et al. Environment International (2025), 196, 109316 | Language: English; Database: Capius

Although microplastics have been detected in human blood, placenta and other tissues, in this study, for

Substances

9003-07-0

(C₃H₆)_x
Polypropylene

Role: Occurrence, Unclassified, Pollutant, Properties, Occurrence

Every publication in this set discusses polypropylene in the context of a pollutant

CAS Lexicon

CAS Lexicon overview

The CAS Lexicon is an ideal tool to understand CAS concept hierarchies, identify scientific expressions, gather relevant keyword synonyms for query building or perform narrow and focused Lexicon searches.

The CAS Lexicon is an ontology of CAS Concepts. CAS Concepts are controlled terms describing the focus of a publication. They are added manually by CAS scientists, based on full-text analysis.

The CAS Lexicon contains subject, chemical class and taxonomic indexing terms in a hierarchy with broader and narrower terms. Concept indexing will be done on the highest level of detail possible, given the information present in the source document. Broader terms do not include more detailed concepts.

Access and navigation



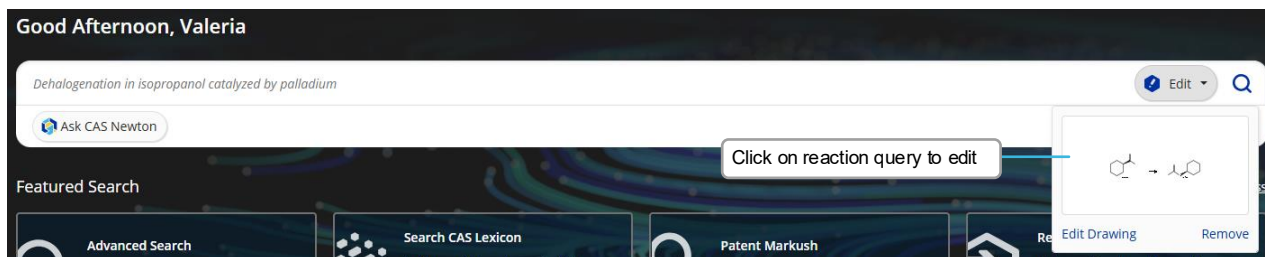
Start by clicking on 'CAS Lexicon' on the landing page, enter a concept or synonym and navigate through the hierarchy of broader and narrower terms. Only one hierarchy level is shown at a time.

Users can build specific CAS Lexicon search queries by selecting concepts and adding them to the query window on the right. Only the selected CAS Concepts will be searched.

Reactions Search

Performing a Reactions search

Reaction queries can be set up using text-based reaction searching, chemical structures, substance names, CAS Registry Numbers, or CAS Reaction Numbers



Reactions search results

By default, reaction search results are grouped into schemes with identical reactants and products. A panel of filters, including yield and steps, allows for further refinement.

Reactions search for drawn structure

CAS Newton NEW All Substances Reactions References Suppliers Patent Markush

Save, alert and share options

View Related Results

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

Group: By Scheme Sort: Relevance View: Expanded

Steps: 4

Send to CAS Draw

Filter Results

View by structure match

Structure Match

As Drawn (0)

Substructure (38K)

Similarity (2,481)

Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (1,240)

80-89% (793)

70-79% (703)

50-69% (1,002)

30-49% (515)

View All

Number of Steps

1 (7,349)

2 (5,838)

Filter reaction results

View Reaction Detail

View reaction details

Suppliers (49)

Suppliers (5)

View suppliers

View reaction reference

Access annotated patent full-text

PatentPak Full Text

Preparation of substituted 3-(4-aminopyrimidin-2-yl)-1H-pyrrolo[2,3-b]pyridines as inhibitors of influenza viruses replication

Assignee: Vertex Pharmaceuticals, Inc.

World Intellectual Property Organization, WO2010148197 A1 2010-12-23

Experimental Protocols

Collapse Scheme

Get similar reactions

Similarity (2,481)

Similarity

Broad (2,481) Medium (15) Narrow (3)

Similar reactions are based on the similarity of adjacent atoms to the specific reaction center.

