

**CAS**  
**SciFinder<sup>®</sup>**  
**Quick Reference Guide**

## **Contents**

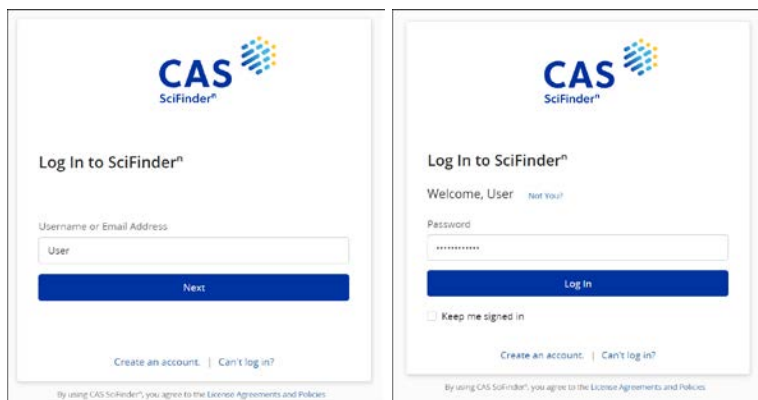
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## Welcome to CAS SciFinder<sup>®</sup>

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

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

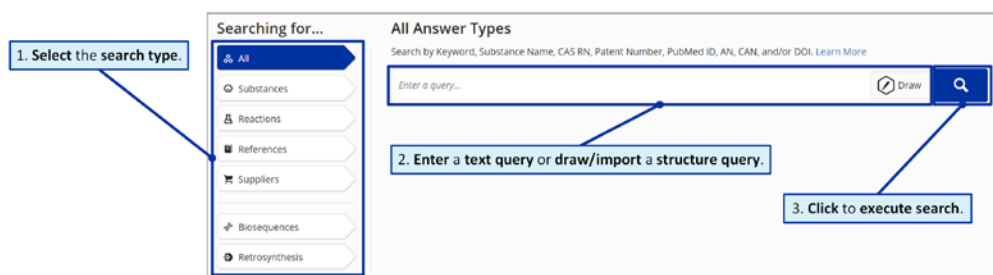
Log in using your CAS SciFinder<sup>®</sup> **Username** and **Password**.



## 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**.



## 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**

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

**Click property name to view more information on Substance Detail.**

**Select filters to focus results.**

**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.**

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

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

Filter Content Report

Download filter data from this result set.

## Substance Detail

### Substance Detail

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

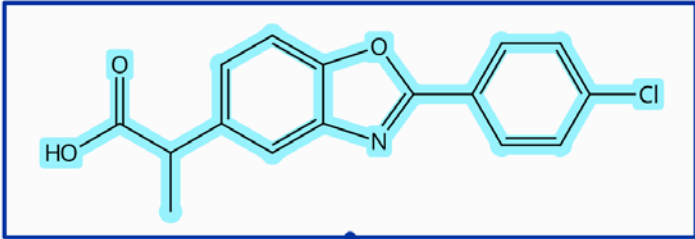
CAS Registry Number  
51234-28-7

Save detail.

Download detail.

Email detail.

Retrieve data related to substance.



C<sub>16</sub>H<sub>12</sub>ClNO<sub>3</sub>  
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 <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C

Click a property name or type to view expanded data below.

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 'References' section of the CAS SciFinder interface. On the left is a 'Filter Behavior' sidebar with categories like Document Type, Substance Role, Language, Publication Year, Author, Organization, Publication Name, Concept, CA Section, CAS Solutions, Formulation Purpose, Database, and Search Within Results. The main area shows a list of search results, with the first two results expanded to show their full text. The interface includes a top navigation bar with 'Substances', 'Reactions', and 'Citing' dropdowns. A 'Filtering' bar shows 'Document Type: 2 Selected' and 'Formulation Purpose: 2 Selected'. A 'Sort' dropdown is set to 'Relevance' and 'View' is set to 'Partial Abstract'. A 'Filter Content Report' section at the bottom left has a 'Download filter data from this result set.' button. Various callouts with arrows point to specific UI elements, providing instructions on how to interact with them.

