Getting Started
with SciFinder Scholar™ 2006
for Mac OS X

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Welcome to SciFinder Scholar 2006 for Mac OS X! This guide provides information you need to start using SciFinder Scholar, a desktop research tool used to locate and process information on a wide variety of chemical and chemical science-related topics.

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SciFinder Scholar Features

Enhancements for SciFinder Scholar 2006 for Mac OS X include:

- Improved navigation – efficiently access Explore and Locate features
- Structure similarity searching – compare your query structure against all substances in the database, and retrieve those with the highest similarity scores
- New structure and reaction drawing tools:
  - Variable Attachment Position tool – define the attachment of a substituent to multiple points on a ring
  - Repeating Group tool – specify variable chain lengths and ring sizes
- "Pre-search" filters for structure searching – limit to:
  - Specific substance classes
  - Single-component substances
  - Commercially available substances
  - Substances with one or more associated references
  - Particular types of studies
- Query highlighting in reaction results – easily identify your query structure within reaction displays
- New visual indicators for related information – click on any substance in a reaction to quickly retrieve retro-synthetic information, references, substance details, commercial sources, and regulatory information
- Improved display of intermediate reaction steps – see all steps within multistep reactions in a single view
- Additional reaction content
  - View experimental conditions (e.g., time, temperature, pressure, pH), when reported, for reactions from 2003 to the present
  - See mixture ratios associated with product yields
  - View all isomers in a reaction
- Locate by Bibliographic Information – quickly find a specific reference using one or more pieces of bibliographic information, such as title words, author/inventor, journal name, publication date, or patent number
- Removal of duplicate references – quickly remove MEDLINE® records that are duplicates of CAplus[SM] records, or set a preference to omit duplicates automatically
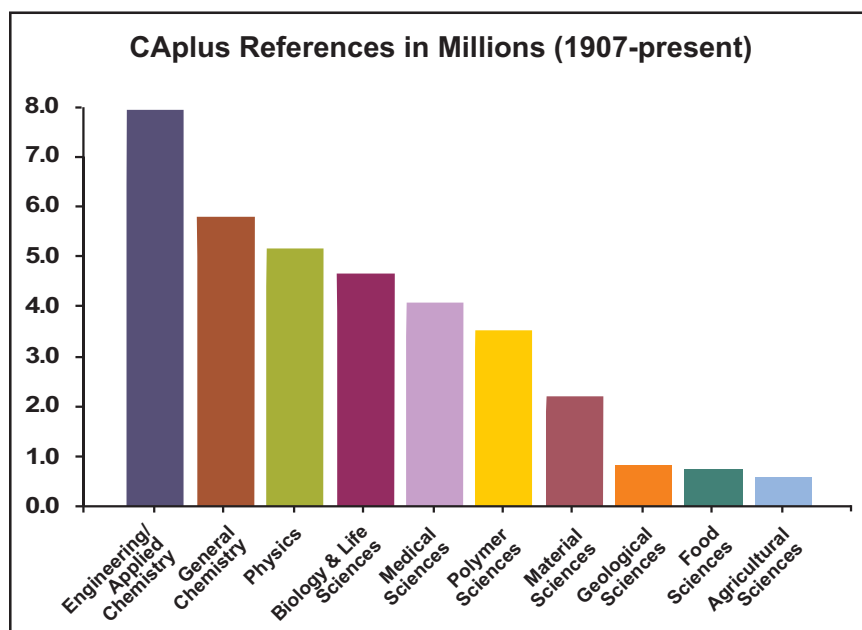
SciFinder Scholar also features:

- Exploring by Chemical Substance (including substructures), Reaction Structure, Research Topic, Author Name, Company Name or Organization, and more
- Sorting, analyzing, and refining answer sets
- Citation searching and linking
- Linking from substance answer sets to detailed records, references, commercial sources, regulatory information, and reactions
- Saving and printing results
- Accessing full-text documents via the ChemPort® Connection[SM]
- Browsing tables of contents of scientific journals
- Linking to Internet resources

SciFinder Scholar Content

SciFinder Scholar retrieves information contained in databases produced by Chemical Abstracts Service (CAS) as well as the MEDLINE database from the National Library of Medicine. All records are in English.

The CAplus database contains over 26 million documents from nearly 9,500 journals and 150 countries, covering literature from 1907 to the present with selected pre-1907 journal and patent references. Sources of the documents include journals, patents, conference proceedings, dissertations, technical reports, books, and more. Patents originate from over 50 active patent-issuing authorities. CAplus covers a wide spectrum of science-related information, including chemistry, biology, engineering, and related sciences.

