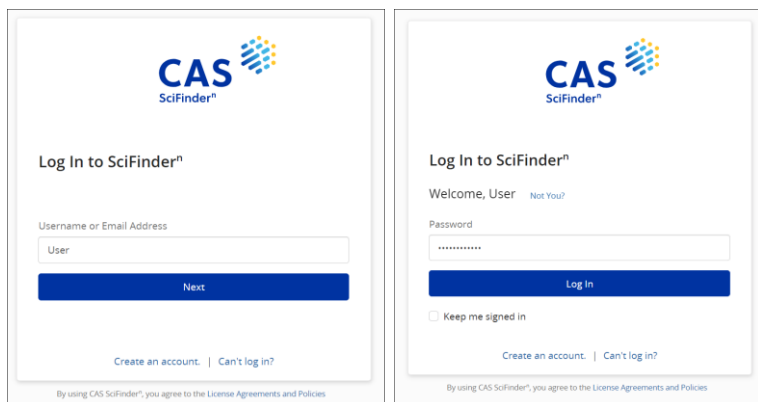


### Welcome to CAS SciFinder<sup>n</sup>

This Quick Reference Guide will show you how to start using CAS SciFinder<sup>n</sup>, the industry's most trusted and comprehensive chemistry relevance engine.

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

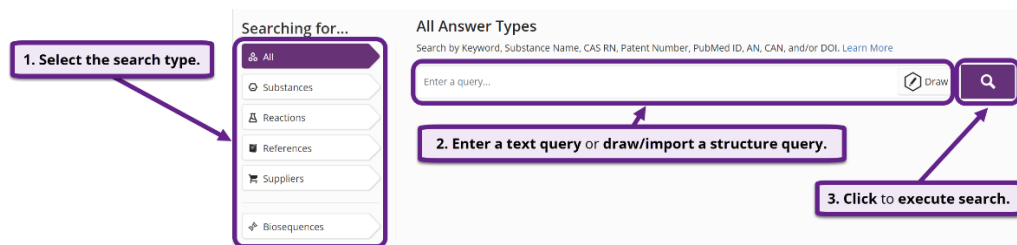
Log in using your CAS SciFinder<sup>®</sup> **Username** and **Password**.



### Search

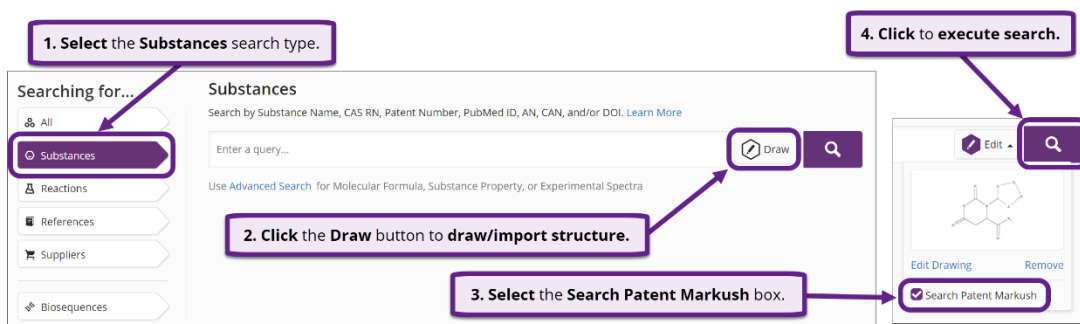
Search for the result type you need using a keyword, substance name, CAS Registry Number<sup>®</sup>, patent number, or structure.

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

**Keep or remove selected results.** Substances (5): 2 Selected

**Retrieve data related to all results.** References, Reactions, Suppliers

**Sort results by relevance or amount of related data.** Sort: Relevance, View: Full

**Change result display.** Download, Email, Save

**View a breakdown of the structure's precision.** Analyze Structure Precision

**View a three-dimensional analysis of the substance results.** Create Chemscape Analysis

**Select filters to focus results.** 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

**Click the X to remove a filter, multiple filters in dropdown menu.** Filtering: Commercial Availability: Available, Reference Role: 2 Selected

