

FOR ACADEMIA

CAS SCIFINDER DISCOVERY PLATFORM™

QUICK REFERENCE GUIDE

CAS

A division of the
American Chemical Society



Contents

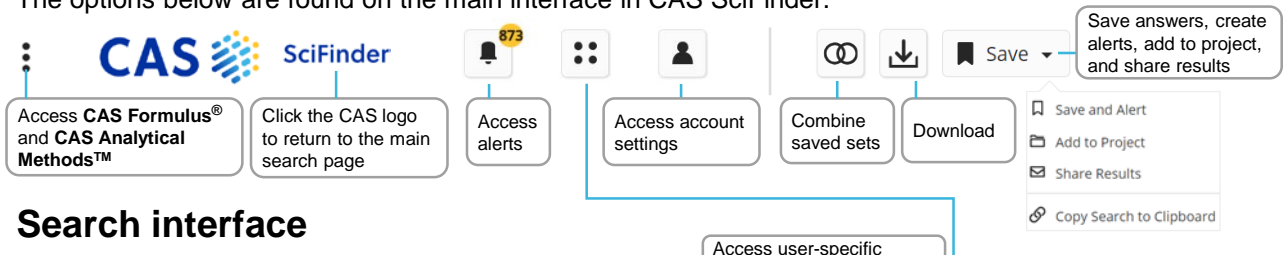
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CAS SciFinder

Solution interface and References search

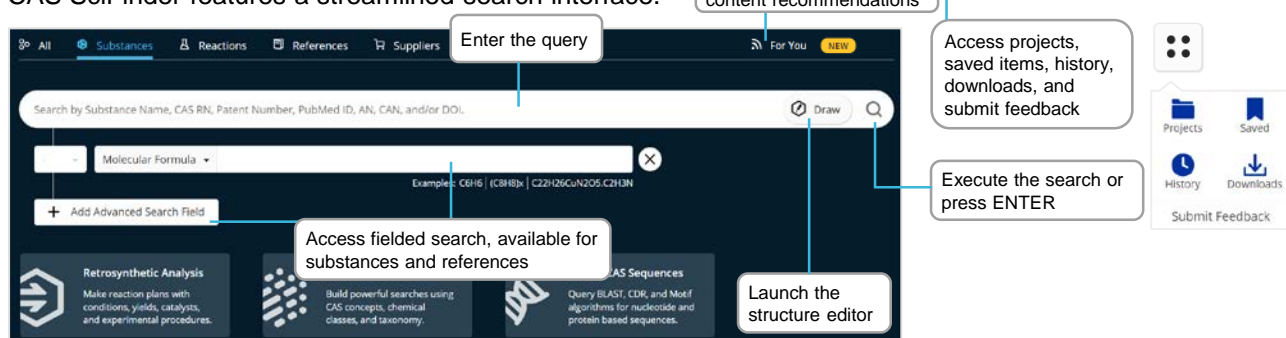
Main interface

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



Search interface

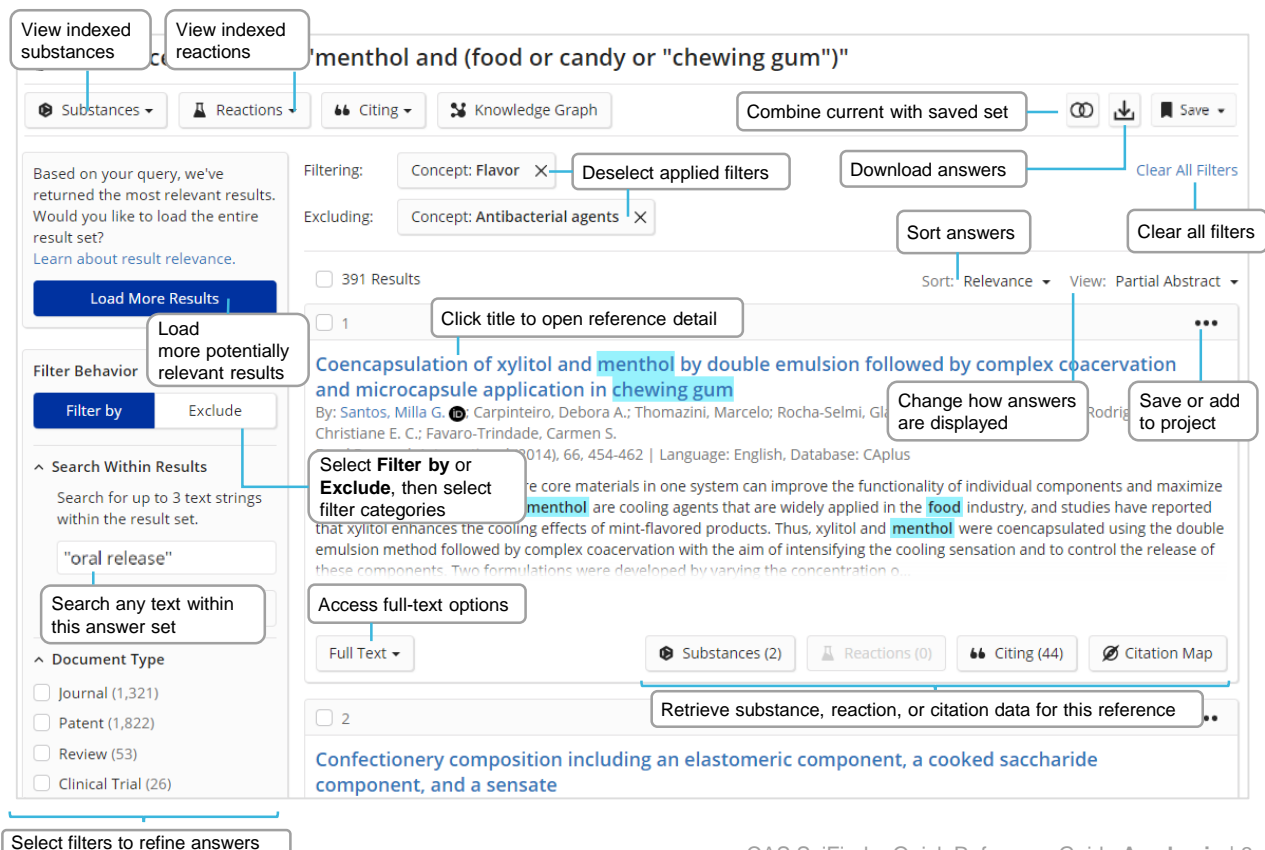
CAS SciFinder features a streamlined search interface.



References search results

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.



Select filters to refine answers

Reference detail

 Fruit juice-containing food products with refreshing and cooling flavors

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

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

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

Keywords: fruit juice flavor food beverage menthol

View bibliographic details

Patent family and priority application information

Boolean operators

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

AND Requires both terms to be present within the document

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

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



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

- | | | |
|---|--|--|
| * | Replaces 0 to any number of characters | ex: polymorph* immunoglobulin*conjugate* |
| ? | Replaces 0 or 1 character in reference searching | 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. At the top, there are navigation tabs: All, Substances, Reactions, References, and Suppliers. Below these is a search bar with the text "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and a button "Enter chemical name query". To the right of the search bar is a button "Click to draw new structure" and a button "Edit". Below the search bar, there are three main search options: "Add Advanced Search Field", "Search CAS Lexicon", and "Search CAS Sequences". Each option has a brief description and a button to "Click query structure to edit". There is also a button "Check to perform Markush search".

Substances search results

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.

