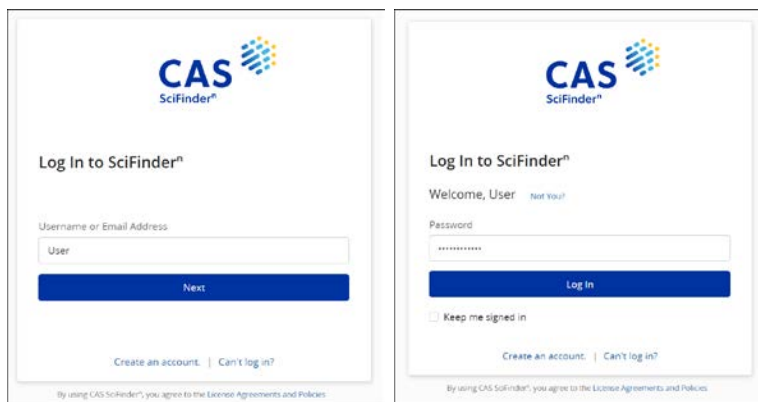


Welcome to CAS SciFinderⁿ

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

First, open the CAS SciFinderⁿ Log In page: <https://scifinder-n.cas.org>.

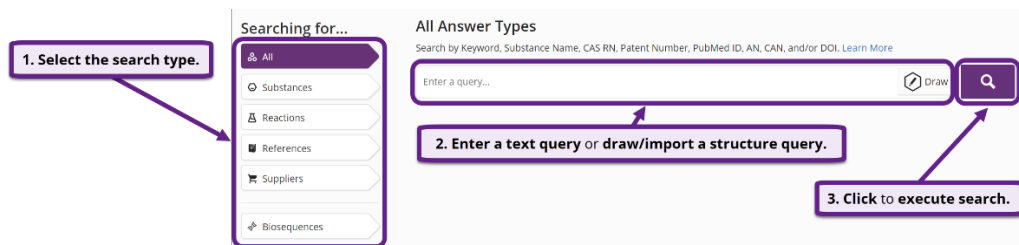
Log in using your CAS SciFinder[®] **Username** and **Password**.



Search

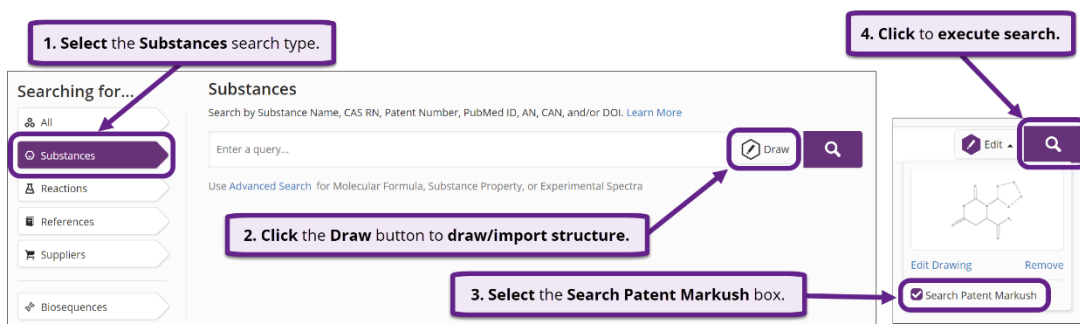
Search for the result type you need using a keyword, substance name, CAS Registry Number[®], patent number, or structure.

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**.



Substances

Select type of structure match.

Keep or remove selected results.

Retrieve data related to all results.

Sort results by relevance or amount of related data.

Change result display.

View a breakdown of the structure's precision.

View a three-dimensional analysis of the substance results.

Select filters to focus results.

Click the X to remove a filter, multiple filters in dropdown menu.

Download results.

Email results.

Save results and/or search.

Retrieve data related to a specific result.

View Key Physical Properties on Substance Detail page.

Click to view substance information window.

Click to open Substance Detail page.

Structure Match: As Drawn (13), Substructure (35), Similarity (21K), Analyze Structure Precision, Create Chemscape Analysis.