CAplus References in Millions (1907-present)

Category	References (Millions)
Engineering/Applied Chemistry	7.9
General Chemistry	5.8
Physics	5.1
Biology & Life Sciences	4.6
Medical Sciences	4.0
Polymer Sciences	3.5
Material Sciences	2.2
Geological Sciences	0.8
Food Sciences	0.7
Agricultural Sciences	0.6

The MEDLINE database covers biomedical literature from more than 4,780 journals and 70 countries. MEDLINE, which includes data from the former OLDMEDLINE database, contains more than 16 million biomedical citations from 1950 to the present. MEDLINE also contains IN-PROCESS records, the most current documents before they have been completely indexed for inclusion in MEDLINE.

In addition to the vast literature sources, the CAS REGISTRY[SM] database provides you with access to more than 28 million organic and inorganic compounds and more than 57 million sequences. From these records, you may access structure diagrams, names, molecular formulas, properties, and more.

The CASREACT® database gives you access to reaction information for more than 10 million single- and multiple-step reactions from journals and patents from 1840 to the present. SciFinder displays reaction diagrams, including structures for reactants, reagents, and products, as well as reference information.

For many substances, you may obtain chemical source and regulatory information from the CHEMCATS® and CHEMLIST® databases. Chemical source information, including supplier addresses and pricing information, for more than 10 million substances is derived from over 900 chemical catalogs and libraries. Over 239,000 regulatory information records from 1979 to the present provide access to substance identity information, inventory status, sources of information, and compliance information.

For more information about the databases and their content, visit the CAS web site at www.cas.org.

The information you can find in SciFinder Scholar includes:

- **Document Information**
  - Title
  - Author/inventor
  - Company name/corporate source/patent assignee
  - Publication year
  - Source, publication, date, publisher, volume, issue, pagination, CODEN, ISSN
  - Patent identification, including patent, application, priority, and patent family information
  - Abstract
  - Indexing
  - Supplementary terms
  - Citations
  - Substances and reactions discussed within the document

- **Substance Information**
  - Chemical names
  - CAS Registry Numbers®
  - Molecular formulas
  - Structure diagrams
  - Sequence information, including GenBank® and patent annotations
  - Property data
  - Commercial source information from chemical substance supplier catalogs
  - Regulatory information
  - Editor notes
  - Documents in which the substance is referenced
  - Reactions in which the substance participates
  - A list of other publicly available databases from the STN online service, where additional information related to the substance may be located

- **Reaction Information**
  - Reaction diagrams, including reactants, reagents, products, catalysts, solvents, and conditions
  - Document in which the reaction is referenced
  - Additional reactions, references, substance details, commercial sources, and regulatory information for all reaction participants

SciFinder Substructure Module

You have the option to purchase the SciFinder Substructure Module (SSM). The module allows you to:

- Search your query as a substructure of a more complex structure
- Conduct a similarity search
- Draw variables and R-groups, i.e., lists of atoms, shortcuts, and/or variables
- Prohibit substitution and ring fusion at particular nodes and bonds
- Preview results to estimate the number of answers and view sample answers
- Draw stereo bonds and automatically analyze answers in terms of the specified stereo features
- Analyze your answers by precision as part of your initial search
- Analyze answers by real-atom attachments, variable group composition, and R-group composition
- Refine structure answer sets by property data

Hardware and Software Requirements

Computer: Macintosh computer with an Intel x86 or PowerPC G4 or G5 processor.

- Mac® OS X (10.2 or higher)
- Minimum of 40-50 MB of available hard disk space
- TCP/IP network-level connection to CAS via the Internet, Z39.50 application-level connection to CAS through port 210
  [Accessing full text via ChemPort and online Help files on the CAS server requires an HTTP application-level connection through port 80.]

Monitor: 13" or larger color monitor capable of displaying 256 colors

Printer: High-quality graphics printer, e.g., laser or inkjet, recommended

Optional Software

Web Browser: Safari® (OS X Default) or a Mac OS X compatible version of Netscape®, Mozilla Firefox™, Microsoft® Internet Explorer (MSIE), or Opera®. A web browser is needed to access full text via ChemPort, online Help, and Internet resources within the **Tools** menu.

- Java™ and JavaScript™ must be enabled for online Help and some features within ChemPort.
- Cookies must be accepted for some features in ChemPort.