The screenshot shows the CAS SciFinder search results interface. On the left, there are several filters: "Structure Match" (As Drawn (117), Substructure (6.2M), Similarity (1,052)), "Analyze Structure Precision", "Chemscape Analysis", "Filter Behavior", and "Search Within Results". The main area displays a list of search results. Each result includes a chemical structure, a CAS Registry Number, and a name. For example, the first result is "90357-06-5" with a chemical structure of a sulfonamide. The second result is "80-08-0" with a chemical structure of Dapsone. The third result is "67-71-0" with a chemical structure of Dimethyl sulfone. Below the list, there is a "Retrieve data related to substance" section with buttons for "Get Substance Details", "Get Bioactivity Data", "Get Reactions (2,494)", "Synthesize (9)", "Start Retrosynthetic Analysis", "Get References (1,404)", and "Get Suppliers (103)". On the right, there is a "Change sort criterion" section with a dropdown menu "Sort: Number of Suppliers" and a "View: Partial" button. Below this is a "Change amount of details displayed" section with a dropdown menu "View: Partial". At the bottom right, there is a "Download .sdf or .mol. Copy Smiles to Clipboard" button and a button "Open editor with this structure".

Substance detail and structure editor

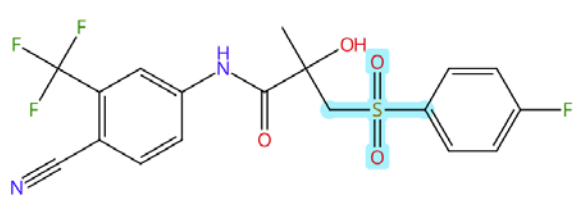
Substance details

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

4,364 233 116

Download Save



GHS Hazard pictograms, full list in tab at bottom of page

C18H14F4N2O4S 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	Press: 760 Torr
Density (Predicted)		

Key properties

Other Names

Experimental Properties

Experimental Spectra

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

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

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

9 Other Names for this Substance

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

CAS Draw editor

You can 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...

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

Bond mapping | Draw reaction arrow

Learn about keyboard shortcuts (e.g., drawing hetero atoms easily)

Hetero atom and H isotope selection

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw

Zoom: 90%

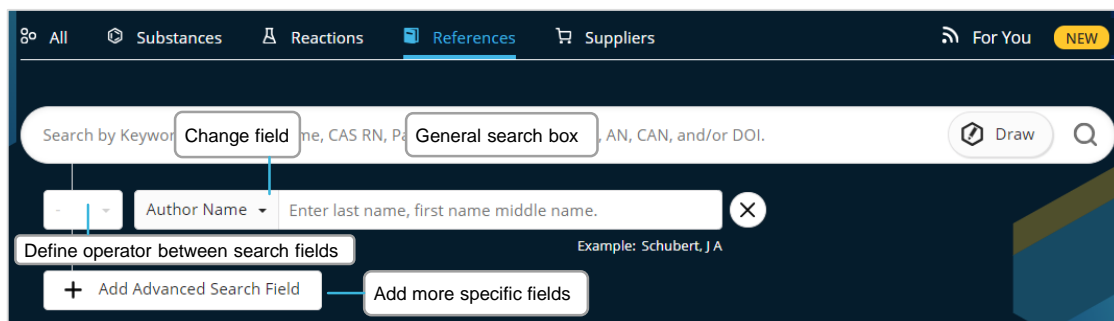
OK Cancel

Advanced Search

Performing an Advanced Search

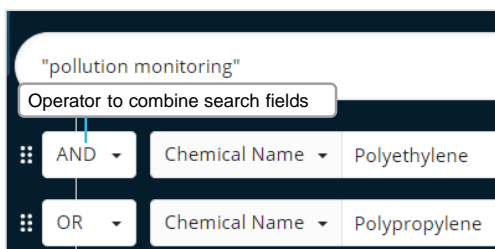
You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinder.

- 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)



Advanced Search examples

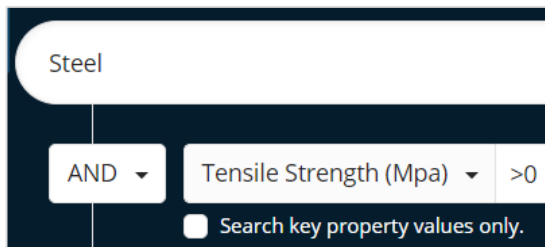
Advanced References Search



Query interpretation:

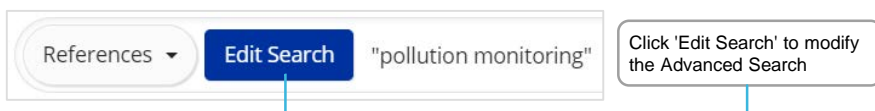
"pollution monitoring" and (polyethylene or polypropylene)

Advanced Substances Search



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

- Authors
- Publication Name
- Organization
- Title
- Abstract/Keywords
- Concept
- Substances
- Bioactivity Data
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Substances Search

- Molecular Formula
- CAS Registry Number
- Chemical Identifier
- Document Identifier
- Patent Identifier
- Experimental Spectra
- Bioactivity Data
- 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, 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)

☐ 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)

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 results 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 3,661 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

321K References 7,909 Reactions 27 Suppliers

Filter Behavior

Filter by ▾ Exclude

Search Within Results

Document Type

Substance Role

- ☐ Uses (268K)
- ☐ Properties (61K)
- ☐ Process (52K)
- ☐ Biological Study (23K)
- ☐ Preparation (19K)

View All

Language

455,514 Results

1

Microstructure of polypropylene

By: Busico, Vincenzo; Cipullo, Roberta
Progress in Polymer Science (2001), 26(3), 443-533 | Language: English, Database: CAPIUS

A review, with 175 references, on catalyst technologies for manufacture of polypropylene with well-controlled microstructure and properties for advanced applications. The development of transition metal catalysts with tunable structure and selectivity is discussed. Polypropylene products with novel and well-controlled microstructure are described. The use of high-field ¹³C NMR methods to study the stereochem. of polypropylene is also discussed.

Full Text ▾

Substance (1) Reactions (0) Citing (395) Citation Map

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

Substance Role

By Count Alphanumeric

1 Selected

- ☐ Uses (268K)
- ☐ Technical or Engineered Material Use (191K)
- ☐ Polymer in Formulation (81K)
- ☐ Properties (61K)
- ☐ Process (52K)
- ☐ Biological Use, Unclassified (3,793)
- ☒ Pollutant (3,661)
- ☐ Biological Study, Unclassified (2,558)
- ☐ Miscellaneous (2,444)


Substance Role

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

View All

Language


Publication Year



No Min to No Max Apply

Microplastics in marine environment review of methods for identification and quantification


By: Hidalgo-Ruz, Valeria; Gutow, Lars; Thompson, Richard C.; Threl, Martin
Environmental Science & Technology (2012), 46(6), 3060-3075 | Language: English, Database: CAPIUS 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-mediated, 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: a) 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 (i.e., specific ID) were also used. The most reliable method to identify the chem. composition of microplastics is by IR spectroscopy. Most studies reported that plastic fragments were polyethylene and polypropylene polymers. Units commonly used for abundance estimates are "items per m³" for sediment and sea surface waters, 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 ranges of microplastics: (i) 500 µm < mm, which are retained by a 100 µm sieve/mesh, 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 (1) Reactions (0) Citing (2,299) Citation Map



Every publication in this set of 3,661 references discusses polypropylene in the context of a p



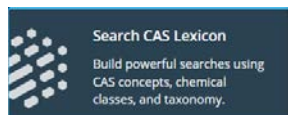
CAS Lexicon

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 highly 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.

Search CAS Sequences

Search options

You can search sequences using three different modalities:

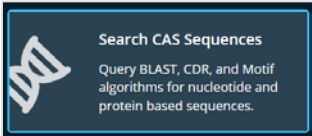
- BLAST: Search similar sequences
- CDR: Search antibodies and t-cell receptors via CDRs
- Motif: Search using variability symbols

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 CAS 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.
- Note 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.



