

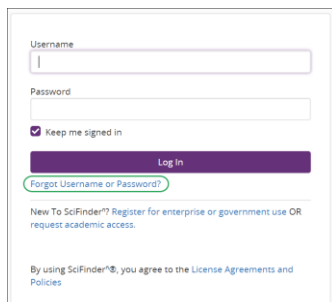
Welcome to CAS SciFinderⁿ

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**.

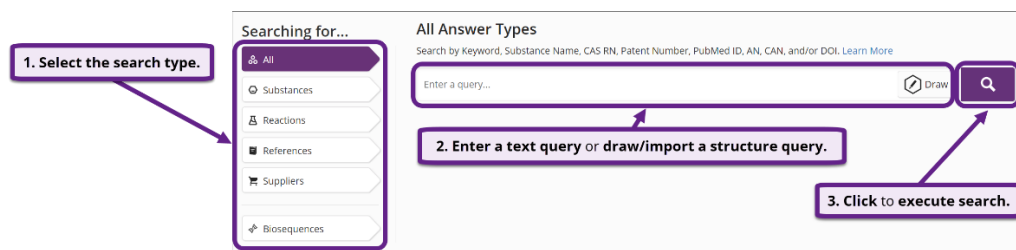
Note: First-time commercial users may self-register by clicking Register for enterprise or government use.



Search

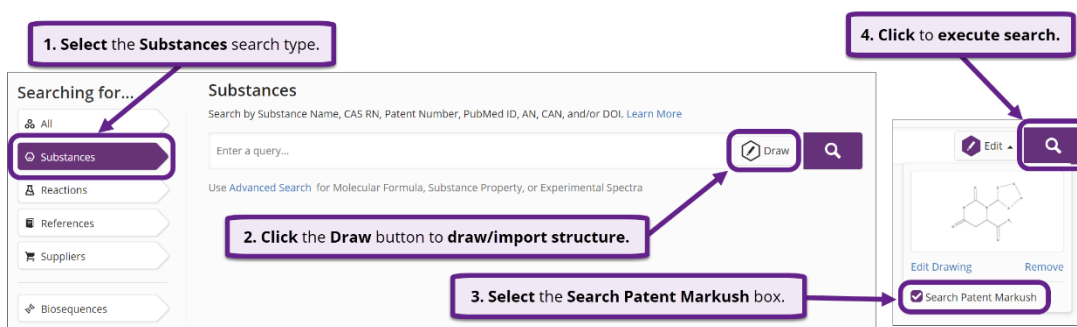
Search for the result type you need using a keyword, substance name, CAS Registry Number[®], patent number, or structure.

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

Keep or remove selected results. 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

Retrieve data related to a specific result. 51234-28-7, 70280-67-0, 66934-19-8

View Key Physical Properties on Substance Detail page. Key Physical Properties table

Click to view substance information window. C₁₆H₁₂ClNO₃ (-)-Benoxaprofen

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. Chemical 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 ³ | Temp: 20 °C; Press: 760 Torr |
| pKa (Predicted) | 4.36±0.30 | Most Acidic Temp: 25 °C |

References

Keep or remove selected results. (2 Selected)

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

Sort results by relevance or amount of related data. (Sort: Relevance)

Change result display. (View: Partial Abstract)

Select filters to focus results. (Filter Behavior sidebar)

Click the X to remove a filter, multiple filters in dropdown menu. (Filtering: Document Type: Patent X Substance Role: 2 Selected X)

Download results. (Download icon)

Email results. (Email icon)

Save results and/or search. (Save icon)

Preparation method of carprofen and intermediates thereof (Title of selected result)

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

Click to open Reference Detail page. (Reference title)

Access options for viewing patent information. (PATENTPAK, Full Text)

Access options for viewing the full text of the reference. (Substances (7), Reactions (3), Cited By (0), Citation Map)

Reference Detail

Retrieve data related to substance. (Substances (6), Reactions (0), Cited By (0), Citation Map)

View map of references this document cites and references that cite this document. (Citation Map icon)

Download detail. (Download icon)

Email detail. (Email icon)

Save detail. (Save icon)

Set citing alert for the reference. (Alert icon)

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

Click a PatentPak option to view the patent source document. (PDF | PDF+ | Viewer)