Adobe® Reader®: Version 5.0.5 or higher and compatible with your version of Mac OS X. The Reader is needed to access PDF documents available via the CAS web site and ChemPort. Adobe Reader can be downloaded at www.adobe.com.

Note: Apple Preview may also be used to view PDF documents.

Starting SciFinder Scholar

The Site Admininistrator for your organization has access to installation information. Please work with your Site Administrator to install SciFinder Scholar 2006 for Mac OS X. Once it is installed properly, you can log on and begin searching.
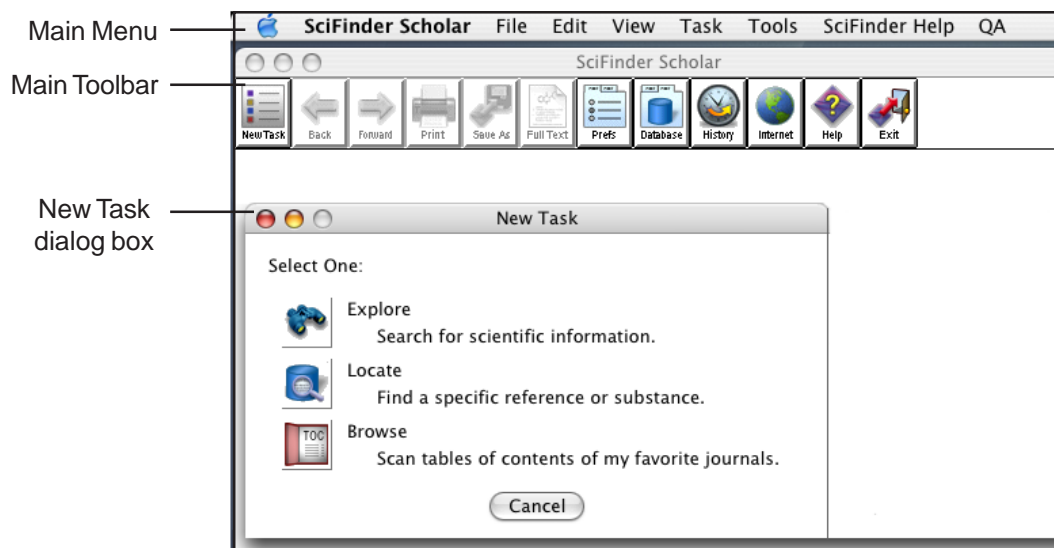
To start SciFinder Scholar:

1. Double-click the SciFinder Scholar icon created during installation or on the Desktop or Dock alias if you have created one.

    The SciFinder Scholar splash screen displays, followed by the License Agreement.

2. If you agree to the terms, click **Accept** to begin searching.
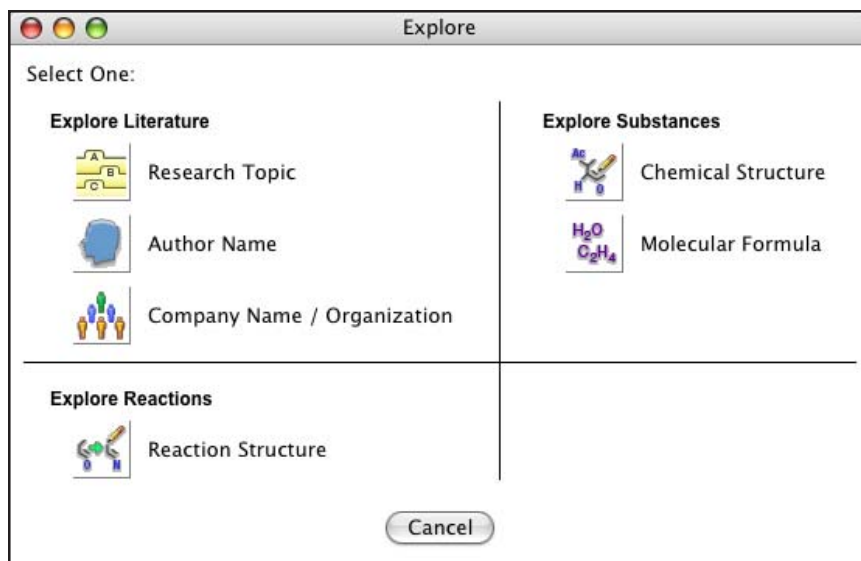
    The main SciFinder Scholar window displays. It contains the Main Menu, Main Toolbar, and New Task dialog box.