BLAST

CDR

Motif

Sequence Search options

Clear Search

> human insulin sequence
fvnqhlcgshlveaylvcgengfftytpktgiveqcctsiclslyqlenycn

Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane

Upload Sequence (.fasta or .txt)

Paste sequence into this window

Sequence Type:
Nucleotide Protein

Search Within:
Nucleotides Proteins

Include NCBI sequences

Include NCBI Sequences

Search Sequences

Advanced Sequence Search

Adjust Parameters for Short Sequences | Reset All

Alignment Identity %
-

Match with Gaps?
Yes No

Gap Costs
Existence 11 Extension 1

Query Coverage %
90

Word Size
3

Scoring Matrix
BLOSUM62

BLAST Algorithm
BLASTp

E-Value
10

Exclude Low Complexity Regions
Yes No

Advanced BLAST parameters



BLAST results analysis

Access results

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

Sequences

1:34 PM

Sequence Type: Protein

Search Within: Proteins

NCBI Included: Yes

BLAST Algorithm: BLASTp

Alignment Identity: -

Query Coverage: 90%

Results will expire on Oct 31, 2023.

> human insulin sequence

fvnqhlcgshlveaylvcgergffytptkgiveqcctsicslyqlenycn

View Results

Edit Search

Complete

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 the '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 (includes a gap of 5 residues)

View Less

Alignment Details

Subject and links to NCBI and substance information in CAS SciFinder

Reference previews

Alignment

Subject

References

Alignment Data

BLAST Score: 231

E-Value: 5.12823e-26

Match

+ Mismatch: Query aa aligned to functionally equivalent subject aa

Get References for this sequence

Q

1

FVNQHLGSH LVEA-YLVCG ERGFFYTPKT ----GIVEQC CTSICSLYQL ENYCN 55

S

1

FVNQHLGSH LVEALYLVCG ERGFFYTPKSDDARGIVEQC CTSICSLYQL ENYCN 55

Start residue of alignment in query and subject sequences

Gap in the query sequence

Filter results

Filtering dynamically changes your results.

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)

Bioactivity data

Searching for targets, ligands, and diseases

The advanced search fields in Substances and References search allow you to find targets, ligands, and diseases with the according bioactivity data. This will search for substance and/or literature within the CAS Life Sciences accordon.

The first screenshot shows the 'Substances' search tab with a dropdown menu for 'Substances with bioactivity data are searched'. The second screenshot shows the 'References' search tab with a dropdown menu for 'Literature with bioactivity data is searched'. The third screenshot shows a combined search interface with a 'Target' dropdown menu and a text input field containing 'Renin receptor ATP6IP2'. A callout box indicates: 'Select target, ligand, or disease (further bioactivity search field can be added and combined)'.

Bioactivity data filter in reference and substance search

The first screenshot shows the 'Life Science Data' filter section with checkboxes for 'Pharmacological Data (56)', 'ADME (113)', and 'Toxicity (5)'. A callout box indicates: 'Filter to refine by the availability of Pharmacological Data, ADME, and Toxicity data'. The second screenshot shows the 'Life Science Data' filter section with checkboxes for 'Pharmacological Data (1,422)', 'ADME (60)', and 'Toxicity (9)'. A callout box indicates: 'Filter to refine by the availability of Pharmacological Data, ADME, and Toxicity data'. Below the filters, a chemical structure is shown with the formula C35H24O7 and the name '2-(2,2-Diphenyl-1,3-benzodioxol-5-yl)-5,7-dihydroxy-3-(phenylmethoxy)-4H-1-benzo...'. A 'Full Text' dropdown is also visible.

Bioactivity data in Substance details

The screenshot shows the 'Substance details' page for 'Toll-like receptor 7'. It includes a table of bioactivity data with columns: Target, Function, Parameter, Value, Disease, Organism, Assay, and Source. The table lists three entries for 'Toll-like receptor 7' as an 'Agonist' with an 'EC50' value of '0.42 µM' and a 'Disease' of 'acute pathogen infection'. A callout box indicates: 'Shows full assay details'. Below the table, there are sections for 'ADME' and 'Toxicity'. An 'Assay Data' popup is shown, displaying the chemical structure of 'Resiquimod' (C11H20N4O2) and its details: Target (Toll-like receptor 7), Assay Name (SEAP reporter assay), Procedure, Assay Comment, Condition, Parameter (EC50), Value (0.42 µM), Measurement Remarks, Ligand Dose, Biological System (Human; HEK cells), and Source (Preparation of 6-amino-7,9-dihydro-8H-purin-8-one derivatives as immunostimulant Toll-like receptor 7 agonists. By: Poudel, Yam B.; Gangwar, Sanjeev; Sivaprakasam, Prasanna; Posy, Shoshana L. World Intellectual Property Organization WO2019036023 A1 2019-02-21 | Language: English; Database: CAPLUS).

Bioactivity data in Reference details

The screenshot shows the 'Reference details' page for 'Pharmacological Data'. It includes a table of bioactivity data with columns: Ligand, Target, Function, Parameter, Value, Disease, Organism, and Assay. The table lists two entries for '621-82-9' as an 'Inhibitor' with an 'IC50' value of '1.017 µM' and a 'Disease' of 'Metabolic syndrome'. A callout box indicates: 'Shows full assay details'.



Reactions search

Performing a Reactions search

Reaction queries can be set up using CAS Reaction Numbers, substance names, CAS Registry Numbers, document identifiers, a chemical structure, or text-based reaction searching.

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.

For single-step, single-stem reactions, you may view similar reactions 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 Azindolyl-Pyrimidine Inhibitor of Influenza Virus Replication

By: Liang, Jiang

View All

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 \(48\)](#)

[Stage 2]
[Suppliers \(149\)](#)

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

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

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

Solvents [Toluene](#)

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

Characterization Data [View characterization data](#)

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

Proton NMR Spectrum (300 MHz, 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, Ilja

🔍 All 📦 Substances ⚗️ Reactions 📄 References 🛒 Suppliers

Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.  Draw 🔍

**Retrosynthetic Analysis**
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

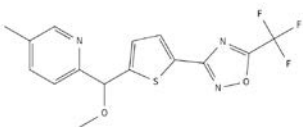
**Search CAS Lexicon**
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

**Search CAS Sequences**
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

1

Retrosynthetic Analysis
Draw or import a structure.

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



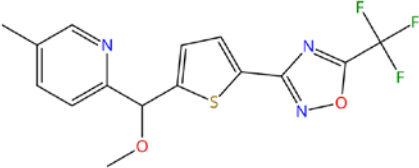
Molecular Formula: C₁₃H₁₂F₃N₃O₂S (355.34)

Start Retrosynthetic Analysis Cancel

CAS RN
2408121-76-4

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

Get Substance Details
Get Bioactivity Data
Get Reactions (1)
Synthesize (1) **2**
Start Retrosynthetic Analysis
Get References (1)
Get Suppliers (0)



Edit Structure Reset

Retrosynthesis planner

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, e.g., poly or heterocyclic molecules.

Once you have selected the desired options, click the 'Create Retrosynthesis Plan' button.

Retrosynthesis Plan Options for drawn structure Powered by ChemPlanner®

Select Synthetic Depth Learn more.

☐ 1
☐ 2
☒ 3
☐ 4

Break and Protect Bonds Learn more.

☒ Break Bond ☒ Protect Bond [Clear All Bond Selections](#)

Set Rules Supporting Predicted Reactions Learn more.

☒ Common
☐ Uncommon (includes Common Rules)
☐ Rare (includes Common and Uncommon Rules)

Set Starting Materials Cost Limit Learn more.

1000 USD/mol

☐ Email me when my plan is complete

[Create Retrosynthesis Plan](#)

Chemical Structure: COc1ccc(NC(=O)C2=CC=CC=C2)cc1

Callouts:

- Change the number of disconnections in the plan (points to Synthetic Depth)
- Break bond in first disconnection (points to Break Bond button)
- Protect bond(s) in entire plan (points to Protect Bond button)
- Clear selections (points to Clear All Bond Selections)
- Select uncommon or rare rules supported by fewer literature examples (points to Uncommon/Rare rules)
- Change upper cost limit for starting materials (USD/mol or USD/g) (points to Cost Limit)
- First bond to be broken (points to the bond between the pyridine ring and the carbonyl group)
- Protected bonds (points to the C-F bonds in the trifluoromethyl group)

Generate plan



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 longer.

