



CAS
SciFinder[®]
Quick Reference Guide

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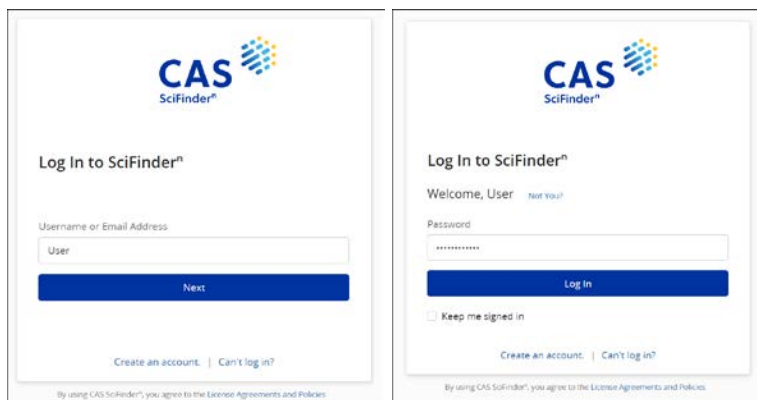
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Welcome to CAS SciFinder[®]

This Quick Reference Guide will show you how to start using CAS SciFinder[®], the industry's most trusted and comprehensive chemistry relevance engine.

First, open the CAS SciFinder[®] Login page: <https://scifinder-n.cas.org>.

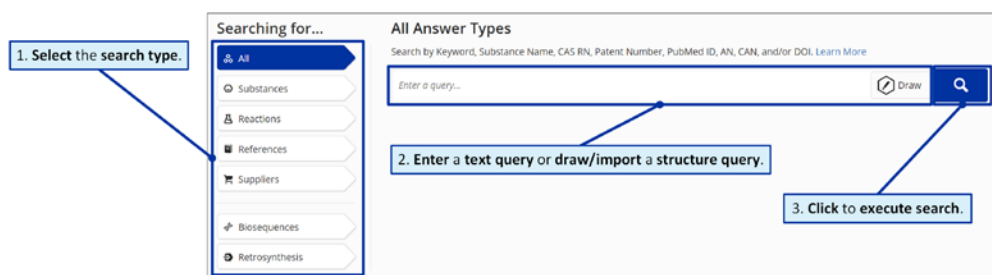
Log in using your CAS SciFinder[®] **Username** and **Password**.



Search

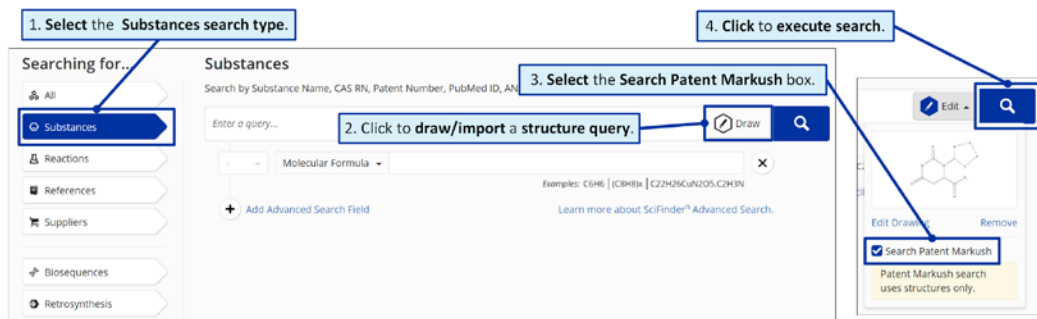
Search for the result type you need using a keyword, substance name, CAS Registry Number[®], patent number, or structure.

Note: You may enter a document object identifier (DOI) in the **All** and **References** searches.



Using **Advanced Search** for **References** and **Substances**, you may search by specific information type (e.g., author name or substance property).

Patent Markush Search: To conduct a patent markush search, select **Substances**, draw/import the query using the Structure Editor, and then check the box for **Search Patent Markush**.



Substance Results

Filter by structure match.

Retrieve related data for all results.

Download results.

Save results/search, create alert.

Email results.

Click the X to remove a filter or Clear All Filters. Multiple filters in dropdown menu.

Clear All Filters

2 Selected 5 Results

Sort: Relevance **View: Full**

Keep or remove selected results.

Change result display.

Sort results by relevance, CAS RN, Molecular Formula or Weight, and Number of References or Suppliers.

Click to display data visualization.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

- Reaction Role
- Reference Role
- Commercial Availability
- Number of Components
- Molecular Weight
- Stereochemistry
- Substance Class
- Isotopes
- Metals
- Experimental Property
- Experimental Spectrum
- Bioactivity Indicator
- Target Indicator
- Regulatory Data by List
- Search Within Results

Select filters to focus results.