**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** 1,086 Results

**Sort: Relevance** **View: Partial Abstract**

**Keep or remove selected results.**

**Change result display.**

**Select filters to focus results.**

**Sort results by relevance, times cited, accession number, or publication date.**

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

**Click to select result.**

**Click to open Reference Detail.**

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

**Click to access full-text viewing options.**

**Click to access patent information viewing options.**

Reference Detail

**Reference Detail** Retrieve data related to reference. Save detail.

Substances (3) Reactions (0) Citing (6) Citation Map Download detail. Email detail.

**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

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

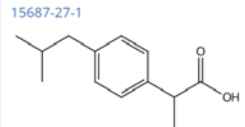
Priority Application

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

IPC Data  
 Concepts  
 Substances

Substances (3)

15687-27-1

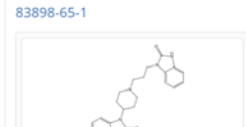


**C<sub>13</sub>H<sub>18</sub>O<sub>2</sub>**  
**Ibuprofen**

PatentPak

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

83898-65-1

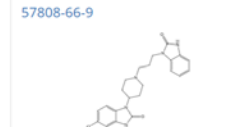


**C<sub>22</sub>H<sub>24</sub>ClN<sub>5</sub>O<sub>2</sub>·C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>**  
**Domperidone maleate**

PatentPak

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

57808-66-9



**C<sub>22</sub>H<sub>24</sub>ClN<sub>5</sub>O<sub>2</sub>**  
**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.** (Points to the References dropdown menu)

**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 removal icons)

**Clear All Filters** (Points to the Clear All Filters button)

**Filter Behavior**

**Filter by** | Exclude

**Yield**

- No Yield Available (29)

**Number of Steps**

- Experimental Procedures (47)

**Experimental Protocols**

- Synthetic Methods (29)
- Experimental Procedure (47)

**Reaction Type**

- Stereochemistry

**Reagent**

- Catalyst

**Solvent**

- Commercial Availability

**Reaction Notes**

- Search Within Results

**Source Reference**

- Document Type
- Language
- Publication Year
- Publication Name
- CA Section

**Filter Content Report**

Download filter data from this result set. (Points to the Download icon)

**1 Selected** | 29 Results

**Group: By Scheme** | **View: Expanded**

**Keep or remove selected results.** (Points to the selection icons)

**Group reactions by scheme or document.** (Points to the Group dropdown menu)

**Change result display.** (Points to the View dropdown menu)

**Suppliers (98)** | **Suppliers (78)** | **Suppliers (17)**

**View substance vendors.** (Points to the Suppliers buttons)

**Expand Scheme** | **View substance vendors.**

**Scheme 2 (1 of 1 Reaction Selected)**

**Click for options to view details, generate retrosynthesis plan, and edit/download structure file.** (Points to the reaction details area)

**Click to open reaction reference's detail page.** (Points to the Suppliers button)

**Reaction Summary** | Steps: 2

1.1 Reagents: [Sodium periodate](#)  
Catalysts: [Benzyltriethylammonium chloride](#)  
Solvents: [Dichloromethane](#), [Water](#); 10 °C; 1 h

1.2 1 min, 25 - 30 °C

1.3 Reagents: [Sodium cyanoborohydride](#)  
Solvents: [Dichloromethane](#); 0 °C; 0 °C → 30 °C; 0.5 - 1 h

2.1 Reagents: [Ammonium formate](#)

**Process for preparing varenicline, varenicline intermediates, and pharmaceutically acceptable salts thereof**

By: Shekhawat, Kundan Singh; et al  
World Intellectual Property Organization, WO2010023561 A1  
2010-03-04

**PatentPak** | **Full Text**

**Click to access full-text viewing options.** (Points to the PatentPak and Full Text buttons)

**Click to access patent information viewing options.** (Points to the PatentPak button)

**View reaction's detail page.** (Points to the View Reaction Detail button)

**View experimental procedure for reaction.** (Points to the Experimental Protocols button)

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

Reaction Detail

**Reaction Detail**

Chemical reaction scheme showing the synthesis of 2,3,4,5-tetrahydro-3-(phenylmethyl)-1,5-methano-1H-3-benzazepine from 1,2,3,4-tetrahydro-1,4-methanonaphthalene-2,3-diol and benzylamine.