- **Broad:** Retrieve reactions that share a reaction center with the selected reaction.
- **Medium:** Retrieve reactions that share a reaction center as well as adjacent atoms.
- **Narrow:** Retrieve reactions with a shared reaction center and extended atoms and bonds.

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.

[Get Similar Reactions](#) [Search for similar reactions](#)

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, Jianglin 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

Absolute stereochemistry shown, Rotation (+)
[Suppliers \(53\)](#)

[Stage 2]
[Suppliers \(155\)](#)

Absolute stereochemistry shown, Rotation (-)
85%
[Suppliers \(2\)](#)

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 [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 'Retrosynthetic Analysis' in CAS SciFinder:

1. Draw or import a structure into the retrosynthesis draw window accessed by clicking on the 'Retrosynthetic Analysis' option on the landing page. The drawn substance can be novel.
2. Click on the 'Start Retrosynthetic Analysis' option found on the substance flyout window.

Good Afternoon, Valeria

Dehalogenation in isopropanol catalyzed by palladium

Ask CAS Newton

Featured Search

- Advanced Search: Select data fields and search operators to create a focused query.
- Search CAS Lexicon: Build powerful searches using CAS concepts, chemical classes, and taxonomy.
- Patent Markush: Search Patent Markush by structure and view associated references.
- Retrosynthetic Analysis: Make reaction plans with conditions, yields, catalysts, and experimental procedures.

CAS Registry Number: 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 Life Science Data
Get Reactions (1)
Synthesize (1)
Start Retrosynthetic Analysis
Get References (1)
Get Suppliers (0)
View in CAS BioFinder

Edit Structure | Reset | Download

Retrosynthetic Analysis

Draw or import a structure.

Enter a CAS Registry Number, SMILES, or InChI

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

Molecular Formula: C₁₅H₁₂F₃N₃O₂S (355.34)

Start Retrosynthetic Analysis | Cancel

Generate plan

Retrosynthesis Planner

Selecting plan options

Retrosynthesis Plan for drawn structure View plan information Build Status: Complete Estimated Yield: 10% Overall Price: \$10311.45

[Download and Save your plan](#)

[Exclude substance](#)

[See Related Suppliers](#)

Green dotted lines indicate predicted steps

Blue lines mark experimental steps

Edit final product structure

Show steps details

Reset

Customize Plan

[Edit](#)

Selected Options: **Common**

Predicted Rules: **Common**

Break and Protect Bonds: **None**

Filters

Break bond in first disconnection

Step Type

☒ Experimental Steps

☐ Predicted Steps

At least one step type must be turned on to display

Starting Material Cost Limit

1000 USD/mol

[Apply](#)

Plan Options

Set Rules Supporting Predicted Reactions

☒ Common

☐ Uncommon (includes common rules)

☐ Rare (includes common and uncommon rules)

Break and Protect Bonds (Optional)

Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. [Learn more](#)

☒ Break Bond ☐ Protect Bond

[Clear selections](#)

[Clear All Bond Selections](#)

Protect bond(s) in entire plan

Protected bond(s)

Broken bond

[Continue to Retrosynthesis Plan](#)

[Generate plan](#)

Viewing All Steps

Reaction	Avg Yield	Options
A → B + C 1.1 Reagents: Sodium carbonate Catalysts: Triphenylphosphine , Palladium diacetate , 1-Butyl-3-methylimidazolium chloride Solvents: Dimethylformamide , Water ; 18 h, reflux	63%	Evidence Alternative Steps Exclude
B → D + E 1.1 Reagents: Sodium hydroxide Solvents: Water ; 45 °C; 3 h, 45 °C; 45 °C → rt	66%	Evidence Alternative Steps Exclude
C → H 1.1 Reagents: Butyllithium	68%	Evidence Alternative Steps Exclude
D → F + G 1.1 Reagents: Butyllithium Solvents: Tetrahydrofuran ; -78 °C; 20 min, -78 °C	65%	Evidence Alternative Steps Exclude

Markush search

CAS SciFinder

Enter a query...