Retrieve related data for a specific result.

Click property name to view more information on Substance Detail.

Click to view substance information.

Click to select result.

Click to open Substance Detail.

Click to download the contents (name and number value) for all or applied filters as an .xlsx file.

Filter Content Report

Download filter data from this result set.

Substances

References Reactions Suppliers

Structure Match

- As Drawn (13)
- Substructure (36)
- Similarity (123K)
- Analyze Structure Precision

Chemscape Analysis

Filtering: Reference Role: 2 Selected Commercial Availability: Available

51234-28-7

C16H12ClNO3
Benoxaprofen

944 References 36 Reactions 35 Suppliers

70280-67-0

C16H12ClNO3
(-)-Benoxaprofen

36 References 0 Reactions 1 Supplier

66934-19-8

C16H12ClNO3
(+)-Benoxaprofen

70062-36-1

C16H12ClNO3
(-)-Benoxaprofen

Key Physical Properties

Key Physical Properties	Value	Condition
Molecular Weight	301.72	-
Boiling Point (Predicted)	446.2±30.0 °C	Press: 760 Torr
Density (Predicted)	1.362±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C

Substance Detail

Substance Detail

References (944)
Reactions (36)
Suppliers (35)

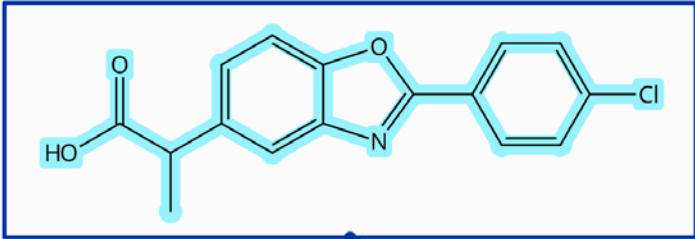
CAS Registry Number
51234-28-7

Save detail.

Download detail.

Email detail.

Retrieve data related to substance.



C₁₆H₁₂ClNO₃
5-Benzoxazoleacetic acid, 2-(4-chlorophenyl)-α-methyl- (94)

Click for options to view details, generate retrosynthesis plan, and edit/download structure file.

Key Physical Properties	Value	Condition
Molecular Weight	301.72	-
Melting Point (Experimental)	189-190 °C	-
Boiling Point (Predicted)	446.2±30.0 °C	Press: 760 Torr
Density (Predicted)	1.362±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C

Expand All | Collapse All

Expand or collapse all categories.

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators

Regulatory Information

Regulatory List: EINECS, REACH, VNECI
Confidential Business Information: Public

Expand All | Collapse All

- Regulatory Synonyms (8)
- Details by Country/International & Other Lists

Additional Details

Reference Results

The screenshot displays the CAS SciFinder interface for reference results. The left sidebar contains a 'Filter Behavior' section with 'Filter by' and 'Exclude' options, and a 'Filter Content Report' section with a download icon. The main results area shows a list of search results with callouts for various actions:

- Retrieve related data for all results.** (Points to the top navigation bar)
- Download results.** (Points to the download icon)
- Save results/search, create alert.** (Points to the 'Save and Alert' icon)
- Email results.** (Points to the email icon)
- Click the X to remove a filter or Clear All Filters. Multiple filters in dropdown menu.** (Points to the filter dropdowns)
- Clear All Filters** (Points to the 'Clear All Filters' button)
- Sort: Relevance** (Points to the sort dropdown)
- View: Partial Abstract** (Points to the view dropdown)
- Keep or remove selected results.** (Points to the selection checkboxes)
- Change result display.** (Points to the view dropdown)
- Select filters to focus results.** (Points to the filter sidebar)
- Sort results by relevance, times cited, accession number, or publication date.** (Points to the sort dropdown)
- Retrieve related data for a specific result.** (Points to the 'Substances (6)', 'Reactions (0)', 'Citing (63)', and 'Citation Map' buttons)
- Click to select result.** (Points to a result checkbox)
- Click to open Reference Detail.** (Points to the 'Full Text' button)
- Click to download the contents (name and number value) for all or applied filters as an .xlsx file.** (Points to the 'Download filter data from this result set.' button)
- Click to access full-text viewing options.** (Points to the 'Full Text' dropdown)
- Click to access patent information viewing options.** (Points to the 'PatentPak' dropdown)

Reference Detail

Reference Detail

Substances (3) Reactions (0) Citing (6) Citation Map

Retrieve data related to reference.

Download detail.

Save detail.

Email detail.

Set citing alert.

View map of references this document cites and references that cite this document.

Click to access full-text viewing options.

View interactive version of patent that highlights specific locations of indexed substances.