Retrosynthesis Plan for drawn structure

View plan information

Plan Information

Estimated Yield: 22%
Overall Price: \$48.62
(USD per 100 grams)

Scoring Profiles

Complexity Reduction
Convergence
Evidence
Cost
Yield
Atom Efficiency

Apply Reset Scoring

Experimental Steps Predicted Steps Edit Plan Options

Exclude steps or substances

Download, Share, and Save your plan

View plan steps

Blue lines mark experimental steps

Green dotted lines indicate predicted steps

Adjust scoring options

Review and select alternative disconnections

Powered by ChemPlanner®

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.

Step Evidence

1.1 Reagents: Butyllithium
Average Yield: 47%
Evidence (16)
Alternative Steps

1.1 Reagents: Potassium *tert*-butoxide
Solvents: Tetrahydrofuran
Average Yield: 59%
Evidence (23)
Alternative Steps (34)
[Experimental Protocols](#) 1

1.1 Reagents: Diisopropylethylamine
Ammonium chloride
O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluoro phosphate
Solvents: Dimethylformamide; 2 d, rt
Average Yield: 50%
Evidence (38)
Alternative Steps (48)
[Experimental Protocols](#)

Predicted Step Only
No reaction summary
Maximum Yield: 79%
Evidence (1)
Alternative Steps (11)
[Experimental Protocols](#)

1.1 Solvents: Carbon tetrachloride
Maximum Yield: 83%
Evidence (1)
Alternative Steps (14)

Filter by

Alternative Step Type
Predicted (48)
Stereochemistry
Non-Selective (48)

5 of 15

Predicted Step

Select View 8 similar Alternatives 2 View Evidence Average Yield: 63%

Grouped similar reactions

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (2)
80-89% (3)
70-79% (10)
50-69% (15)
30-49% (2)
View All

Number of Steps

1 (55)

Non-Participating Functional Groups

55 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction)

Steps: 1

Suppliers (49) Suppliers (51) Suppliers (61)

31-614-CAS-29434160

Steps: 1

Preparation of piperidine-containing compounds for treating and preventing metabolic and cerebrovascular diseases

By: Rodríguez, Maritza E.; et al
World Intellectual Property Organization,
WO2010080664 A1 2010-07-15

PatentPak 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.

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 Information

Estimated Yield: 79%
Overall Price: \$599.28
(USD per 100 grams)

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 shows the CAS SciFinder interface for a Patent Markush search. The top navigation bar includes the CAS logo, SciFinder, and a search bar. The main section 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 displays a chemical structure with Markush symbols (G1, G2, G3, G4) and a list of patent matches. The first match is 'Preparation of deuterated dihydrofuranones for the treatment of irritation symptoms of joint degeneration, as well as of acute pain, and dysmenorrhea' by Berolina Drug Development AB. The second match is 'Heterocycle derivatives and methods of use' by The University of Texas System. The interface also includes a 'Markush search option' button, a 'Link to a specific patent reference' button, and a 'Link to CAS PatentPak Viewer' button.

CAS PatentPak

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

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

The screenshot shows the CAS PatentPak interface for viewing a patent PDF. The top navigation bar includes the CAS logo, PatentPak, and a search bar. The main section is titled 'Key Substances in Patent'. On the left, there is a list of key substances with their CAS RNs and chemical structures. The central area displays a patent PDF with marked-up key substances. The first key substance is 'Li' (CAS RN 33454-82-9) and the second is 'Li+' (CAS RN 14283-67-9). The interface also includes a 'Download PDF' button, a 'Link to related information' button, and a 'Highlighted key substance is marked' button. The bottom section shows a detailed view of a key substance, including its chemical structure, CAS RN, and a list of related information.

Suppliers search and ChemDoodle

Suppliers search

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

Suppliers search for "7664-93-9"

490 Results

Filter Behavior: Filter by (selected), Exclude

Preferred Suppliers:

- ☐ Preferred (52)
- ☐ No Preference (438)

Supplier:

- ☐ Hayashi Pure Chemical Products Catalog (106)
- ☐ Thermo Fisher Scientific Product List (66)
- ☐ KANTO CHEMICAL (43)
- ☐ Aladdin Scientific Product Listing (37)
- ☐ FUJIFILM Wako Chemicals Europe GmbH Product List (37)

View All

Purity:

- ☐ ≥99% (8)
- ☐ 95-98% (132)
- ☐ 90-94% (9)
- ☐ <90% (14)

Sort options: Sort: Relevance (selected)

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

Preferred/non-preferred supplier tagging

Supplier	Substance	Purity	Purchasing Det
<input type="checkbox"/> 1 Oakwood Chemical United States Last Updated: 1 Mar 2024	7664-93-9 Sulfuric Acid, ACS Grade	95-98%	Order From Sup 100 ml, USD 25 1 L, USD 40.00 2.5 L, USD 80.00
<input type="checkbox"/> 2 Link to detail Oakwood Chemical United States Last Updated: 1 Mar 2024			
<input type="checkbox"/> 3 Oakwood Chemical United States Last Updated: 1 Mar 2024			

Reactivity of information

Reactivity of information

Link to detail

Oakwood Chemical Product List

Preferred Supplier

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

Email: sales@oakwoodchemical.com

Phone: 1-800-467-3386

Substance Information

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

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

Item Details

Chemical Name: Sulfuric Acid, ACS Grade

Order Number: 25494

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 2024

Order From Supplier

ChemDoodle

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

ChemDoodle interface showing various tools and a chemical structure.

Tools:

- Select
- Center
- Flip fragment
- Cut | Copy | Paste
- ChemDoodle
- Clear | Eraser
- Labeling
- Undo | Redo
- Draw bonds
- Draw rings
- Add charges
- Chain tool
- Repeating groups
- Variable point of attachment
- Lock atoms/chains/rings
- Add attachment point to fragment
- Make reaction
- Reaction mapping
- Break/form bonds
- Templates
- Open | Save
- Zoom

Model with CAS Registry Number

ChemDoodle®



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 is how it works:

- 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)

13 | 0 | 1 | Citation Map

In this Reference

- [IPC Data](#)
- [CAS Concepts](#)
- [Substances](#)

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 (PAMAM), at least one isothiazolone biocide, and a binder.

Keywords: aqueous dendritic amine coatings

PatentPak Viewer | Get Prior Art Analysis | Full Text

Initiate the analysis from the detailed record view

References

1:52 PM

Prior Art Analysis (195)

[Aqueous dendritic amine coatings containing dendritic poly\(amido\)amine \(PAMAM\)](#)

View Results

Complete

View Results from the search history

CAS Formulus

Search

CAS Formulus

Help & Support

Alerts

Saved


Good Afternoon, Liu

Formulations


Ingredients

celecoxib

Enter a formulation ingredient, purpose, physical form, function or document identifier (including patent number, DOI number, etc.), and then click the magnifying glass.



Formulation Designer
Design custom formulation templates based on selections and ingredients



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

Browse and select field

All Fields
Form
Function
Ingredient
Purpose
Route
Target

Add another term

Add Another Term

Advanced Formulations Search

Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.
At least two search terms are required.

Search For

Operator

Enter one term

Ingredient

Required

Celecoxib

Ex: caffeine, sodium, 50-00-0

Delete this

Search For

Operator

Enter one term

Purpose

Required

Analgesics

Ex: herbicide, fertilizer, bakery product

Search For

Operator

Enter one term

Form

Required

Tablets

Ex: spray, granules

Choose an operator to connect different terms for searching

Optional

Excluded

Clear all

Clear All

Click for formulation search

Search

Download results as PDF or Excel format.

Formulations search for "celecoxib"

Get Additional References

Compare (2/3) | Save

Sort: Relevance | Group: By Family

Filter by — Refine results by applying filters.