Filter Behavior: Filter by, Exclude

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

Substances (5)

2 Selected | References | Reactions | Suppliers

Filtering: Commercial Availability: Available | Reference Role: 2 Selected

1 51234-28-7

2 70280-67-0

3 66934-19-8

Key Physical Properties

Property	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 (1 of 13)

References (1,028) | Reactions (28) | Suppliers (36)

CAS Registry Number
51234-28-7

Chemical Structure: CC(=O)Oc1ccc2nc(c1)ccc2-c1ccc(Cl)cc1

Key Physical Properties

Property	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

Experimental Properties | Spectra

Other Names

- Experimental Properties
- Experimental Spectra
- Predicted Properties
- Predicted Spectra

Expand All | Collapse All

Retrieve data related to substance.

Download detail.

Email detail.

Save detail.

Click the structure image to display its substance information window, which displays options to view details, generate retrosynthesis plan, and edit/download structure file.

Click to view expanded data in category below.

Click a category to expand and view additional substance information.

Expand or collapse all categories.

References

Keep or remove selected results. (Callout to '2 Selected' button)

Retrieve data related to all results. (Callout to 'Substances', 'Reactions', 'Cited By' buttons)

Sort results by relevance or amount of related data. (Callout to 'Sort: Relevance' dropdown)

Change result display. (Callout to 'View: Partial Abstract' dropdown)

Select filters to focus results. (Callout to 'Filter Behavior' sidebar)

Click the X to remove a filter, multiple filters in dropdown menu. (Callout to filter removal X icon)

Download results. (Callout to download icon)

Email results. (Callout to email icon)

Save results and/or search. (Callout to star icon)

Click to open Reference Detail page. (Callout to 'View More' link)

Access options for viewing patent information. (Callout to 'PATENTPAK' dropdown)

Access options for viewing the full text of the reference. (Callout to 'Full Text' dropdown)

Retrieve data related to a specific result. (Callout to 'Substances (2)', 'Reaction (1)', 'Cited By (2)', 'Citation Map' buttons)

Preparation method of carprofen and intermediates thereof (Callout to specific reference title)

Reference Detail

Retrieve data related to substance. (Callout to 'Substances (6)' button)

View map of references this document cites and references that cite this document. (Callout to 'Citation Map' button)

Download detail. (Callout to download icon)

Email detail. (Callout to email icon)

Save detail. (Callout to star icon)

Set citing alert for the reference. (Callout to bell icon)

Access options for viewing the full text of the reference. (Callout to 'PATENTPAK Viewer', 'Full Text' dropdown)

Click a PatentPak option to view the patent source document. (Callout to 'PDF', 'PDF+', 'Viewer' links)

Expand to view concepts that characterize the general subject matter of the reference. (Callout to 'Concepts' dropdown)

Expand to view substances indexed in the reference. (Callout to 'Substances' dropdown)

Expand to view citations from this reference. (Callout to 'Citations' dropdown)

Expand to view formulation information in the reference. (Callout to 'Formulations' dropdown)

View interactive version of the patent that highlights specific locations of indexed substances. (Callout to 'Patent' section)

Patent Information:
 Patent Number: WO2015095199
 Publication Date: 2015-06-25
 Application Number: WO2014-US70615

Abstract: A method and composition for treating osteoarthritis including administering an anti-inflammatory agent to a patient, wherein the anti-inflammatory agent is Et (α-guanido-methyl) ethanoate. Et (α-guanido-methyl) ethanoate provides a safe, non-toxic anti-inflammatory treatment for osteoarthritis.

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2015095199	English	A1	PDF PDF+ Viewer	2015-06-25		
US20150164847	English	A1	PDF PDF+ Viewer	2015-06-18	US2014-14572159	2014-12-16

Reactions

Keep or remove selected results.

Retrieve data related to all results.

Change result display.

Select filters to focus results.

Click the X to remove a filter, multiple filters in dropdown menu.

Download results.

Save results and/or search.

Email results.

Retrieve suppliers for the substance.

Click any structure image or substance name to display its substance information window, which displays options to view details, generate retrosynthesis plan, and edit/download structure file.

Click to open reaction reference's detail page.

Access options for viewing the full text of the reference.

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

Display experimental procedure for reaction.