Request a prior art analysis that contains both patent and non-patent literature.

Click a PatentPak option view the patent source document.

View IPC codes for basic patent and patent family members.

View concepts that characterize the reference's general subject matter.

View the reference's indexed substances.

View the reference's formulation data.

View the reference's citations.

Patent

Patent Number: WO9834612
 Publication Date: 1998-08-13
 Application Number: WO1998-EP648
 Application Date: 1998-02-03
 Kind Code: A1
 Assignee: The Boots Company PLC, United Kingdom

Source: World Intellectual Property Organization
 CODEN: PIXXD2

Database Information: AN: 1998:548531, CAN: 129:180142, CPlus

Language: English

Pharmaceutical compositions containing **ibuprofen** and domperidone for the treatment of migraine

By: Pankhania, Manendra Govind; Yurdakul, Saruhan

Migraine, a therapeutically effective amount of **ibuprofen** or a salt thereof and a therapeutically effective amount of domperidone or a salt thereof. A pharmaceutical tablet contained 5.9, PVP 3.9, croscarmellose sodium 9.6, and stearic acid 0.6%.

Keywords: pharmaceutical tablet **ibuprofen** domperidone migraine treatment

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO9834612	English	A1	PDF PDF+ Viewer	1998-08-13	WO1998-EP648	1998-02-03
CA2279184	Undetermined	A1		1998-08-13	CA1998-2279184	1998-02-03
EP1017300	Undetermined	A1		2000-07-12	EP1998-906926	1998-02-03
HU225043	Hungarian	B1		2006-05-29	HU2000-1104	1998-02-03

View All

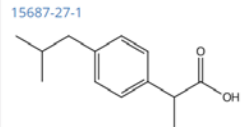
Priority Application

Priority Application Number	Application Date
GB1997-2392	1997-02-06
WO1998-EP648	

Expand All | Collapse All

Substances (3)

15687-27-1

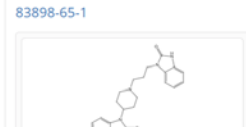


C₁₃H₁₈O₂
Ibuprofen

PatentPak

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Therapeutic Use, Biological Study, Uses

83898-65-1

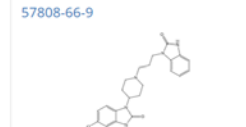


C₂₂H₂₄ClN₅O₂·C₄H₄O₄
Domperidone maleate

PatentPak

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Therapeutic Use, Biological Study, Uses

57808-66-9



C₂₂H₂₄ClN₅O₂
Domperidone

PatentPak

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Therapeutic Use, Biological Study, Uses

Formulations

Cited Documents

Reaction Results

Retrieve related data for all results. (References dropdown)

Download results. (Download icon)

Save results/search, create alert. (Save and Alert icon)

Email results. (Email icon)

Click the X to remove a filter or Clear All Filters. Multiple filters in dropdown menu. (Filtering: Number of Steps: 2 X Experimental Protocols: Synthetic Methods X)

Clear All Filters. (Clear All Filters button)

1 Selected 29 Results

Keep or remove selected results. (1 Selected dropdown)

Group reactions by scheme or document. (Group: By Scheme dropdown)

Change result display. (View: Expanded dropdown)

Select filters to focus results. (Filter Behavior sidebar)

View substance vendors. (Suppliers (98) button)

Click for options to view details, generate retrosynthesis plan, and edit/download structure file. (Expand Scheme dropdown)

Click to open reaction reference's detail page. (Reaction Summary section)

Process for preparing varenicline, varenicline intermediates, and pharmaceutically acceptable salts thereof (Reaction Summary text)

Click to access full-text viewing options. (PatentPak Full Text dropdown)

Click to access patent information viewing options. (PatentPak dropdown)

View reaction's detail page. (View Reaction Detail button)

View experimental procedure for reaction. (Experimental Protocols button)

Click to download the contents (name and number value) for all or applied filters as an .xlsx file. (Download filter data icon)

Reaction Detail

Reaction Detail

Suppliers (19) Suppliers (78) Suppliers (40)

Download detail. Save detail. Email detail. View substance vendors. Click to open reaction reference's detail page.