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

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

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

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

View interactive version of the patent that highlights specific locations of indexed substances. (Patent information sidebar)

| 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. (Buttons: 1 Selected, References)

Retrieve data related to all results. (Buttons: Keep Selected Results, Remove Selected Results)

Change result display. (Buttons: Group: By Scheme, View: Expanded, Download, Save, Clear All Filters)

Select filters to focus results. (Filter Behavior sidebar)

Click the X to remove a filter, multiple filters in dropdown menu. (Buttons: Experimental Protocols: MethodsNow: Synthesis, X)

Download results. (Download icon)

Save results and/or search. (Save icon)

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. (Structure images)

Retrieve suppliers for the substance. (Suppliers buttons: Suppliers (102), Suppliers (90), Suppliers (15), Suppliers (33))

View reaction's detail page. (Buttons: View Reaction Detail, Experimental Protocols)

Collapse or expand a scheme's reaction summaries. (Buttons: Collapse Scheme, Expand Scheme)

Display experimental procedure for reaction. (Buttons: Experimental Protocols)

View interactive version of the patent that highlights specific locations of indexed substances. (Buttons: PATENTPAK, Full Text)

Click to open reaction reference's detail page. (Buttons: PATENTPAK, Full Text)

Access options for viewing the full text of the reference. (Buttons: PATENTPAK, Full Text)

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

Reaction Detail

Retrieve suppliers for the substance. (Buttons: Suppliers (99), Suppliers (86), Suppliers (45), Suppliers (14))

Download detail. (Buttons: Download, Save, Email detail, Save detail)

Click to open reaction reference's detail page. (Buttons: PATENTPAK, Full Text)

View alternative reactions for the same product. (Buttons: Alternative Steps (13))

View all reference authors. (Buttons: View All, World Intellectual Property Organization)

View interactive version of the patent that highlights specific locations of indexed substances. (Buttons: PATENTPAK, Full Text)

Access options for viewing the full text of the reference. (Buttons: PATENTPAK, Full Text)

Click the tabs to view the steps in a multi-step reaction. (Buttons: Step 1, Step 2)

Click the tabs to view available experimental protocols. (Buttons: MethodsNow[™], Experimental Procedure)

Reference:
 process for preparation of arformoterol via asymmetric reduction of nitroacetophenones.
 By: Dixit, Girish; et al
 World Intellectual Property Organization
 Patent Number: WO2010128355
 Publication Date: 2010-11-11
 Application Number: WIO2009-1B8097
 Application Date: 2009-12-28

| Stage | Reagents | Catalysts | Solvents | Conditions |
|-------|----------|----------------|-----------------|--|
| 1 | - | - | Tetrahydrofuran | 2 h, 20 - 40 °C |
| 2 | Hydrogen | Platinum oxide | - | 8 - 15 h, 4 - 5 kg/cm ² , 20 °C |

CAS Reaction Number: 31-313-CAS-12687628

Notes: autoclave used

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

Reactants: Benzylamine

Suppliers

Keep or remove selected results.

Select filters to focus results.

Change result display.

Download results.

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

Email results.

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

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

Click to open Supplier Detail page.

Click to select a quantity.

Supplier List (24)

Filter Behavior: Filter by, Exclude

- Preferred Suppliers
- Supplier
- Purity
 - ≥99% (4)
 - 95-98% (23)
 - 90-94% (1)
- Quantity
- Ships Within
- Stock Status
- Order From Supplier
- Country

Filtering: Purity: 2 Selected X

- 95-98%
- 90-94%

Supplier: 1 Selected

| Supplier | Product List | CAS Registry Number | Purity | Price | Ships Within |
|------------------------|---------------|---------------------|--------|-------------------|----------------------|
| Arspichem Product List | United States | 51234-28-7 | 95-98% | Price Unavailable | Ships within 2 weeks |
| Alchem Pharmtech, Inc. | United States | 51234-28-7 | 95-98% | USD 6900 | Ships within 8 weeks |
| AstaTech Product List | United States | 51234-28-7 | 95-98% | USD 6900 | 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.