**Download results.** Download

**Save results and/or search.** Save

**View Key Physical Properties on Substance Detail page.** Key Physical Properties table for 51234-28-7 and 70280-67-0

**Retrieve data related to a specific result.** 70280-67-0: 36 References, 0 Reactions, 1 Supplier

**Click to view substance information window.** 66934-19-8

**Click to open Substance Detail page.** 66934-19-8

## Substance Detail

**Retrieve data related to substance.** Substance Detail (1 of 13): References (1,028), Reactions (28), Suppliers (36)

**Download detail.** Download

**Email detail.** Email

**Save detail.** Save

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

**Click to view expanded data in category below.** Key Physical Properties table

**Click a category to expand and view additional substance information.** Experimental Properties

**Expand or collapse all categories.** Expand All | Collapse All

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 <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C

## References

**Keep or remove selected results.**

**Retrieve data related to all results.**

**Sort results by relevance or amount of related data.**

**Change result display.**

**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.**

**Preparation method of carprofen and intermediates thereof**

**Retrieve data related to a specific result.**

**Click to open Reference Detail page.**

**Access options for viewing patent information.**

**Access options for viewing the full text of the reference.**

## Reference Detail

**Retrieve data related to substance.**

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

**Download detail.**

**Email detail.**

**Save detail.**

**Set citing alert for the reference.**

**Access options for viewing the full text of the reference.**

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

**Click a PatentPak option to view the patent source document.**

**Expand to view concepts that characterize the general subject matter of the reference.**

**Expand to view substances indexed in the reference.**

**Expand to view citations from this reference.**

**Expand to view formulation information in the reference.**

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2015095199	English	A1	PDF   PDF+   Viewer	2015-06-25		
P						
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.**

**View reaction's detail page.**

**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.**

**Experimental Protocols: MethodsNow: Synthesis**

**Suppliers (102)**

**Suppliers (90)**

**Suppliers (15)**

**Suppliers (33)**

**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, WO2010/2010-11-11

**process for preparation of arformoterol via asymmetric reduction of nitroacetophenones.**

**PATENTPAK**

**Full Text**

**View Reaction Detail**

**Experimental Protocols**

**Patent Information**

**Patent Number** WO2010128355  
**Publication Date** 2010-11-11  
**Application Number** WO2009-1B8097  
**Application Date** 2009-12-28

## Reaction Detail

**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.**

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

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

**Click the tabs to view available experimental protocols.**

**Access options for viewing the full text of the reference.**

**Suppliers (99)**

**Suppliers (86)**

**Suppliers (45)**

**Suppliers (14)**

**Step 1**

**Step 2**

**Alternative Steps (13)**

**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** WO2009-1B8097  
**Application Date** 2009-12-28

Stage	Reagents	Catalyst	Solvents	Conditions
1	-	-	Tetrahydrofuran	2 h, 20 - 40 °C
2	Hydrogen	Platinum oxide	-	8 - 15 h, 4 - 5 kg/cm <sup>2</sup> , 20 - 30 °C