Steps: 2

Suppliers (63)

View alternative reactions for the same product. Alternative Steps (7)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Sodium periodate	Benzyltriethylammonium chloride	Dichloromethane Water	10 °C; 1 h
2	-	-	-	1 min, 25 - 30 °C
3	Sodium cyanoborohydride	-	Dichloromethane	0 °C; 0 °C → 30 °C; 0.5 - 1 h
4	Sodium carbonate	-	Water	1 h, pH 9

CAS Reaction Number: 31-032-CAS-650575

Experimental Protocols
Synthetic Methods Experimental Procedure

Products: 2,3,4,5-Tetrahydro-3-(phenylmethyl)-1,5-methano-1H-3-benzazepine

Reactants: 1,2,3,4-Tetrahydro-1,4-methanonaphthalene-2,3-diol
Benzylamine

Reagents: Sodium periodate
Sodium cyanoborohydride
Sodium carbonate

Catalysts: Benzyltriethylammonium chloride

Solvents: Dichloromethane
Water

Procedure: 1. Stir a 1,2,3,4-tetrahydro-1,4-methanonaphthalene-2,3-diol (100 g) in a mixture of water (2600 ml) and methylene chloride (1040 ml) under nitrogen at 10 °C.
2. Add sodium periodate (127.6 g) and triethylbenzyl ammonium chloride (10 g) and stir the resulting mixture for 1 hour.

PATENT
Process for preparing varenicline, varenicline intermediates, and pharmaceutically acceptable salts thereof
By: Shekhawat, Kundan Singh; et al
View All
World Intellectual Property Organization
PatentPak Full Text
Patent Number: WO2010023561
Publication Date: 2010-03-04
Application Number: WO2009-1B7081
Application Date: 2009-08-31
Kind Code: A1
Assignee: Actavis Group PTC ehf, Iceland

Click tabs to view steps in multi-step reactions.

Click to access patent information viewing options.

Click to access full-text viewing options.

Click tabs to view available experimental protocols.

Supplier Results

Suppliers

Click the X to remove a filter or Clear All Filters. Multiple filters in dropdown menu.

Download results. Email results.

Clear All Filters

Sort results by relevance, supplier name, shipping speed, or purity.

Sort: Relevance

Select filters to focus results.

Filter Behavior

Filter by Exclude

Preferred Suppliers

Supplier

Purity

Quantity

Ships Within

Stock Status

Order From Supplier

Country/Region

Filter Content Report

Download filter data from this result set.

Filtering: Purity: 95-98% X

1 Selected 21 Results

Supplier Substance Purity Purchasing Details Availability

1 ASTATECH 51234-28-7 BENOXAPROFEN 95-98% 0.1 g, USD 3500 Synthesis on demand

Click to open Substance Detail.

AstaTech Product List

United States

Last Updated: 31 Mar 2022

View details, generate retrosynthesis plan, and edit/download structure file.

Order From Supplier

Open product ordering page on supplier's website.

2 Arspichem Product List 51234-28-7 2-(2-(4-chlorophenyl)benzo[d]oxazol-5-yl)propanoic acid 95-98% Typically in stock

Product Information

Open product information page on supplier's website.

3 Alchem Pharmtech, Inc. 51234-28-7 2-(2-(4-chlorophenyl)benzo[d]oxazol-5-yl)propanoic acid 95-98% Maintained in stock

Click to select result.

Click thumbs up/down to set supplier preference.

Click to download the contents (name and number value) for all or applied filters as an .xlsx file.

Supplier Detail

Supplier Detail

Click thumbs up to set supplier as Preferred or thumbs down for Non-Preferred.

Download detail. Email detail.

Click to open Substance Detail.

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

Email sales@astatechinc.com

Phone 215-785-3197

Substance Information

CAS Registry Number 51234-28-7

CAS Name Benoxaprofen

Chemical Name BENOXAPROFEN

Order Number C90147

Purity 95%

Quantity, Price 0.1 g, USD 3500
0.25 g, USD 6900

Stock Status Synthesis on demand

Ships Within 8 weeks

Pricing Information 31 Mar 2022

Last Updated

Order From Supplier

Open product ordering page on supplier's website.

Additional Contact Information

AstaTech, Inc.
Keystone Business Park
2525 Pearl Buck Road
Bristol, PA, 19007
United States

Fax 215-785-2656

Click to view details, generate retrosynthesis plan, and edit/download structure file.

Biosequence Results

Biosequences

Retrieve related data for all results. | Download results. | Email results.

References | Click to select another sequence.

BLAST Search Details

- Sequence Type: Protein
- Search Within: Nucleotides
- BLAST Algorithm: TBLASTn-fast
- NCBI Included: No
- Alignment Identity: -
- Query Coverage: 90%
- E-Value: 10
- Match with Gaps?: Yes
- Gap Costs: Existence 11
- Extension 1

Query Details View More

> pdb|1E57|C Chain C, Physalis Mottle Virus

83 Results

Sort: Alignment Identity | View: Expanded

Sort results by Alignment Identity, E-Value, Query Coverage, or Subject Coverage.

Change result display.

Click to display data visualization.

Bioscape Analysis

Visually explore sequence similarity with a new tool. Learn more about Bioscape.