- Industry
 - ☒ Pharmaceutical
 - ☐ Unclassified
- Purpose
 - ☐ Drug delivery systems (108)
 - ☒ Analgesics (81)
 - ☐ Anti-inflammatory agents (80)
 - ☐ Antiarthritics (57)
 - ☐ Pharmaceutical formulations (31)
- Physical Form
 - ☐ Capsules (85)
 - ☒ Tablets (81)
 - ☐ Solutions (54)
 - ☐ Suspensions (31)
 - ☐ Liquids (17)
- State of Matter
- Delivery Route
 - ☒ Oral drug delivery systems (81)
 - ☐ Controlled-release drug delivery systems (11)
 - ☐ Topical drug delivery systems (5)
 - ☐ Parenteral drug delivery systems (4)
 - ☐ Inhalation drug delivery systems (2)
- Information Included
 - ☒ Component Amount (80)
 - ☐ Process (59)
 - ☒ Experimental Activity (49)
 - ☐ Effective Dose (5)
- Document Type
- Organization
- Language
- Publication Year

View All

Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics

Location: Comparative Example 2B, Table 2, 5
Purpose: Analgesics, Anti-inflammatory agents
Target: Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis
Delivery Route: Oral drug delivery systems
Physical Form: Tablets

Formulation components, function, and amount reported

Component	Function	Amount Reported
Group: granulated celecoxib	Formulation active agents	1008 g
Celecoxib	Nonsteroidal anti-inflammatory agents [Ⓢ]	1200 g
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:7)	Formulation excipients	264 g
Hydroxypropyl cellulose	Disintegrants	-
Cellulose, carboxymethyl ether	Disintegrants	102 g
Additional group components reported		
Group: Additional ingredients	-	-
Magnesium stearate	Lubricants	12 g

Patent PDF | View in CAS SciFinder

View or download the patent full text.

View in CAS SciFinder

Remove from Compare

View Formulation Detail

11 Similar Formulations - View All | View similar formulations.

Oral Pulsatile Drug Delivery System of Celecoxib: Antiinflammatory Agents or Analgesics--Controlled Release Drug Delivery Systems for Pharmaceutical Formulation

Location: Article Page 1, 3, 4, Table 1
Purpose: Analgesics, Anti-inflammatory agents
Delivery Route: Oral drug delivery systems
Physical Form: Tablets

Add to Compare

Component	Function	Amount Reported
Group: celecoxib granules	Formulation active agents	-
Celecoxib	Nonsteroidal anti-inflammatory agents	-
Mannitol	-	-

JOURNAL

Formulation and evaluation of pulsatile drug delivery system of celecoxib
World Journal of Pharmaceutical Research
Language: English
View in CAS SciFinder

Click the hyperlink to view more information about this ingredient



Explore detailed formulation information

Download result as PDF format.

Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics

Download icon

Save

Purpose

Target

Delivery Route

Physical Form

Analgesics, Anti-inflammatory agents

Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis

Oral drug delivery systems

Tablets

Save the result

View

Predicted value

Formulation Ingredients

Ingredients details about this formulation

Expand All Groups | Collapse All Groups

Feedback

Component	Function	Amount Reported	Optionality
Group: granulated celecoxib	Formulation active agents	1008 g	Mandatory
Celecoxib	Nonsteroidal anti-inflammatory agents	1200 g	Mandatory
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)	Formulation excipients	264 g	Mandatory
Hydroxypropyl cellulose	Disintegrants	384 g	Mandatory
Cellulose, carboxymethyl ether	Disintegrants	102 g	Mandatory
Poly(vinyl alcohol)	Binders	42 g	Mandatory
Sodium dodecyl sulfate	Surfactants	24 g	Mandatory
Magnesium stearate	Lubricants	12 g	Mandatory

More Formulations like this...

View more related similar formulations

Celecoxib Tablet Composition: Antiarthritics Purpose: Antiarthritics Target: Arthritis, Homo sapiens Delivery Route: Oral drug delivery syst... Physical Form: Tablets

Celecoxib Tablet: Antiarthritics Purpose: Antiarthritics Target: Homo sapiens, Osteoarthritis, ... Delivery Route: Physical Form: Tablets

Pharmaceutical Composition: Antiarthritics-Immediate Release Purpose: Antiarthritics Target: Homo sapiens Delivery Route: Oral drug delivery syst... Physical Form: Sachets, Tablets, disinte...

Antiarthritic Pharmaceutical Composition Purpose: Antiarthritics Target: Arthritis, Homo sapiens Delivery Route: Oral drug delivery syst... Physical Form: Tablets

Process

The process for this formulation

celecoxib, lactose hydrate, low-substituted hydroxypropyl cellulose and carmellose were added into a high-speed stirring granulator to obtain a mixture. polyvinyl alcohol and sodium lauryl sulfate were dissolved in purified water to obtain a solution. the obtained solution was added dropwise or sprayed over the mixture obtained above and wet granulated to a particle diameter of 4 mm in a crusher. the granulated product was put into a fluid bed dryer supplied with air at a temperature of 85 °C and dried at 40 °C. the dried product was further crushed to obtain granulated celecoxib of diameter 1 mm. the obtained celecoxib granulated product was mixed with magnesium stearate and tableted at 600 kgf pressure to obtain a circular tablet of 340 mg and 9.5 mm diameter.

Experimental Activity

Reported experimental activity about this formulation

Descriptor	Notes	Details
dissolution rate of celecoxib	after 15 minutes	27.6 %
dissolution rate of celecoxib	after 30 minutes	75.1 %
dissolution rate of celecoxib	after 45 minutes	88.7 %
dissolution rate of celecoxib	after 60 minutes	93 %

Source Patent

View the source patent

Pharmaceutical tablet containing celecoxib as anti-inflammatory and analgesic agent

Assignee : Ohara Pharmaceutical Co., Ltd.
JP2019089758
Language: Japanese
Location: Comparative Example 2B, Table 2, 5

Patent PDF

View in CAS SciFinder

CAS SciFinder Quick Reference Guide Academic | 25

Search for ingredients

CAS

Formulus

Help & Support

Alerts

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Good Afternoon, Liu

Click Ingredients

Formulations

Ingredients

propylene glycol

Enter an ingredient name, CAS Registry Number, or function, and click the magnifying glass to search.

Ingredients search for "propylene glycol"

Refine results by applying filters

Filter by

Industry

☐ Agrochemical

☐ Cleaning & Surfactant Products

☐ Cosmetics & Personal Care

☐ Food & Related

☐ Inks, Paints, & Coatings

☒ Pharmaceutical

View All

Regulatory Information

☐ REACH (6)

☐ Cosing: Cosmetic Ingredient Inventory (3)

☐ EPA Pesticide Inactive Ingredients (3)

☒ FDA Inactive Ingredients Database (3)

Experimental Properties

Commercial Availability

1 Selected 3 Results

CAS RN: 57-55-6

View Details

HO

CH2

OH

C3H8O2

(z)-Propylene glycol

Propylene glycol

Key Physical Properties

Value

Condition

Molecular Weight

76.09

Melting Point (Experimental)

-59 °C

Boiling Point (Experimental)

188.2 °C

Density (Experimental)

1.036 g/cm³

Commonly Used As: Solvents; Humectants; Pl

Similar Ingredients with Regulatory Information

Propylene glycol monolaurate

Propylene glycol butyl ether

Propylene glycol monopropyl ether

View 14 More

Commonly Formulated With | Regulatory Information | Experimental Properties

Get Formulations

Get Suppliers

Add to Formulation Designer

Share results via email.

Save results

Download results as an Excel file

View ingredient suppliers

View experimental properties.