Supplier Detail (3)

AstaTech Product List

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 Structure: CC(O)C(=O)c1ccc2nc(c1)C(=O)c3ccc(Cl)cc32

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

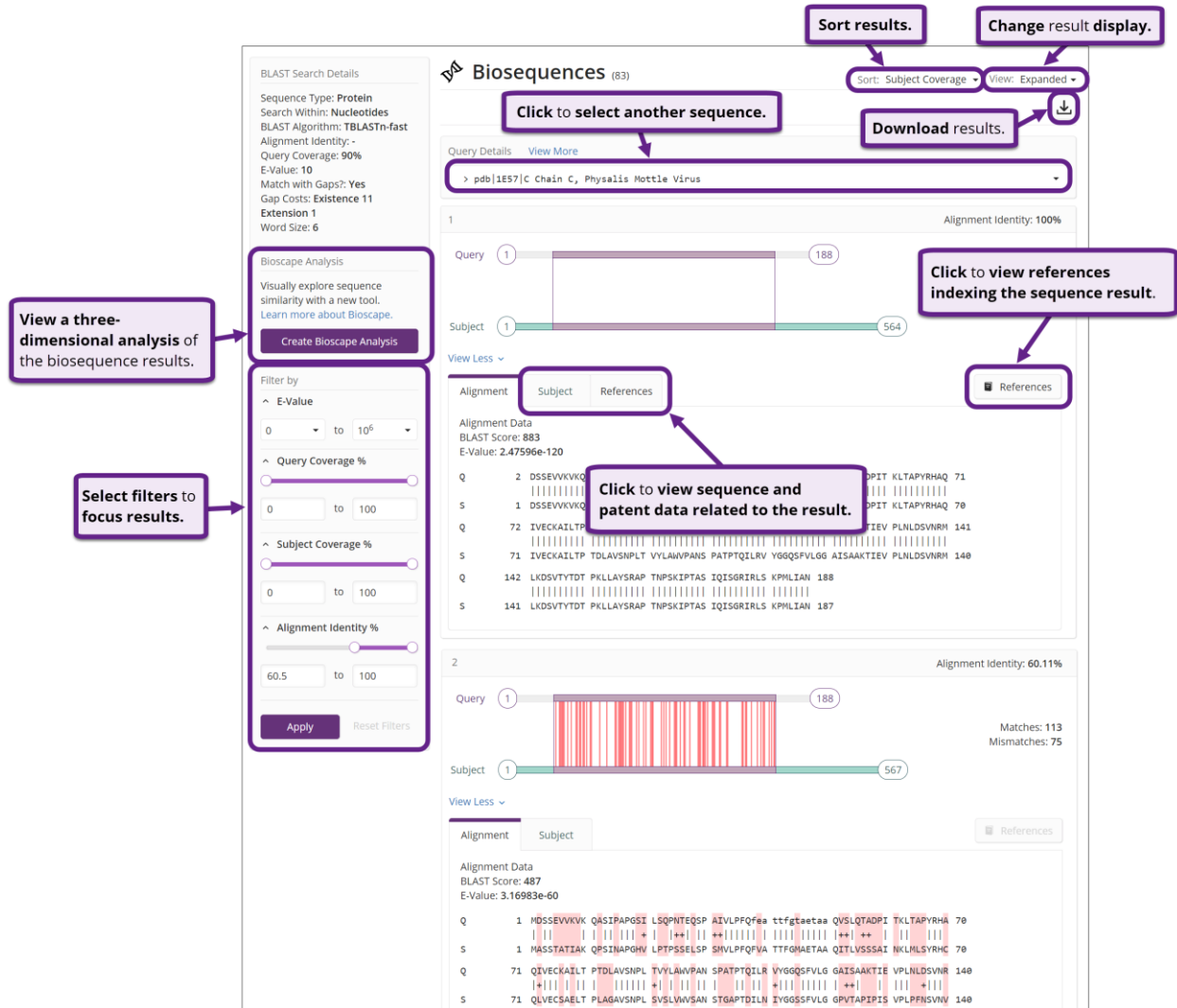
Order From Supplier

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. Key features and callouts include:

- Sort results.**: Callout pointing to the 'Sort: Subject Coverage' dropdown menu.
- Change result display.**: Callout pointing to the 'View: Expanded' dropdown menu.
- Click to select another sequence.**: Callout pointing to the search bar containing 'pdb|1E57|C Chain C, Physalis Mottle Virus'.
- Download results.**: Callout pointing to the download icon.
- View a three-dimensional analysis of the biosequence results.**: Callout pointing to the 'Bioscape Analysis' section.
- Select filters to focus results.**: Callout pointing to the 'Filter by' section with sliders for E-Value, Query Coverage %, Subject Coverage %, and Alignment Identity %.
- Click to view references indexing the sequence result.**: Callout pointing to the 'References' button.
- Click to view sequence and patent data related to the result.**: Callout pointing to the 'References' tab in the alignment view.