Create Bioscape Analysis

Filter by

- E-Value: 0 to 10⁶
- Query Coverage %: 0 to 100
- Subject Coverage %: 0 to 100
- Alignment Identity %: 60.5 to 100

Apply | Reset Filters

Alignment | Subject | References

Alignment Data

BLAST Score: 889
E-Value: 3.1542e-118

Click to view CAS RN, NCBI Identifier, sequence length, NCBI Organism, and tabular sequence.

Click to patent/journal results containing a matching sequence.

Click to view references indexing the sequence.

References

Query 1 | 188

Subject 1 | 1,255

Alignment Identity: 100%

Matches: 188
Mismatches: 0

Query 2 | 188

Subject 1 | 6,673

Alignment Identity: 100%

Matches: 188
Mismatches: 0

Bioscape

Bioscape visualizes the similarity and patent landscape for a set of sequence results. The location of the sequence bar in the visualization corresponds to the similarity of the sequence to the query, and the height of the sequence bar corresponds to the number of patents in which the sequence has been published.

The screenshot shows the Bioscape interface with several callout boxes:

- Refine sequence result bars by similarity.** Points to the 'Sequence Similarity' slider, which ranges from 97% to 100%.
- Refine sequence result bars by patent keyword and simple legal status.** Points to the search and filter icons on the left.
- Change how sequence result bars display.** Points to a bar style selection icon.
- Multiple CAS RNs Associated with this Sequence.** Points to a table with columns for 'Patents' and 'Sequence Length' (660). A callout box says: 'If present, click to view substances.' Another callout box says: 'Click to view relevant patents.'
- Queried sequence.** Points to a specific bar in the visualization.
- Click a bar to view its patent count and sequence length.** Points to a bar in the visualization.
- Click the Select Sequence button and then click-and-drag to select multiple sequence results for viewing.** Points to the 'Select Sequence' button at the bottom.

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Chemscape

Chemscape visualizes the similarity and patent landscape for a set of substance results. The location of the substance bar in the visualization corresponds to the similarity of the substance to the query and the height of the substance in the visualization corresponds to the number of patents in which the substance has been published.

The screenshot shows the Chemscape visualization in CAS SciFinder. The interface includes a top navigation bar with the CAS SciFinder logo, a search bar, and a 'Structural Similarity' slider ranging from 80% (Less Similar) to 100% (More Similar). The main visualization is a 3D bar chart where the x-axis represents similarity and the z-axis represents the number of patents. A 'Queried sequence' is highlighted with a red bar. A callout box for 'Olanarib' (763113-22-0) is open, showing its chemical structure and a list of relevant patents, including AZD 2281 and KU 0059436. The interface also features a 'Select Structure' button and a 'Save' button for MyChemscape.

View and manage your saved Chemscape.

Group and refine Chemscape structures to show key information.

Add new structures to your Chemscape and indicate their position.

Refine your Chemscape by keyword or an exact match to a chemical structure.

Change how structure result bars display.

Click to open Substance Detail page.

Click to view relevant patents.

Click a bar to view its structure and number of associated patents.

Click the Select Structure button and then click-and-drag to select multiple structure results for viewing or a new Chemscape.

Click to save your Chemscape for later access in MyChemscape.

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Saved Searches and Results

Filter by

- Result Type
 - Reactions (4)
 - References (4)
 - Substances (2)
- Alerts
 - Unviewed (1)
 - Alerts Set (2)
 - No Alerts (8)
- Tags
 - Citing Alert (1)
 - For Review (1)
 - NSAID (1)

Combine Saved Results

Combine

Set/edit an alert on saved query or view and manage alert results.

Filter saved items.

Click to select item.

Delete selected item.

Email selected item.

Click to open Reference Detail.

View references citing the saved item.

Edit name.

Run a saved query.

Combine previously saved queries or selected results.

Create/add tags.

Click to remove tag.

Display saved result set.

View Saved

Search History

Filter history by selected search types.

Filter by

- Result Type
 - All (4)
 - Biosequences (19)
 - Patent Markush (1)
 - Reactions (13)
 - References (64)
 - Retrosynthesis (16)
 - Substances (36)
 - Suppliers (8)
- Date
 - Start Date: mm/dd/yyyy
 - End Date: mm/dd/yyyy
 - Calendar: May 2022

Display search history for a specified date range.

Your Search History
53 Searches

Delete searches.

Rerun search to retrieve latest results.

Edit search and then rerun.

Open retrosynthesis plan or edit options and rerun.