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[Return to Home](#)

Patent Markush search for drawn structure

[CAS Newton](#) [NEW](#) [All](#) [Substances](#) [Reactions](#) [References](#) [Suppliers](#) [Patent Markush](#)

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Patent Markush Match

☒ As Drawn (96)

☐ Substructure (120)

Behavior

[Filter by](#) [Exclude](#)

Patent Office

☐ World Intellectual Property Organization (55)

☐ United States (25)

☐ European Patent Organization (8)

☐ China (3)

☐ United Kingdom (2)

Markush details

DE10162120 Markush Details

Preparation of deuterated dihydrofuranones for the treatment of irritation symptoms of joint degeneration, as well as of acute pain, and dysmenorrhea

Assignee: Berolinda Drug Development AB
Germany; DE10162120 A1 2003-06-18 | Language: German, Database: CAPLUS

Patent Status: ● Dead

Patent claim 1

[PatentPak](#) [Full Text](#)

There are no notes to display for this structure.

Markush location

[Link to a specific patent](#)

Markush structure search type

Assembled Markush hit structure

Filter by patent authority

Link to CAS PatentPak Viewer

WO2001094369 Markush Details

Heterocycle derivatives and methods of use

Aspirin, The University of Texas System

Download it as **PDF** (Full-text patent as text-searchable PDF only) or **PDF+** (Full-text patent as text-searchable PDF with marked-up Key Substances)

CAS PatentPak

PAGE 65 67

CLAIMS ZOOM DOWNLOAD

Download PDF including list of marked-up substances and annotations

Jump To

Jump to Claims Download PDF

Key Substances in Patent

CAS RN 2649770-30-7

Analyst Markup Locations (1)

Page 65

CAS RN 2289636-49-1

Analyst Markup Locations (1)

Page 65

CAS RN 2289634-36-0

Analyst Markup Locations (1)

Page 65

CAS RN 60633-25-2

Link to location of substance in patent

Link to related information

WO 2021/126593

Highlighted key substance is marked

T/US2020/063766

Key substances identified in the patent

CAS SciFinder Quick Reference Guide Academic 1.17

Prior Art Discovery

Prior art refers to scientific, technical, or other publicly available information that existed before the filing date of a patent application. In simple terms it answers: "What was already known before?"

CAS SciFinder uses AI to automatically retrieve a list of similar publications, starting from a patent that is already published and indexed, or from any text describing the topic of interest.

From a published patent

Select 'Get Prior Art Analysis' from the patent reference detail page.

- Uses a single patent as the starting point.
- Draws on indexed CAS concepts, substances, IPC/CPC codes, and full text of the claims to identify relevant prior art.
- Retrieves documents published before the patent's application date in the answer set.

Aqueous dendritic amine coatings containing dendritic poly(amid...

13 0 1 1 Citation Map

In This Patent

- [Claims](#)
- [Classifications](#)
- [CAS Concepts](#)
- [Substances](#)
- [Formulations](#)

Assignee: NIPSEA Technologies Pte. Ltd.
Inventors: Wang, Shaofeng; Li, Hairong; Seow, Swee How

The poly...

Keywords: aqueous dendritic coating PAMAM polyamidoamine

[PatentPak](#) [Get Prior Art Analysis](#) [Full Text](#) [View in CAS](#)

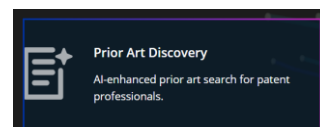
Results

Access results from search history.

- Provides an AI-based relevance prediction.
- Generates a list of relevance-ranked previously known documents
- Patent and non-patent literature are divided in separate tabs.

From free text

Access the input interface via the Prior Art Discovery button on the landing page.



Add descriptive text, such as the abstract of a publication or the claims section of a patent. Optionally, add a chemical structure and adjust the priority date if needed. Results can be limited to documents published before the selected date.

Prior Art Discovery

Prior Art Discovery uses CAS AI tools to find similar patents and non-patent literature results. Please input a mini [Discovery](#).

An aqueous antimicrobial coating composition containing: (A) a specific multistage polymer bearing specific he to 1000 ppm, by weight based on the weight of the aqueous antimicrobial coating composition, of silver ions; w composition is 10: 1 or higher; (C) from 0.04-1.0% of zinc oxide, by weight based on the weight of the aqueous

Change the date up to which you want to see results

Priority Date: 2026-09-04 [Edit](#)

Optionally add a structure

Add Structure (Optional)
[Edit](#)

[Edit Drawing](#) [Remove](#)

Prior Art Discovery for "An aqueous antimicrobial coating composition containing: (A) a specific multistage polymer bearing s..."