3. Select one of the options from the New Task dialog box.
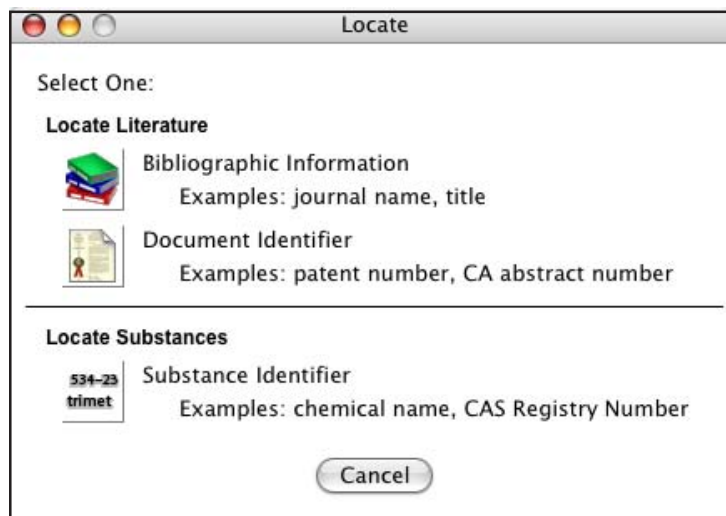
Explore

Explore allows you to look for scientific information in the CAS databases as well as the MEDLINE database.

Click the icon for the task you want to perform. SciFinder Scholar prompts you for the appropriate information to conduct your search. For details about the Explore features, see the SciFinder Scholar online Help.

Locate

Locate allows you to quickly find a specific reference based on one or more pieces of bibliographic information or a document identifier. It also lets you search for specific substances by using a name or CAS Registry Number.

Click the icon for the task you want to perform. SciFinder Scholar prompts you for the appropriate information to conduct your search. For details about the Locate features, see the SciFinder Scholar online Help.

Browse

Browse allows you to scan a list of over 1,900 key scientific journals covered by the CAS databases. You can view the tables of contents and link to full-text options for selected journals.
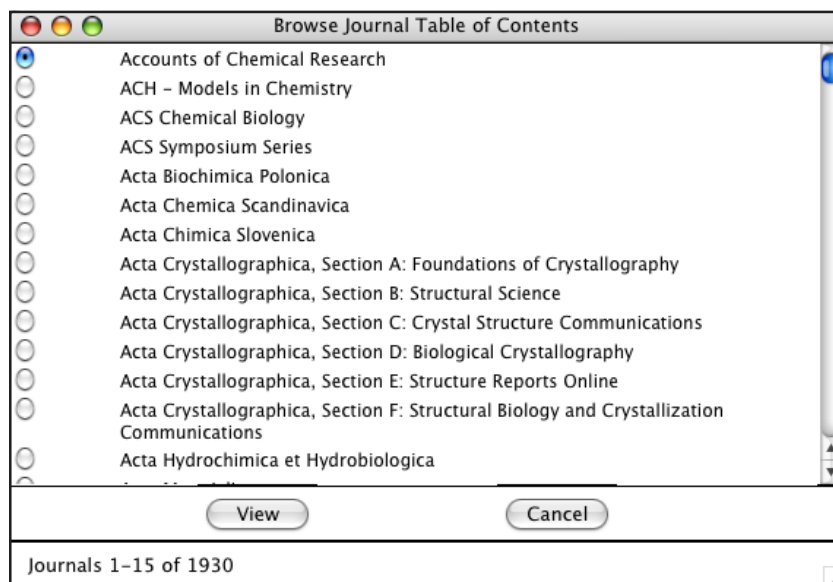
To view a table of contents, select a journal. Then click **View**. For details about the Browse feature, see the SciFinder Scholar online Help.

SciFinder Scholar Help and Resources

SciFinder Scholar Online Help

Comprehensive Help files that include search tips, troubleshooting information, and links to "how to" examples are provided within SciFinder Scholar.

To access the Help files, click the **Help** button located on the Main Toolbar. Or, select **SciFinder Help** from the **SciFinder Help** menu.

SciFinder Scholar Web Sites

For more information about SciFinder Scholar, visit www.cas.org/ SCIFINDER/SCHOLAR/. Click the **SciFinder Scholar Resources** link to access easy-to-follow examples and tips to help make your exploration with SciFinder Scholar more productive.

To quickly access these and other SciFinder Scholar resources, click the **Internet** button on the Main Toolbar or select an Internet option from the **Tools** menu. Select the resource of interest, and click **OK**.

Additional Support

If you have questions, need technical assistance, or have suggestions concerning SciFinder Scholar, please contact your Site Administrator.