CAS Reaction Number: 31-313-CAS-12647628

**Notes**

autoclave used

**Experimental Protocols**

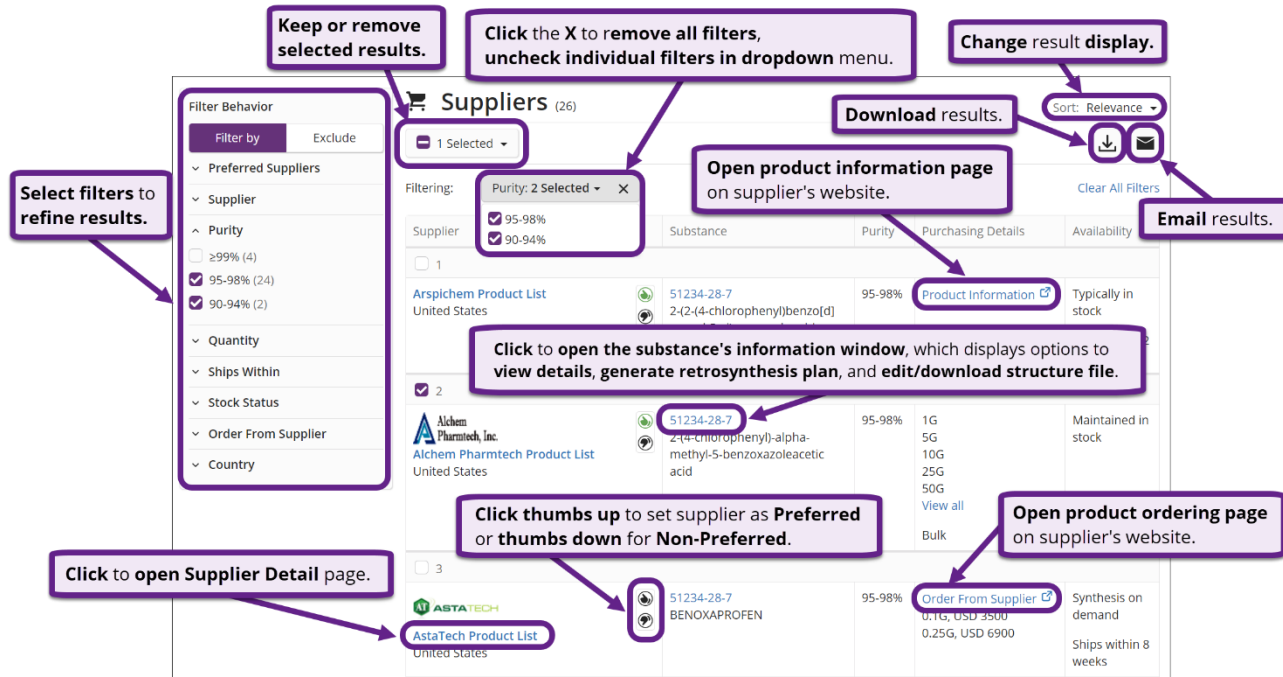
**Synthetic Methods**

**Experimental Procedure**

**Products** 4-Methoxy-*o*-methyl-*N*-(phenylmethyl)benzeneethanamine

**Reactants** Benzylamine

## Suppliers



**Keep or remove selected results.**

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

**Change result display.**

**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.**

**Open product ordering page on supplier's website.**

**Click to open Supplier Detail page.