Collapse or expand a scheme's reaction summaries.

View reaction's detail page.

Filter Behavior

Filter by

Exclude

Yield

☐ No Yield Available (9)

Number of Steps

☐ Experimental Procedure (9)

Experimental Protocols

☒ MethodsNow: Synthesis (9)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

☒ Document Type

Language

Publication Year

Publication Name

Reactions (9)

1 Selected

References

Keep Selected Results

Remove Selected Results

Steps: 2

Experimental Protocols: MethodsNow: Synthesis

Scheme 1 (3 Reactions)

Suppliers (102)

Suppliers (90)

Suppliers (15)

Expand Scheme

Scheme 2 (1 of 1 Reaction Selected)

Steps: 2

Reaction Summary

1.1 Reagents: Potassium carbonate

Solvents: Methanol, Tetrahydrofuran; 2 - 4 h, 20 - 30 °C

2.1 20 - 30 °C; 30 °C → 110 °C; 10 h, 100 - 110 °C

By: Dixit, Girish; et al

World Intellectual Property Organization, WO2010/128355

2010-11-11

PATENTPAK

Full Text

process for preparation of arformoterol via asymmetric reduction of nitroacetophenones.

Click to open reaction reference's detail page.

Access options for viewing the full text of the reference.

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

Display experimental procedure for reaction.

Collapse or expand a scheme's reaction summaries.

View reaction's detail page.

Reaction Detail

Reaction Detail (Scheme 1, Reaction 1 of 3)

Retrieve suppliers for the substance.

Download detail.

Email detail.

Save detail.

Click to open reaction reference's detail page.

View alternative reactions for the same product.

View all reference authors.

Click the tabs to view the steps in a multi-step reaction.

Click the tabs to view available experimental protocols.

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

Access options for viewing the full text of the reference.

Step 1

Step 2

Alternative Steps (13)

Stage

Reagents

Catalyst

Solvents

Conditions

1

2

Hydrogen

Platinum oxide

Tetrahydrofuran

2 h, 20 - 40 °C

8 - 15 h, 4 - 5 kg/cm², 20 °C

CAS Reaction Number: 31-313-CAS-12647628

Notes

autoclave used

Experimental Protocols

Synthetic Methods

Experimental Procedure

Products

4-Methoxy- α -methyl-N-(phenylmethyl)benzeneethanamine

Reactants

Benzylamine

Reference

process for preparation of arformoterol via asymmetric reduction of nitroacetophenones.

By: Dixit, Girish; et al

World Intellectual Property Organization

PATENTPAK

Full Text

Patent Information

Patent Number

WO2010128355

Publication Date

2010-11-11

Application Number

WO2009-1B097

Application Date

2009-12-28

Suppliers

Suppliers (26)

Filter Behavior

- Filter by: Exclude
- Preferred Suppliers
- Supplier
- Purity
 - ≥99% (4)
 - 95-98% (24)
 - 90-94% (2)
- Quantity
- Ships Within
- Stock Status
- Order From Supplier
- Country

1 Selected

Keep or remove selected results.

Click the X to remove all filters, uncheck individual filters in dropdown menu.

Change result display.

Sort: Relevance

Download results.

Email results.

Select filters to refine results.

Open product information page on supplier's website.

Click to open the substance's information window, which displays options to view details, generate retrosynthesis plan, and edit/download structure file.

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

Click to open Supplier Detail page.

Open product ordering page on supplier's website.

Supplier	Substance	Purity	Purchasing Details	Availability
Arspichem Product List United States	51234-28-7 2-(2-(4-chlorophenyl)benzo[d]	95-98%	Typically in stock	
Alchem Pharmtech, Inc. Alchem Pharmtech Product List United States	51234-28-7 2-(4-chlorophenyl)-alpha-methyl-S-benzoxazoleacetic acid	95-98%	1G 5G 10G 25G 50G Bulk View all	Maintained in stock
ASTATECH AstaTech Product List United States	51234-28-7 BENOXAPROFEN	95-98%	Order From Supplier 0.1G, USD 3500 0.25G, USD 6900	Synthesis on demand Ships within 8 weeks

Supplier Detail

Supplier Detail (3)

AstaTech Product List

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

Download detail.