View regulatory information and inventory lists

View components used as ingredients in formulations

Add ingredients to the Formulation Designer

Commonly Formulated With

Ingredient	CAS RN/CAS SCN	As Active Ingredients	As Inactive Ingredients	As Any Role
Water	7732-18-5	View Formulations	View Formulations	View Formulations
Glycerol	56-81-5	View Formulations	View Formulations	View Formulations
Ethanol	64-17-5	View Formulations	View Formulations	View Formulations
Carb. acid	7732-18-5	View Formulations	View Formulations	View Formulations
Sodium hydroxide	1310-73-2	View Formulations	View Formulations	View Formulations
Oleic acid	112-80-1	View Formulations	View Formulations	View Formulations
Dioctyl sebacate	139-33-3	View Formulations	View Formulations	View Formulations
Sodium sulfate	7757-83-7	View Formulations	View Formulations	View Formulations
Diphenyl glycol monomethyl ether	111-90-0	View Formulations	View Formulations	View Formulations
(S)-Nonylphenylglycidyl ether	30574-66-0	View Formulations	View Formulations	View Formulations
Karbitan	11138-96-2	View Formulations	View Formulations	View Formulations
Alcohol, C12-15, aliphatic	68131-39-0	View Formulations	View Formulations	View Formulations
Isopropyl	67-63-0	View Formulations	View Formulations	View Formulations
Polyethylene glycol monomethyl ether	9004-96-2	View Formulations	View Formulations	View Formulations
Hydrogen peroxide	7721-84-1	View Formulations	View Formulations	View Formulations
Propylene glycol	2552-60-5	View Formulations	View Formulations	View Formulations
Triacetin	12463-47-7	View Formulations	View Formulations	View Formulations
Methylparaben	99-75-3	View Formulations	View Formulations	View Formulations
Ammonia	7664-41-7	View Formulations	View Formulations	View Formulations
Ethylhexane	141-43-5	View Formulations	View Formulations	View Formulations

ANMAT

Cosing: Cosmetic Ingredients Inventory

Drug Master File List

EMA Excipients List

Original Name (translation)	Applicant Name	Event Date	Category	Packaging	Strength	Form
PROPLENGLICOL* (PROPYLENE GLYCOL)	ALCON LABORATORIOS ARGENTINA S.A.	March 2019	EYE LUBRICANT	1 Dropper Bottle of 10 ml	0.6 g/100 ml	OPHTHALMIC SOLUTION

* SEE PROSPECTUS IN VVM

Source

Marketing Authorizations for Medicines is produced by Argentine National Administration of Medicines, Food and Medical Technology

Inventory Lists

Ingredient is on the following inventory lists:

Acronym	Inventory List	Country
ABC	Australian Inventory of Industrial Chemicals	Australia
AREC	South Korean Act on the Registration and Evaluation of Chemicals	Korea (Republic of)



Explore ingredient suppliers

Refine results by applying filters.

Download results as an Excel file

Suppliers (160)

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- Grade
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 - ☐ ACS reagent (2)
 - ☐ pharmaceutical primary standard (2)
 - ☐ 10mM in DMSO (1)
- Certificate of Analysis
 - ☐ Available (10)
- Bulk Availability
 - ☐ Available (40)
- Supplier
 - ☐ Thermo Fisher Scientific - Laboratory Chemicals (16)
 - ☐ Sigma-Aldrich (15)
 - ☐ FUJIFILM Wako Pure Chemical Corporation (14)
 - ☐ LGC Standards (12)
 - ☐ KANTO CHEMICAL CO., INC. (9)
- Supplier-Reported Properties
 - ☐ Molecular Weight (42)
 - ☐ Product Category (32)
 - ☐ Storage (24)
 - ☐ Boiling Point (23)
 - ☐ Melting Point (23)
- Order from Supplier
 - ☐ Available (56)

View All

Results for (1)-Propylene glycol
CAS RN: 57-55-6

Aaron Chemicals LLC
View Details

View contact information, shipping details, and distribution options.

Product Information	Quantity Information	Ordering & Shipping
Name: 1,2-Propanediol Molecular Weight: 76.0944	Available Amounts: 500 g USD 5.00 100 g USD 4.00 1000 g USD 7.00	Order from Supplier Order from Supplier Ships Within: 1 week Status: Maintained in stock

First Scientific LLC
View Details

Product Information	Quantity Information	Ordering & Shipping
Name: 1,2-Propanediol	Available Amounts: 500 g USD 8.00 100 g USD 6.00 25 g USD 5.00	Order from Supplier Order from Supplier Ships Within: 1 week Status: Maintained in stock

Enamine US Inc.
View Details

Product Information	Quantity Information	Ordering & Shipping
Name: propane-1,2-diol Molecular Weight: 76.09 Weight: 21726&&senderid=0&&lang=en SDS Availability: https://enamine.enamine.net/pub/msds?code=EN300-21726&&senderid=0&&lang=en Shipping: Room temperature Storage: Room temperature	Available Amounts: 2.5 g USD 27.00 50 g USD 50.00 5 g USD 29.00 250 mg USD 19.00 100 mg USD 19.00 100 g USD 67.00 10 g USD 32.00 1 g USD 26.00 500 mg USD 21.00 25 g USD 38.00	Order from Supplier Order from Supplier Ships Within: 1 week Status: Maintained in stock

Design formulations

Formulation Designer

Browse and select physical form.

Clear All Selections

Industry

- Pharmaceutical
- Cosmetics & Personal Care
- Agrochemical
- Cleaning & Surfactant Products
- Inks, Paints, & Coatings
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Browse and select industry.

Browse and select purpose.

- Drug delivery systems
- Pharmaceutical formulations
- Antitumor agents
- Anti-inflammatory agents
- Analgesics**
- Antibacterial agents
- Ophthalmic agents
- Antidiabetic agents
- Antiviral agents
- Antihypertensives
- View More Purposes -

Physical Form

- Tablets**
- Capsules
- Solutions
- Gels
- Liquids
- Pharmaceutical ointments
- Cream preparations
- Suspensions
- Sprays
- Powders
- View More Physical Forms -

Add up to 5 Ingredients

- Celecoxib
- Polyethylene glycol
- + Add Another Ingredient

click to add another ingredient

Delete the ingredient

Create Template

Click to search

View more.

Formulation Designer

Clear All Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Pharmaceutical	Analgesics	Tablets	Celecoxib Polyethylene glycol

Edit Selections

Click and edit the industry, purpose, physical form, and ingredient of formulation

Save the result

SaveDownload

Download results as an Excel file

Your Template

Unit SizemgGoClear

Function	Ingredient	Regulatory Lists	Top Alternatives	Amounts
Active or Featured Ingredient:	Celecoxib	Drug Master File List; EMA EPARS; FDA Orange Book; Japanese Approved Drugs List; NMPA	-	Amount not available
Active or Featured Ingredient:	Polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available
Lubricants	Talc (Mg ₃ H ₂ (SiO ₃) ₄) View More Alternatives	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA Color Additives;	Sodium dodecyl sulfate; Glyceryl tribehenate; Sodium stearyl fumarate; Magnesium stearate;	Approximate Range: 3 - 4%
Binders	Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer View More Alternatives	<div>Alternative Ingredients (Showing all 10)<div>Select the ingredient you would like to use:<div><div>Sodium dodecyl sulfate</div><div>Glyceryl tribehenate</div><div>Sodium stearyl fumarate</div><div>Magnesium stearate</div><div>Stearic acid</div><div>Silica</div><div>Polyoxyethylene sorbitan monooleate</div><div>Calcium stearate</div><div>Polyethylene glycol</div><div>Glycerol behenate</div></div></div></div>		
Disintegrants	Croscarmellose sodium View More Alternatives	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Silica; Starch; Sodium carboxymethyl cellulose; Poly(vinylpyrrolidone); Hydroxypropyl cellulose	Approximate Range: 4 - 5%
Diluents	Magnesium oxide View More Alternatives	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients;	Talc (Mg ₃ H ₂ (SiO ₃) ₄); Butyl methacrylate-dimethylaminoethyl methacrylate	Approximate Range: 8 - 16%

+ Add Function

Click to add function

Function

Anti-inflammatory agents

Add FunctionCancel

Add function then click to have a new formulation design



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blood plasma

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Click to execute search.

Advanced Search

Analyte palmitic acid

AND Matrix blood plasma

Add Search Criteria

Search

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Select the search field: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, or Publication Name.