**

**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

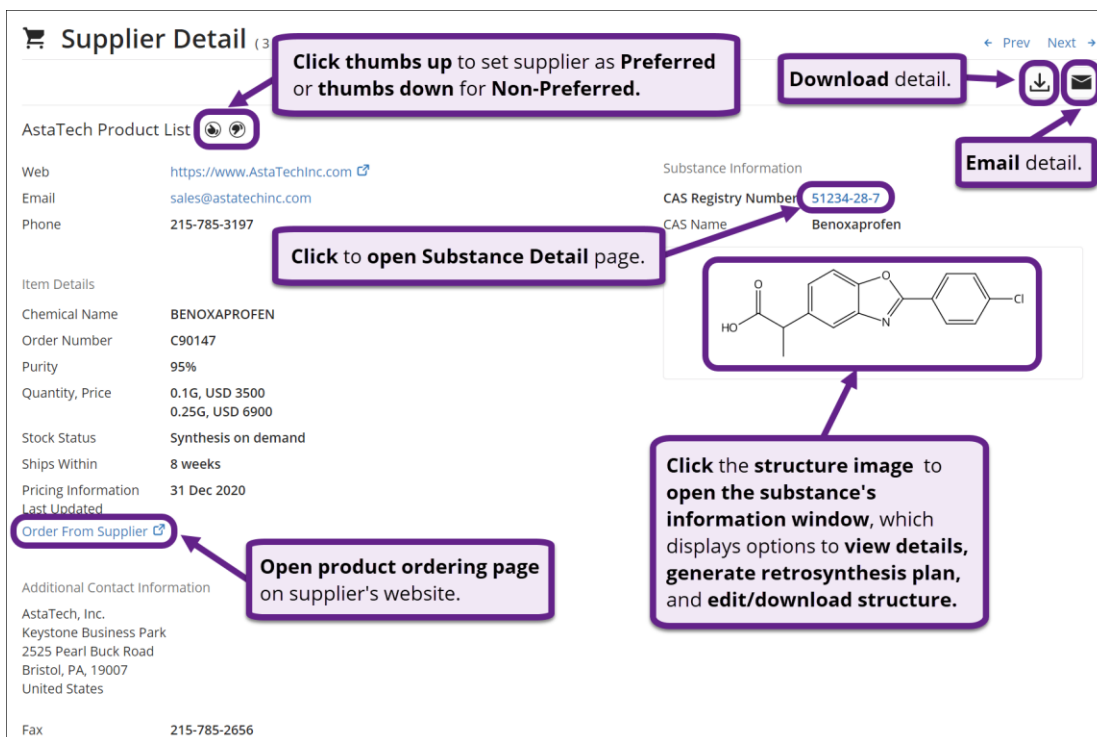
**Suppliers (26)**

Filtering: Purity: 2 Selected X

Supplier: 1 Selected

Supplier	Substance	Purity	Purchasing Details	Availability
1 Arsphichem Product List United States	51234-28-7 2-(2-(4-chlorophenyl)benzo[d]	95-98%		Typically in stock
2 Alchem Pharmtech, Inc. Alchem Pharmtech Product List United States	51234-28-7 2-(4-chlorophenyl)-alpha-methyl-5-benzoxazoleacetic acid	95-98%	1G 5G 10G 25G 50G Bulk	Maintained in stock
3 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)**