Email detail.

Click to open Substance Detail page.

Click the structure image to open the substance's information window, which displays options to view details, generate retrosynthesis plan, and edit/download structure.

Open product ordering page on supplier's website.

Order From Supplier

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

Email: sales@astatechinc.com

Phone: 215-785-3197

Item Details

Chemical Name: BENOXAPROFEN

Order Number: C90147

Purity: 95%

Quantity, Price: 0.1G, USD 3500
0.25G, USD 6900

Stock Status: Synthesis on demand

Ships Within: 8 weeks

Pricing Information: 31 Dec 2020

Last Updated:

Additional Contact Information

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

Fax: 215-785-2656

Substance Information

CAS Registry Number: 51234-28-7

CAS Name: Benoxaprofen

Chemical Structure: CC(=O)Oc1ccc2c(c1)oc(c2)c3ccc(Cl)cc3

Biosequences

The screenshot displays the CAS SciFinder Biosequences search results page. The interface includes a sidebar on the left for search details and filters, and a main content area showing sequence alignments and analysis options.

Callouts and Annotations:

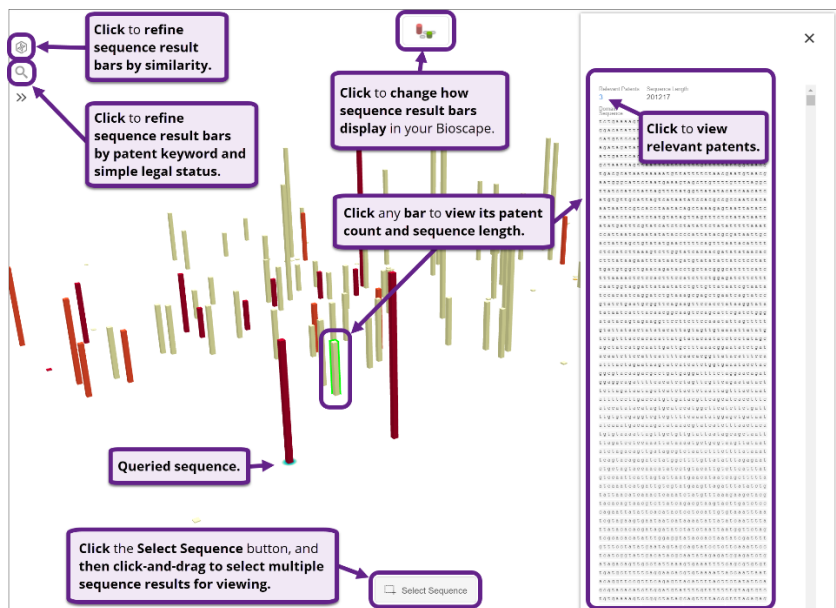
- Sort results.** Points to the "Sort: Subject Coverage" dropdown menu.
- Change result display.** Points to the "View: Expanded" dropdown menu.
- Click to select another sequence.** Points to the search bar containing "pdb|1B57|C Chain C, Physalis Mottle Virus".
- Download results.** Points to the download icon (downward arrow) in the top right.
- Click to view references indexing the sequence result.** Points to the "References" button in the bottom right of the alignment section.
- Click to view sequence and patent data related to the result.** Points to the "References" tab in the alignment section.
- Select filters to focus results.** Points to the "Filter by" section in the sidebar, which includes sliders for E-Value, Query Coverage %, Subject Coverage %, and Alignment Identity %.
- View a three-dimensional analysis of the biosequence results.** Points to the "Create Bioscape Analysis" button in the sidebar.