Rerun Search

Edit Search

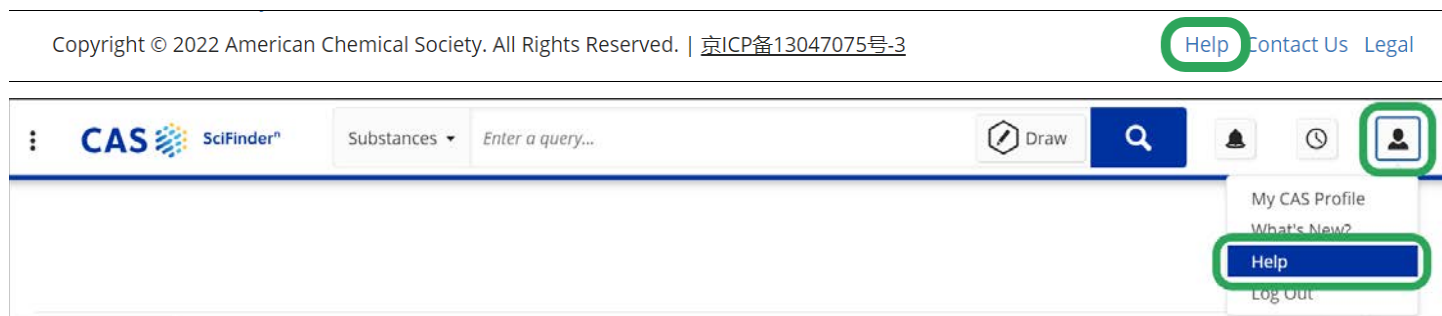
Open Plan

Edit Search

Complete

CAS SciFinder[®] Support

To access CAS SciFinder[®] in-application support, click the **Help** link at the bottom of any page or select **Help** from the **Account** menu.



For additional assistance using CAS SciFinder[®], please contact the **CAS Customer Center**:

- **Hours:** 8:00 a.m. to 6:00 p.m. EST Monday – Friday.
- **Phone:**
 - 1-800-753-4227 (North America)
 - +1-614-447-3700 (outside North America)
 - **Option 2:** General information or account-related questions
 - **Option 3:** Assistance with search strategies, database content, or using a product
 - **Option 4:** Technical assistance with software set up, installation, and configuration
- **Email:** help@cas.org
- **Web:** <https://www.cas.org/contact>

If desired, ask for a CAS SciFinder[®] Familiarization Training Session visit or online session.

Advanced Search

The screenshot shows the 'Advanced Search' interface with the following components and callouts:

- Select the search field: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, or Publication Name.** (Callout pointing to the 'Analyte' dropdown menu)
- Enter the query for the search field.** (Callout pointing to the text input field containing 'palmitic acid')
- Select the logical operator: AND, OR, NOT.** (Callout pointing to the 'AND' dropdown menu)
- Click to remove a query.** (Callout pointing to the 'x' icon on the right side of the search criteria row)
- Click to add another query.** (Callout pointing to the 'Add Search Criteria' button)
- Click to execute search.** (Callout pointing to the search button with a magnifying glass icon)
- Click to reset form.** (Callout pointing to the 'Clear' button)

The interface includes a dropdown menu for 'Analyte' (set to 'palmitic acid'), a logical operator dropdown (set to 'AND'), a dropdown for 'Matrix' (set to 'blood plasma'), and a text input field for the query. Below these are buttons for 'Add Search Criteria', 'Search', and 'Clear'.



Results

The screenshot displays the 'Results' page for a search query. The interface includes a left-hand navigation panel with filters for Matrix, Method Category, Technique, and Year. The main content area shows a list of search results, with the first result selected. Callout boxes provide instructions on how to interact with the interface:

- Select individual methods to export or save, or check box at top to select all methods on page.** (Points to the selection checkboxes at the top of the results list.)
- Save methods.** (Points to the download icon.)
- Sort methods by Relevance or Publication Year.** (Points to the 'Sort Relevance' dropdown menu.)
- Download methods to PDF or XLS format.** (Points to the download icon.)
- Click method title or View Details & Instructions to view method details.** (Points to the 'View Details & Instructions' button for the first result.)
- Click Compare to view selected methods for comparison.** (Points to the 'Compare (2/3)' button.)
- Click Add to Compare to select methods for comparison.** (Points to the 'Add to Compare' button.)
- Select boxes to filter methods by data values.** (Points to the filter checkboxes in the left-hand panel.)
- Remove a selected comparison method.** (Points to the 'Remove from Compare' button.)

Method Detail


Method Detail (1 of 38) ← Prev Next →


Download method to PDF or XLS format.  

Analysis of (±)-Pentobarbital in Blood plasma by Gas chromatography-mass spectrometry


CAS MN: 1-101-CAS-168942

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: Gas chromatography-mass spectrometry

Save method. 

View structure image. 