**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.**

**Substance Information**

CAS Registry Number: 51234-28-7

CAS Name: Benoxaprofen

CC(C)C(=O)Oc1ccc2nc3ccc(Cl)cc3o2

**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

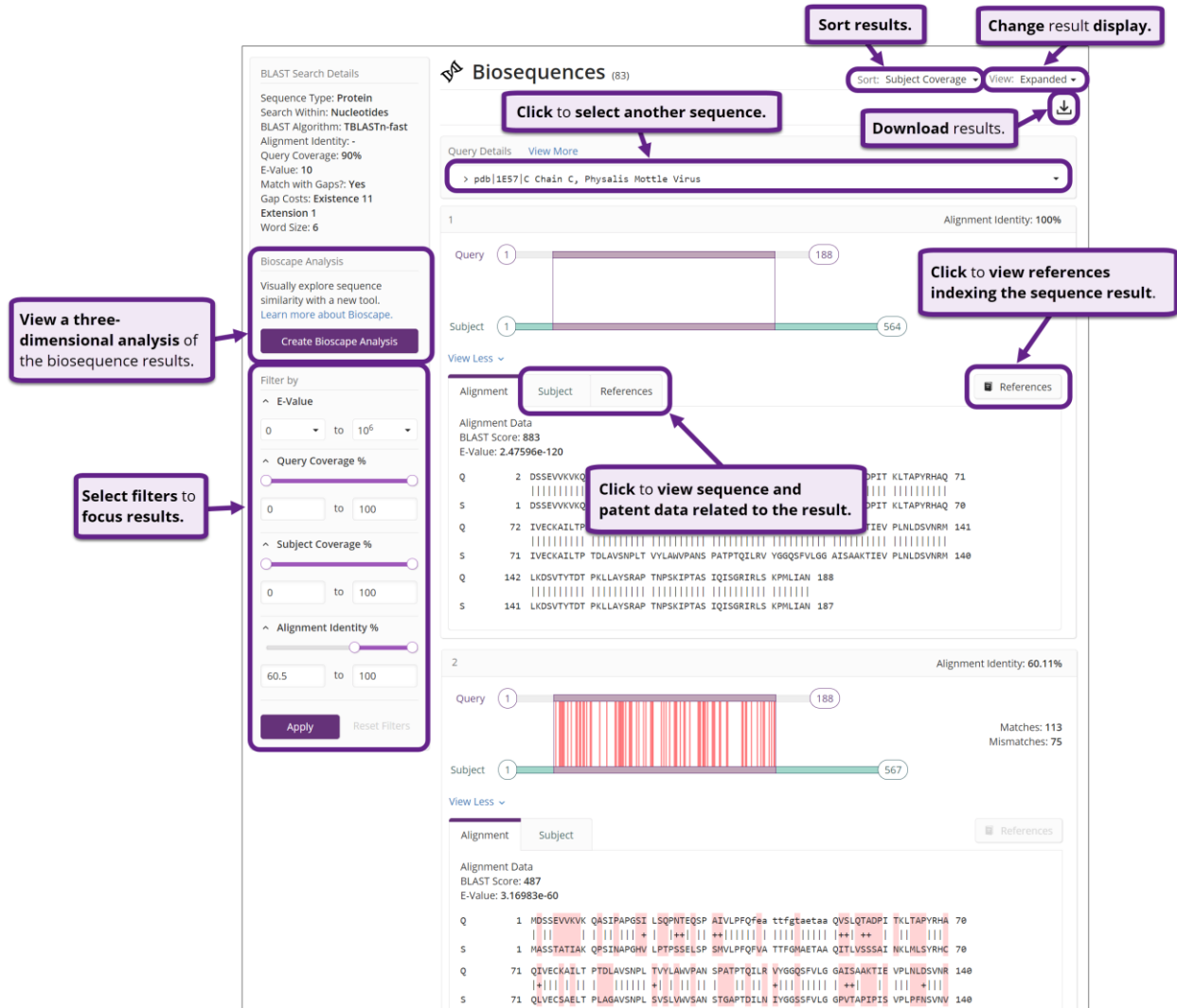
Last Updated: Order From Supplier

**Additional Contact Information**

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

Fax: 215-785-2656

## Biosequences



The screenshot displays the Biosequences search results page. On the left, the 'BLAST Search Details' panel shows search parameters: Sequence Type: Protein, Search Within: Nucleotides, BLAST Algorithm: TBLASTn-fast, Alignment Identity: -, Query Coverage: 90%, E-Value: 10, Match with Gaps?: Yes, Gap Costs: Existence 11, Extension 1, Word Size: 6. Below this is the 'Bioscape Analysis' section, which includes a 'Create Bioscape Analysis' button and a 'Filter by' section with sliders for E-Value, Query Coverage %, Subject Coverage %, and Alignment Identity %.

The main results area shows two alignments. Alignment 1 has an identity of 100% and shows a perfect match between the query (188) and subject (564). Alignment 2 has an identity of 60.11% and shows 113 matches and 75 mismatches between the query (188) and subject (567). The alignment data for both shows sequence alignments with gaps and scores.

Callout boxes highlight the following features:

- Sort results.** and **Change result display.** (pointing to 'Sort: Subject Coverage' and 'View: Expanded')
- Click to select another sequence.** (pointing to the search bar)
- Download results.** (pointing to the download icon)
- View a three-dimensional analysis of the biosequence results.** (pointing to the 'Create Bioscape Analysis' button)
- Select filters to focus results.** (pointing to the 'Filter by' section)
- Click to view references indexing the sequence result.** (pointing to the 'References' button)
- Click to view sequence and patent data related to the result.** (pointing to the 'References' button in the alignment details)



## 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.

Click to refine sequence result bars by similarity.

Click to refine sequence result bars by patent keyword and simple legal status.

Click to change how sequence result bars display in your Bioscape.

Click any bar to view its patent count and sequence length.

Click to view relevant patents.

Queried sequence.

Click the Select Sequence button, and then click-and-drag to select multiple sequence results for viewing.

Select Sequence

## 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.

Click to view and manage your saved Chemscape.

Click to group and refine Chemscape structures to show key information.

Click to add new structures to your Chemscape and indicate their position.

Click to further refine your Chemscape by keyword or an exact match to a chemical structure.

Click to change how structure result bars display in your Chemscape.

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

Click to open Substance Detail page.

Queried substance.

Click to view relevant patents.

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

Click to save your Chemscape for later access on My Chemscape.