Search Results Summary:

- BLAST Search Details:**
 - Sequence Type: Protein
 - Search Within: Nucleotides
 - BLAST Algorithm: TBLASTn-fast
 - Alignment Identity: 90%
 - Query Coverage: 90%
 - E-Value: 10
 - Match with Gaps: Yes
 - Gap Costs: Existence 11
 - Extension 1
 - Word Size: 6
- Bioscape Analysis:**
 - Visually explore sequence similarity with a new tool.
 - [Learn more about Bioscape.](#)
 - [Create Bioscape Analysis](#)
- Filter by:**
 - E-Value: 0 to 10⁵
 - Query Coverage %: 0 to 100
 - Subject Coverage %: 0 to 100
 - Alignment Identity %: 60.5 to 100
 - [Apply](#) [Reset Filters](#)
- Alignment 1:**
 - Query: 1 (188)
 - Subject: 1 (564)
 - Alignment Identity: 100%
 - Alignment Data: BLAST Score: 883, E-Value: 2.47566e-120
 - Sequence alignment shown with gaps and matches.
- Alignment 2:**
 - Query: 1 (188)
 - Subject: 1 (567)
 - Alignment Identity: 60.11%
 - Matches: 113, Mismatches: 75
 - Alignment Data: BLAST Score: 487, E-Value: 3.16983e-60
 - Sequence alignment shown with gaps and matches.

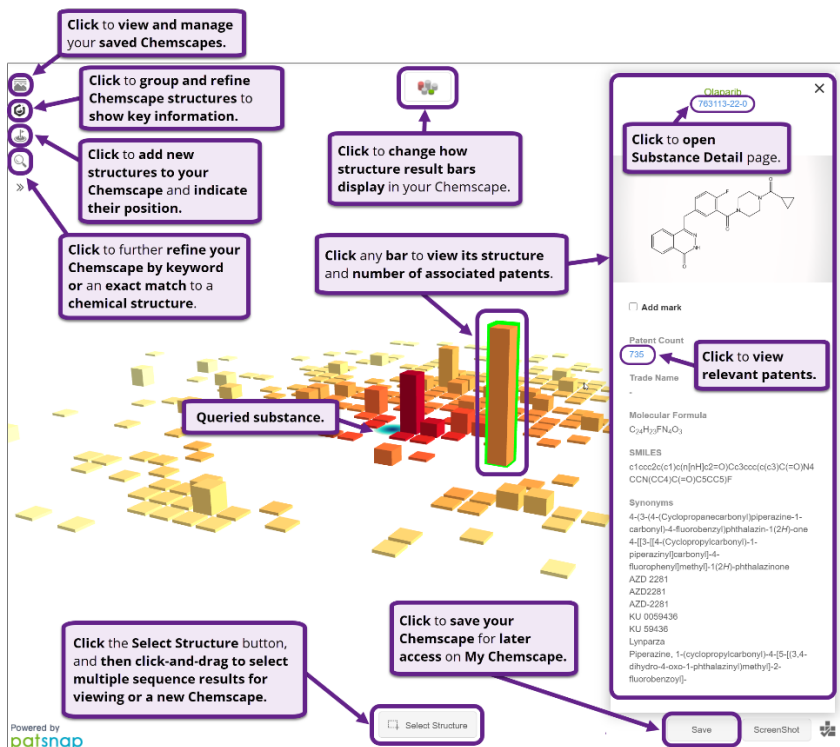
Bioscope

Bioscope 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.



Chemscope

Chemscope 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.



Search History

The screenshot shows the 'Search History' page with several annotations in purple boxes and arrows:

- Delete searches from your history.** Points to a trash can icon in the top right of the history list.
- Filter search history for selected search types.** Points to the 'Filter by' section on the left, where 'Substances' is checked under 'Result Type'.
- Rerun search to retrieve the latest results.** Points to the 'Rerun Search' button for a search from January 6, 2021.
- Rerun retrosynthesis plan or edit options and rerun.** Points to the 'Rerun Plan' and 'Edit Options' buttons for a retrosynthesis search from August 11, 2020.
- Edit search and then rerun.** Points to the 'Edit Search' button for a 'Patent Markush' search from June 19, 2019.
- Display search history for a specified date range.** Points to the 'Date' filter section on the left, which includes a calendar for selecting a date range.

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.

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[Help](#) [Contact Us](#) [Legal](#)

The screenshot shows the top navigation bar with 'Saved', 'History', and 'Account' links. The 'Account' link is highlighted with a purple box. Below it, a dropdown menu is visible with options: 'My CAS Profile', 'What's New?', 'Help' (highlighted with a purple box), and 'Log Out'.

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.