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Keyword

Analyte

Matrix

Method Category

Technique

CAS Method Number

Publication Name



Explore methods

Explore Methods

Category

Agricultural Applications / Bioassays Biomolecule Isolation Environmental Analysis Food Analysis Fuels / Geology / Biofuels Historical Analysis / Dating Miscellaneous Organic Compound Analysis Organometallics / Inorganics Pharmacology / Toxicology Polymer Analysis Water Analysis

Category Name

Bioassay Bioassay Synthetic Probes Biomarker Biological Process Biomarker Cell Assay Biomarker Medicine Assay Biomedicine Material Analysis Biomolecule Isolation Assay Bioorganism Isolation Assay Genetic Analysis Nanomaterial Analysis

Enter Keywords

Include Keywords (Optional)

Palmitic acid

+ Add Another Keyword

Add Another Keyword

Clear all selections

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Click for methods search.

Search Methods

Results

Results for Custom query

Filter by Analyte, Matrix, Method Category, Technique, and Year.

Filter By

Analyte

☐ Palmitic acid (7)☐ Stearic acid (7)☐ Linoleic acid (6)☐ Oleic acid (5)☐ Arachidonic acid (4)[View All](#)

Matrix

☐ Blood plasma (7)☐ Hazelnut oil (1)

Method Category

Technique

☐ Gas chromatography (82)☐ Extraction (49)☐ Solvent extraction (48)☐ Flame ionization detectors (39)☐ Gas chromatography-mass spectrometry (26)☒ HPLC (7)[View All](#)

Year

1 Selected 7 Results

Sort: Relevance Group: By Method

1

Check the result before downloading or saving

Analysis of Myristic acid in Blood plasma by Solvent extraction

Click to view the result details.

By: Furukawa, Eri; Chen, Zhen; Ueshiba, Hiroki; Wu, Yue; Chiba, Hitoshi; Yanagawa, Yojiro; Katagiri, Seiji; Nagano, Masashi; Hui, Shu-Ping
Postpartum cows showed high oocyte triacylglycerols concurrently with high plasma free fatty acids
Theriogenology (2021), 176, 174-182. Elsevier Inc.

Analyte

cis-Octadecenoic acid; (Z)-Hexadecenoic acid; cis-Octadecadienoic acid; Palmitic acid; Myristic acid; Stearic acid

Matrix

Blood plasma

Other Materials

Reagent: Chloroform; Methanol
Material: Atlantic T3 C18 column (2.1 × 150 mm, 3 μm); Ethylenediaminetetraacetic acid-loaded vacuum tubes

Method Category

Fatty Acid Analysis

Click to view the abstract

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Full Text

View in CAS SciFinder

Click and jump to CAS SciFinder for display.

2

Analysis of Palmitic acid in Blood plasma by Solvent extraction

By: Forest, Anik; Ruiz, Matthieu; Bouchard, Bertrand; Boucher, Gabrielle; Gingras, Olivier; Daneault, Caroline; Robillard Frayne, Isabelle; Rhainds, David; Tardif, Jean-Claude; Rioux, John D.; Des Rosiers, Christine
Comprehensive and Reproducible Untargeted Lipidomic Workflow Using LC-QTOF Validated for Human Plasma Analysis

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CAS SciFinder Quick Reference Guide Academic | 31

Method details

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■ Analysis of Myristic acid in Blood plasma by Solvent extraction

CAS Method Number

1-122-CAS-534418

Method Category

The analytes, matrix, materials, reagents, etc. are displayed.

Technique

Mass spectrometry: HPLC: Solvent extraction

Analyte

- cis*-Octadecenoic acid
- (*Z*)-Hexadecenoic acid
- cis*-Octadecadienoic acid
- Palmitic acid**
- Myristic acid

Equipment Information

Equipment Used

HPLC system, Prominence, Shimadzu Corp, Kyoto, Japan

Mass spectrometer, LTQ Orbitrap, Thermo-Fisher Scientific Inc. San Jose, CA, USA

Source

Bibliography

JOURNAL

Postpartum cows showed high oocyte triacylglycerols concurrently with high plasma free fatty acids

Furukawa, Eri; Chen, Zhen; Ueshiba,
Hiroki; Wu, Yue; Chiba, Hitoshi;
Yanagawa, Yojiro; Katagiri, Seiji; Nagano,
Masashi; Hui, Shu-Ping

Theriogenology (2021), 176, 174 - 182.
Elsevier Inc.

CODEN : THGNBO | ISSN : 0093691X |
DOI :
10.1016/j.theriogenology.2021.09.034

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Validation

Data Validation

Retention Time

7.53 min, Tetradecanoic acid
9.91 min, Hexadecanoic acid
8.35 min, n-Hexadecenoic acid
11.85 min, Octadecanoic acid
10.5 min, Octadecenoic acid (Z)-
9.25 min, Octadecadienoic acid

Concentration

0.26 ± 0.11 nmol/100 µL (sample data), Tetradecanoic acid
3.68 ± 1.04 nmol/100 µL (sample data), Hexadecanoic acid
0.66 ± 0.28 nmol/100 µL (sample data), n-Hexadecenoic acid
5.34 ± 0.79 nmol/100 µL (sample data), Octadecanoic acid
7.57 ± 2.25 nmol/100 µL (sample data), Octadecenoic acid (Z)-
1.14 ± 0.24 nmol/100 µL (sample data), Octadecadienoic acid



Compare methods

Compare up to 3 Methods

Click X to remove the method.

Remove all methods.

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Analysis of Palmitic acid in Blood plasma by Solvent extraction

Analyte(s): Palmitoleic acid; **Palmitic acid**; Elaidic...

Matrix: **Blood plasma**

Method Category: Biomolecule Isolation Assay

Analysis of Fatty acids in Blood plasma by HPLC

Analyte(s): Stearic acid; Linoleic acid; **Palmitic...**

Matrix: **Blood plasma**

Method Category: Fatty Acid Analysis

Analysis of Lauric acid in Blood plasma by Electrochemiluminescence

Analyte(s): **Palmitic acid**; Stearic...

Matrix: **Blood plasma**

Method Category: Fatty Acid Analysis

Up to three different methods can be compared at a time. And the content of all method information details can be compared.

Comparing your 3 selected Methods

Click X to remove method from the table.

Download the comparison table with PDF or XLS format.