Select Structure

Save

ScreenShot

Patent Count  
735

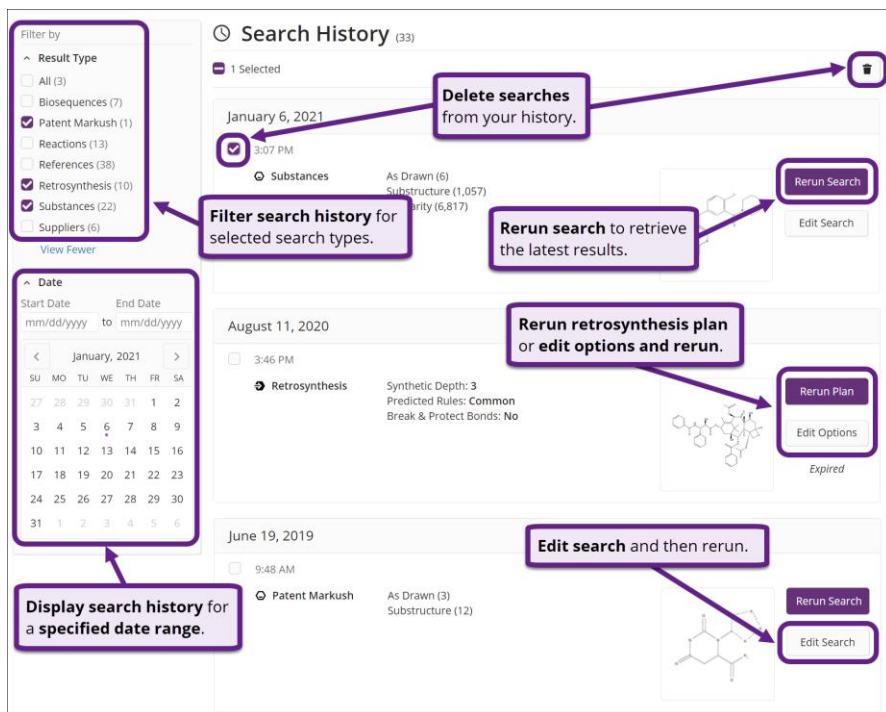
Trade Name

Molecular Formula  
 $C_{24}H_{27}FN_3O_3$

SMILES  
c1ccc2c(c1)[nH]c2=O[C@@]3Cc4cc(c3)C(=O)N4  
CCN(CC4)C(=O)C5CC5)F

Synonyms  
4-(3-(4-(Cyclopropylcarbonyl)piperazine-1-carbonyl)-4-fluorobenzyl)phthalazin-1(2H)-one  
4-([3-[[4-(Cyclopropylcarbonyl)-1-piperazinyl]carbonyl]-4-fluorophenyl]methyl)-1(2H)-phthalazinone  
AZD 2281  
AZD2281  
AZD-2281  
KU 009436  
KU 009430  
Lymparza  
Piperazine, 1-(cyclopropylcarbonyl)-4-[[5-[[3,4-dihydro-4-oxo-1-phthalazinyl]methyl]-2-fluorobenzoyl]-

## Search History



The screenshot shows the 'Search History' interface with several callouts:

- Delete searches from your history.** Points to a trash icon in the top right of the history list.
- Filter search history for selected search types.** Points to the 'Filter by' sidebar on the left, which includes categories like Result Type, Date, and Substances.
- Rerun search to retrieve the latest results.** Points to the 'Rerun Search' button for a specific search entry.
- Rerun retrosynthesis plan or edit options and rerun.** Points to the 'Rerun Plan' and 'Edit Options' buttons for a retrosynthesis search.
- Edit search and then rerun.** Points to the 'Edit Search' button for a search entry.
- Display search history for a specified date range.** Points to the date selection calendar in the 'Date' filter section.

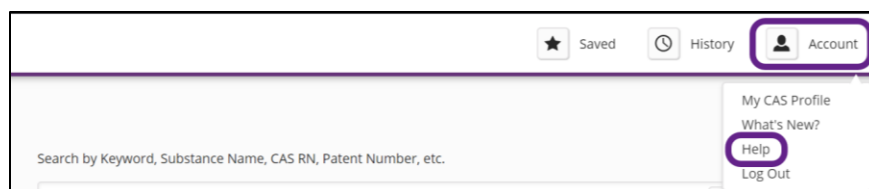
## CAS SciFinder<sup>n</sup> Support

To access CAS SciFinder<sup>n</sup> in-application support, click the **Help** link at the bottom of any page or select **Help** from the **Account** menu.



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Account menu options: My CAS Profile, What's New?, **Help**, Log Out.

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- **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](mailto:help@cas.org)
- **Web:** <https://www.cas.org/contact>

If desired, ask for a CAS SciFinder<sup>n</sup> Familiarization Training Session visit or online session.