**Callout Boxes:**

- Save detail.** (Save icon)
- Download detail.** (Download icon)
- Email detail.** (Email icon)
- View substance vendors.** (Suppliers (63) link)
- Click to open reaction reference's detail page.** (Reaction reference link)
- View alternative reactions for the same product.** (Alternative Steps (7) link)
- Click tabs to view steps in multi-step reactions.** (Step 1, Step 2 tabs)
- Click to access patent information viewing options.** (PatentPak, Full Text dropdowns)
- Click to access full-text viewing options.** (Full Text dropdown)
- Click tabs to view available experimental protocols.** (Synthetic Methods, Experimental Procedure tabs)

**Table: Reaction Conditions**

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

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



## 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.

Open product ordering page on supplier's website.

Order From Supplier

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

Open product information page on supplier's website.

Product Information

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.

Order From Supplier

Open product ordering page on supplier's website.

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

AstaTech Product List

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

Email [sales@astatechinc.com](mailto: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

Additional Contact Information

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

Fax 215-785-2656



## 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 instructional callouts:

- Refine sequence result bars by similarity.** Points to the 'Sequence Similarity' slider, which is set from 97% to 100%.
- Refine sequence result bars by patent keyword and simple legal status.** Points to the search filters on the left.
- Change how sequence result bars display.** Points to a bar style selection icon.
- Multiple CAS RNs Associated with this Sequence** (with a close button 'X') points to a detailed view of a sequence. Inside this view:
  - If present, click to view substances.** Points to a 'Substances' button.
  - Click to view relevant patents.** Points to a 'Patents' button.
- Queried sequence.** Points to a specific bar in the main visualization.
- Click a bar to view its patent count and sequence length.** Points to a bar in the main 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.

At the bottom of the interface, it says 'Powered by patSnap' and 'Copyright © 2022 American Chemical Society. All Rights Reserved. | 京ICP备13047075号-3'. There are also links for 'Help', 'Contact Us', and 'Legal'.

## 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 interface with several callout boxes:

- View and manage your saved Chemscape.** (Points to the top-left navigation icons)
- Group and refine Chemscape structures to show key information.** (Points to the top-left navigation icons)
- Add new structures to your Chemscape and indicate their position.** (Points to the top-left navigation icons)
- Refine your Chemscape by keyword or an exact match to a chemical structure.** (Points to the top-left navigation icons)
- Change how structure result bars display.** (Points to the 'Structural Similarity' slider)
- Queried sequence.** (Points to a specific bar in the visualization)
- Click a bar to view its structure and number of associated patents.** (Points to a bar in the visualization)
- Click to save your Chemscape for later access in MyChemscape.** (Points to the 'Save' button)
- Click to open Substance Detail page.** (Points to the substance detail panel)
- Click to view relevant patents.** (Points to the 'Patent Count' in the substance detail panel)
- Click the Select Structure button and then click-and-drag to select multiple structure results for viewing or a new Chemscape.** (Points to the 'Select Structure' button)

The substance detail panel for Olanarib (763113-22-0) includes:

- Patent Count:** 906
- Molecular Formula:** C<sub>24</sub>H<sub>29</sub>FN<sub>4</sub>O<sub>3</sub>
- SMILES:** c1ccc2c(c1)c(n[nH]c2=O)C(c3ccc(c(c3)C(=O)N4CCN(CC4)C(=O)C5CC5)F
- Synonyms:** 4-(3-(4-(Cyclopropanecarbonyl)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, KU 0059436, KU 59436, Lynparza, Piperazine, 1-(cyclopropylcarbonyl)-4-[5-[[3,4-dihydro-4-oxo-1-phthalazinyl]methyl]-2-fluorobenzoyl]-

## 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.**

**View Citing**

**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<sup>®</sup> Support

To access CAS SciFinder<sup>®</sup> 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<sup>®</sup>, please contact the **CAS Customer Center**:

- **Hours:** 8:00 a.m. to 12:30 a.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](mailto:help@cas.org)
- **Web:** <https://www.cas.org/contact>

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