	Method 1 ×	Method 2 ×	Method 3 ×
	Analysis of Palmitic acid in Blood plasma by Solvent extraction	Analysis of Fatty acids in Blood plasma by HPLC	Analysis of Lauric acid in Blood plasma by Electrochemiluminescence
CAS Method Number	2-114-CAS-225380	1-122-CAS-96286	1-122-CAS-3193044
Method Category	Biomolecule Isolation Assay	Fatty Acid Analysis	Fatty Acid Analysis
Technique	Time-of-flight mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction	Electrochemical analysis; Atmospheric precipitation; HPLC	Electrochemiluminescence; HPLC
Analyte	Palmitoleic acid; Palmitic acid ; Elaidic acid; Linoleic acid; Stearic acid; Arachidonic acid; Docosahexaenoic acid	Stearic acid; Linoleic acid; Palmitic acid ; Arachidonic acid; Oleic acid; Fatty acids	Palmitic acid ; Stearic acid; Myristoleic acid; Palmitoleic acid; Lauric acid; Arachidonic acid; Oleic acid; Linoleic acid; Linolenic acid; Myristic acid; Fatty acids
Matrix	Blood plasma	Blood plasma	Blood plasma
Other Materials	<i>tert</i> -Butyl methyl ether; Chloroform; Formic acid; Methanol; Ethyl acetate; Hydrochloric acid; Sodium chloride; Glass vial; Zorbax Eclipse plus C ₁₈ column (2.1 × 100 mm, 1.8 μm)	Alloxan; Acetonitrile; Lithium perchlorate; 3,5-Di- <i>tert</i> -butyl-1,2-benzoquinone; Maltose; Diethyl ether; Reverse-phase C30 microbore column (250 mm × 1.0 mm i.d.); Membrane filter (pore size, 0.45 μm); Glucose meter (Glucocard)	1-Pyrrolidinepropanamine; 3,4-Dihydro-9-methyl-2H-pyrido[1,2- <i>a</i>]pyrimidin-2-one; Phosphoric acid; Sodium hydroxide; Acetic acid; Acetonitrile; Boric acid (H ₃ BO ₃); 2-Bromo-1-ethylpyridinium tetrafluoroborate; Chloroform; Heptane; Phosphate-buffered saline solutions; Photomultiplier tube; TSK-gel Octyl-80TS (4.6 × 150 mm, Tosoh) column; Cosmosil 5C18-MS (4.6 × 250 mm) column
Equipment Used	Vortexer, Glas-Col, Terre-Haute, IN, USA; Centrifuge, RVC 2-25, Christ, Osterode, Germany; HPLC system, 1290 Infinity, Agilent Technologies Inc., Santa Clara, CA, USA; Time of flight mass spectrometer, 6550, Agilent Technologies Inc., Santa Clara, CA, USA	HPLC system; Degasser, DG-980-50, Jasco, Tokyo, Japan; HPLC pumps, 301M, Flom, Tokyo, Japan; Sample injector, 7725, Rheodyne, Cotati, CA, USA; Electrochemical detector, LC-4C, BAS, Tokyo, Japan; Electrochemical cell (Radial flow cell), BAS; Electrochemical recorder, 807-IT, Jasco	Degasser, DGU-10B, Shimadzu, Japan; Degasser, DGU-3A, Shimadzu, Japan; Pump, LC-10AD, Shimadzu; Autosampler, SIL-6A, Shimadzu; Chemiluminescence detector, CLD-10A, Shimadzu; HPLC system
Conditions	Instrument: column: Zorbax Eclipse plus C ₁₈ column (2.1 × 100 mm, 1.8 μm); column temperature: 40 °C; mobile phase A: 0.2% formic acid and 10 mM ammonium formate in water; mobile phase B: 0.2% formic acid	Instrument: Column: reverse-phase C30 microbore column (Develosil C30-UG-3, 250 mm × 1.0 mm i.d., Nomura Chemical, Aichi, Japan); mobile phase: acetonitrile-ethanol (90:10, v/v) mixture and one containing 6	Instrument: column: TSK-gel Octyl-80TS (4.6 × 150 mm, Tosoh) column; mobile phase: 50 mM BR buffer (pH 2.5) containing 50% acetonitrile and reagent solution of 0.8 mM Ru(bpy) ₃ Cl ₂ in 10 mM H ₂ SO ₄ ; flow rate:

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CAS

Analytical Methods

blood plasma

Q

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Analysis of Formaldehyde in Air by Amperometry		11 August 2023	Copy Link for URL to share item or Delete saved item.

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Newly introduced medicaments and pharmaceutical specialities. Laxovit

By: Zernik

Chemisches Zentralblatt (1933), 104 Book 2(8), 1217-1217 | Language: German, Database: CHEMZENT

Machine Translated: Chem. FABR. DR. J. WIERNIK U. CO. A.-G., Berlin-Waidmannslust: tablets with each 12.5 mg sodium cholate and 2-oxo-3.3 with (p-oxyphenyl)-indolin. The evacuant with effect on Dünn-u. Thick intestine. — Lygal (DR. GEORG HENNING, Berlin-Tempelhof): compound of 50% phenyl quinolinecarboxylic acid Ca (or Na) 29% dimethyl amino phenazone and 21% Coffein-Natriumsalicylat. Antiarthriticum. — Pantaplant (chemical. Structures KOLBERG G. mass forming H., Kolberg): fluid extracts from

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2

Messages of the drug testing station [APA] of the Swiss tables Apotheker-Vereins

No author and editor data available

Chemisches Zentralblatt (1940), 111 Book 2(22), 3065-3065 | Language: German, Database: CHEMZENT

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1933. II. F. PHARMAZIE. DESINFektion. 1217

Katagel-Kreidl (Herst. ders.): gifftfreie Spezialtrockenbeize für Saatgut. — Medoform (Herst. ders.): Liqu. Formaldehydi saponat. — Meissol (ANT. MEISZL'S NACHF., Wien): Ungeziefervertilgungsmittel. — Oma (OMA-NÄHRSTOFF-GES., St. Veit a. d. Glan, Kärnten): Kindernährmittel. — Oma-Kinder- u. Wundpulver (Herst. ders.): peledol (Pellidol? Ref.) haltiger Fettpuder. — Pommelte (POMMETTE-KELLEREI, Wien XI): naturreiner Apfelsaft. (Pharmaz. Mh. 14. 42—44. Febr. 1933.) HARMS.

—, Neue Arzneimittel, Spezialitäten und Geheimmittel. Anustypsalbe u. Anustypzäpfchen (BÄREN-APOTHEKE, ROB. RADITZ, Wien II): Hämorrhoidalpräparate mit Tannalbin, Ichthyol u. Bi-Salzen. — Gynosupp (Herst. ders.): Vaginal-„Kugeln“ in Form eines gerade abgestutzten Kegels mit Milchsäure, Bor-Salicylsäure u. Hydrarg. salicylicum. Anticoncipiens usw. Auch mit 10% Ichthyol als Gynosupp cum Ichthyolo. (Pharmaz. Mh. 14. 63—66. März 1933.) HARMS.

F. Zernik, Neue pharmazeutische Präparate in Deutschland. Douchin (Dr. R. u. Dr. O. WEIL, Frankfurt a. M.): Cachets mit 0,2 g Pyrasulf (C. 1933. I. 2278), 0,2 g Chinin „Weil“ (C. 1931. II. 1599), 0,4 g Somnacetin (C. 1931. I. 2223) u. 0,00033 g Scopolamin. Zur Schmerzlinderung in der Austreibungsperiode. (Manufactur. Chemist pharmac. Cosmetic Perfum. Trade J. 4. 50—52. Febr. 1933.) HARMS.

F. Zernik, Neue pharmazeutische Präparate in Deutschland. Intramin pervesival (Dr. GEORG HENNING, Berlin-Tempelhof): neuer Name für Intramin (C. 1931. I. 484). — Intramin intravenös (Herst. ders.): diiodmethansulfosaures Na in 40%ig. wss. Lsg. zur Röntgendarst. der Harnwege. — Stomachysatum Bürger (YSATFABRIK G. M. B. H., Wernigerode): Extrakte von Artemisia Absinthium, Achillea millefolium, Gnaphalium arenarium u. Rheum palmatum. Gegen Magenstörungen. — Progynon oleosum (SCHERING-KAHLBAUM A.-G., Berlin): ölige Lsg. des Follikulinbenzoats. Die 1-ccm-Ampulle enthält 10000 Mäuseeinheiten. 1 × wöchentlich intramuskulär als Depot. (Manufactur. Chemist pharmac. Cosmetic Perfum. Trade J. 4. 146—48. Mai 1933.) HARMS.

Zernik, Neu eingeführte Arzneimittel und pharmazeutische Spezialitäten. Laxovit (CHEM. FABR. DR. J. WIERNIK U. CO. A.-G., Berlin-Waidmannslust): Tabletten mit je 12,5 mg Natriumcholat u. 2-Oxo-3,3-bis-(p-oxyphenyl)-indolin. Abführmittel mit Wrkg. auf Dünn- u. Dickdarm. — Lygal (DR. GEORG HENNING, Berlin-Tempelhof): Verb. von 50% phenylquinolinecarbonsaurem Ca (bzw. Na), 29% Dimethylaminophenazon u. 21% Coffein-Natriumsalicylat. Antiarthriticum. — Pantaplant (CHEM. WERKE

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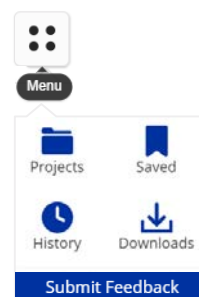
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