The interface shows two alignment results. The first alignment (1) has an identity of 100% and shows a perfect match between the query and subject sequences. The second alignment (2) has an identity of 60.11% and shows several mismatches between the query and subject sequences.

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.

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 Bioscope.

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

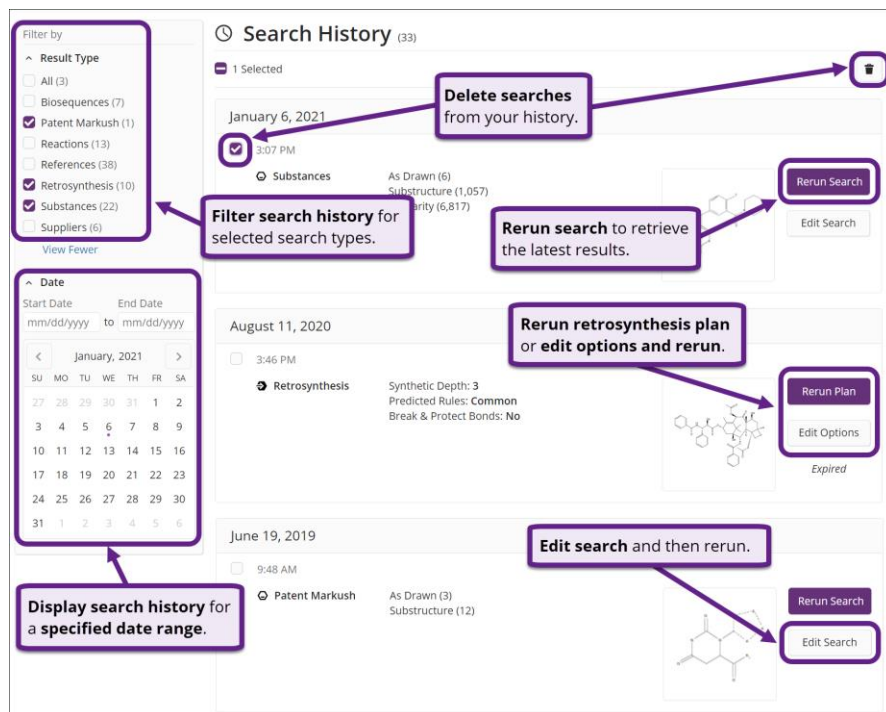
Trade Name

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

SMILES
c1ccc2c(c1)[nH]c2=O(c3ccc(c(c3)C(=O)N4CCN(C4)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
Lynparza
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:

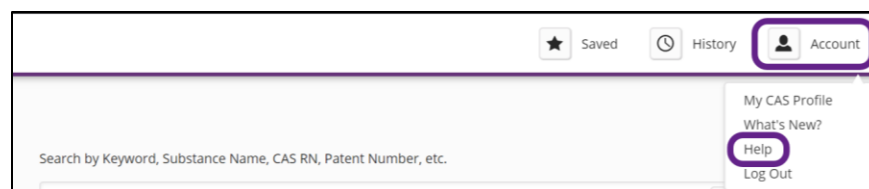
- Delete searches from your history.** Points to a trash icon in the top right of the history list.
- Filter search history for selected search types.** Points to the 'Filter by' sidebar on the left, which includes categories like Result Type, Date, and Substances.
- Rerun search to retrieve the latest 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 SciFinderⁿ Support

To access CAS SciFinderⁿ 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 'Account' menu with the following options:

- My CAS Profile
- What's New?
- Help** (highlighted with a red circle)
- Log Out

For additional assistance using CAS SciFinderⁿ, 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 SciFinderⁿ Familiarization Training Session visit or online session.