Materials	Role	Image	CAS RN
(±)-Pentobarbital	analyte	View Structure	76-74-4
(±)-Thiopental	analyte	View Structure	76-75-5
Propofol	analyte	View Structure	2078-54-8
2,4,6-(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>)-Pyrimidinetrione, 1-methyl-5-(1-methyl-2-propenyl)-			151-83-7
Diazepam			439-14-5
Phenobarbital	analyte	View Structure	50-06-6
Midazolam	analyte	View Structure	59467-70-8
Nordiazepam	analyte	View Structure	1088-11-5
Blood plasma	matrix		
GC capillary column (12 m x 0.2 mm ID, 330-nm film thickness)	material		

Scroll the display to see method details such as: Materials, Source, Equipment Used, Conditions, Instrument, Instructions, and Validation. 

Source

Fast, Simple, and Validated Gas Chromatographic-Mass Spectrometric Assay for Quantification of Drugs Relevant to Diagnosis of Brain Death in Human Blood Plasma Samples

Peters, Frank T.; Jung, Julia; Kraemer, Thomas; Maurer, Hans H.

Therapeutic Drug Monitoring (2005), 27 (3), 334 - 344. Lippincott Williams & Wilkins

CODEN: TDMODV | ISSN: 01634356 | DOI: 10.1097/01.ftd.0000158079.53577.46

Full Text ▾

Abstract ^

In addition to total anamnesis, one of the important aspects in diagnosis of brain death is the exclusion of effective plasma concentrations of drugs that

Compare Methods

Compare Methods

Click X to remove method from the table.

Download the comparison table.

Expand All data items on table or Collapse All.

Expand All | Collapse All

	1	2	3
Title	Analysis of Hyperoside in Blood plasma by HPLC	Analysis of Carbamazepine in Blood plasma by HPLC	Analysis of 5-Fluorouracil in Blood plasma by Liquid-liquid extraction
CAS Method Number	1-101-CAS-135904	1-101-CAS-184445	1-101-CAS-158452
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Liquid chromatographic UV detectors; HPLC; Extraction	HPLC; Solid phase extraction	HPLC; Liquid-liquid extraction
Analyte	Hyperoside	<i>trans</i> -10,11-Dihydroxy-10,11-dihydrocarbamazepine; Carbamazepine 10,11-epoxide; View All	Uracil; 5-Fluorouracil; Dihydrouracil; Antitumor agents
Matrix	Blood plasma	Blood plasma	Blood plasma
Other Materials	Acetic acid; Methanol; Analytical column (Diamonsil C18, 4.6 mm X 150 mm, i.d., 5 µm); Guard column (KR View All	0.45 µm regenerated cellulose membrane filter; analytical column (250 mm x 4.6 mm; 5 µm); cartridges View All	RP-18 X-Terra'column (5 µm particles, 25 cm)
Equipment Used	High performance liquid chromatography system, Shimadzu, Kyoto, Japan; Milli-Q Biocel Ultrapure View All	HPLC system, 1200, Agilent Technologies, Wilmington, DE, USA; Vacuum Manifold, 12-port, Supelco, View All	HPLC system, 1100, Agilent

Search for Existing Formulations

Enter a formulation **ingredient, purpose, physical form, function, or document identifier**, and then click the magnifying glass.

Search for Formulations by Ingredient, Purpose, Form, Function, etc.

celcecoxib

Try **Advanced Search** for a more precise search experience

Explore Formulation Results

Click the **Suggested References** tab to view reference results matching your search term.

Refine results by applying filters.

Download results as PDF or Excel.

Compare selected formulations.

Formulation components with function and amount reported.

Component	Function	Amount Reported
Group: granulated celecoxib	active agent	1008 g
Celecoxib	nonsteroidal antiinflammatory agent	1200 g
Mannitol	excipient	102 g
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:2)	excipient	264 g
Hydroxypropyl cellulose	disintegrating agent	384 g
Additional group components reported		
Magnesium stearate	lubricants	12 g

View or download full-text patent document.

View full component list with optionality, production process, effective dose, and experimental activity.

Click a blue component ingredient name to view more information.

Search for Ingredients

The screenshot shows the search interface with three callouts:

- Click Ingredients.** points to the 'Ingredients' button in the search filters.
- Enter an ingredient name, CAS Registry Number, or function.** points to the search input field containing 'propylene glycol'.
- Execute search.** points to the search icon (magnifying glass).