Search Details

Your Inputs

Text
An aqueous antimicrobial coating composition containing: (A) a specific multistage polym...
[View All](#)

Priority Date
2026-09-04

Structure

C=CN1C=CC=C1

Full Text

4

Diffusion coefficients of silver ions in aqueous phosphoric and fluoroboric acid solutions
By: Koczorowski, Zbigniew
Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1981), 125 (1), 225-9 | 10.1016/s0022-0728(81)80338-5
In aqueous H3PO4 (3.25-9.20 mol/dm3) and aqueous HBF4 (2.50-5.43 mol/dm3) solutions at 25°, the diffusion coefficient (D) of Ag+ was determined by the chronopotentiometric method. D Decreased with increasing acid concentration; D was larger in aqueous HBF4 than in aqueous H3PO4.

Full Text

5

Fungicidal paint for outdoor use
By: Singh, I. D.; Chandel, B. S.; Maithani, D.; Tandon, R. N.
Labdev, Part A: Physical Sciences (1971), 9 (3-4), 155-7
...afforded to metal telegraph poles and towers used in communication systems in the jungles of India by application of one coat of primers containing fungistatic/alk. pigments, e.g. aluminum [7429-90-5], zinc oxide [1314-13-2], or pigment BR in an alkyd resin medium, and 2 coats...

Full Text

Fungicidal paint for outdoor use

By: Singh, I. D.; Chandel, B. S.; Maithani, D.; Tandon, R. N.

Non-Patent Literature
[View Reference Details](#)

Protection against attack by fungi and lichens was afforded to metal telegraph poles and towers used in communication systems in the jungles of India by application of one coat of primers containing fungistatic/alk. pigments, e.g. aluminum [7429-90-5], zinc oxide [1314-13-2], or pigment BR in an alkyd resin medium, and 2 coats of a finishing paint containing the same materials. **Keywords:** coat of primers, alkaline pigments, finishing paint, metal telegraph poles, coats, pigment BR, lichens, alkyd resin medium, same materials, fungistatic, zinc oxide, aluminum, towers, communication systems, application

[Publication Information](#) [View More](#)

Substances

Concepts

Suppliers Search

Suppliers search

Find Supplier information on substances via the result navigation bar, from a specific substance, or query it directly.

Results for "Where can I buy 1kg HMF"

CAS Newton **NEW** All Substances Reactions References Suppliers Patent Markush

67-47-0
HMF

Estimated Commercial Pricing
\$13.3 USD/kg

Supplier price is the average of HMF
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Suppliers

Showing 3 of 128 Suppliers

AstaTech AstaTech Product List
2026-07-28

BOC Sciences BOC Sciences Product List
2024-10-09

ALFA Chemistry Alfa Chemistry Product List
2026-05-07

67-47-0
5-HYDROXYMETHYLFURFURAL

67-47-0
5-Hydroxymethyl-2-furaldehyde

67-47-0
5-Hydroxymethyl-2-Furaldehyde

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[Order From Supplier](#)
25 g, USD 112.00

Order Number: NP4241

Order Number: ACM67470-1

Suppliers search for "7664-93-9"

CAS Newton **NEW** All Substances Reactions References **Suppliers** Patent Markush

Filter Results

Behavior

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Preferred Suppliers

Supplier

Purity

- ☐ ≥99% (4)
- ☐ 95-98% (141)
- ☐ 90-94% (10)
- ☐ <90% (10)

498 Results

[Link to detail](#)

Oakwood Chemical Product List

Substance	Purity	Quantity Information	Availability	Ordering
7664-93-9 Sulfuric Acid, ACS Grade	95-98%	100 ml, USD 28.00 1 L, USD 43.00 2.5 L, USD 88.00 Bulk	Maintained in stock Ships within 1 week United States	Order From Supplier Order Number: 080325

Sort options

Sort: [Relevance](#)

- Relevance
- Price: Low to High
- Price: High to Low
- Supplier: A to Z
- Supplier: Z to A
- Ships Within
- Purity

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