Explore Ingredient Results

The screenshot displays the results for Propylene glycol (CAS RN: 57-55-6) with several callouts:

- Refine results by applying filters.** points to the 'Pharmaceutical' filter in the 'Industry' section.
- Download results as an Excel file.** points to the download icon.
- View ingredient suppliers.** points to the 'Suppliers' button.
- View formulations using the ingredient.** points to the 'Formulations' button.
- Add ingredient to the Formulation Designer.** points to the 'Send to Designer' button.
- View experimental properties.** points to the 'Experimental Properties' tab.
- View components used with the ingredient in formulations.** points to the 'Commonly Formulated With' table.
- View regulatory information and inventory lists.** points to the 'Regulatory Information' and 'Inventory Lists' sections.

Commonly Formulated With Table:

Ingredient	CAS RN/CAS SCN	All Active Ingredients
Water	7732-18-5	View Formulation
Glycerol	56-81-5	View Formulation
Ethanol	64-17-5	View Formulation
Cholic acid	77-05-9	View Formulation
Cholic acid	112-80-1	View Formulation
Sodium sulfite	7757-83-7	View Formulation
Polyethylene glycol	25322-68-3	View Formulation
(1S)-hydroxyethane-1,1-diphosphonic acid	2809-21-4	View Formulation


Regulatory Information Table:


DMF Number	Original Name	Applicant	Event	Event Date	Classification
E30	PROPYLENE GLYCOL--TRADE NAME SPLENEGLYCOL	DOW CHEMICAL CO	submission	8/21/1963	status: I type: II
E230	PROPYLENE GLYCOL	AVANTAR CORP	submission	9/25/1989	status: I type: II

Explore Ingredient Suppliers

Filter by

- Grade
 - Molecular Biology Grade (8)
 - Reagent Grade (5)
 - Reference Material (4)
 - Reference Material, ISO 17025 (2)
 - Reference Material, ISO 17034 (2)
- Certificate of Analysis
 - Available (1)
- Bulk Availability
 - Available (24)
- Supplier
 - LGC (8)
 - FUJIFILM Wako Pure Chemical Corporation (6)
 - Sigma-Aldrich (4)
 - A2B Chem LLC (3)
 - AA BLOCKS LLC (3)
- Supplier-Reported Properties
 - Hazard Information (5)
 - Solubility (5)
 - Description (3)
 - Primary Action (1)
- Order from Supplier
 - Available (53)

 Suppliers (124)

Download results as an Excel file. 

Refine results by applying filters.

Results for Celecoxib
CAS RN: 169590-42-5

View contact information, shipping details, and distribution options.

BIONET/Key Organics Ltd.

[View Details](#)

Product Information	Quantity Information	Ordering & Shipping						
<p>Name: Celecoxib</p> <p>Description: Celecoxib is used in management of arthritis (OA), arthritis (RA) and ankylosing spondylitis. It is a selective noncompetitive inhibitor of cyclooxygenase-2 (COX-2). Ref: Drugs. 2000; 59 (4), 957-980.</p> <p>Solubility: 70 mg/ml DMSO</p>	<p>Available Amounts:</p> <table style="width: 100%; border-collapse: collapse;"> <tr><td>1 mg</td><td>GBP 30.00</td></tr> <tr><td>5 mg</td><td>GBP 41.00</td></tr> <tr><td>10 mg</td><td>GBP 51.00</td></tr> </table>	1 mg	GBP 30.00	5 mg	GBP 41.00	10 mg	GBP 51.00	<p>Order from Supplier</p> <p>Ships Within: 1 week</p> <p>Status: Typically in stock</p>
1 mg	GBP 30.00							
5 mg	GBP 41.00							
10 mg	GBP 51.00							

Open supplier's ordering page.

Tokyo Chemical Industry Co., Ltd. (Tokyo Kasei Kogyo Co., Ltd.) (Overseas Sales Office)

[View Details](#)

Product Information	Quantity Information	Ordering & Shipping				
<p>Name: Celecoxib</p>	<p>Available Amounts:</p> <table style="width: 100%; border-collapse: collapse;"> <tr><td>200 mg</td><td>JPY 5100</td></tr> <tr><td>1 g</td><td>JPY 17500</td></tr> </table>	200 mg	JPY 5100	1 g	JPY 17500	<p>Product Information</p> <p>Ships Within: 1 week</p> <p>Status: Maintained in stock</p>
200 mg	JPY 5100					
1 g	JPY 17500					

Open supplier's product page for ingredient.

TCI America

[View Details](#)

Product Information	Quantity Information	Ordering & Shipping				
<p>Name: Celecoxib</p>	<p>Available Amounts:</p> <table style="width: 100%; border-collapse: collapse;"> <tr><td>200 mg</td><td>USD 27</td></tr> <tr><td>1 g</td><td>USD 79</td></tr> </table>	200 mg	USD 27	1 g	USD 79	<p>Order from Supplier</p> <p>Ships Within: 1 week</p> <p>Status: Maintained in stock</p>
200 mg	USD 27					
1 g	USD 79					