

# Getting Started with SciFinder<sup>®</sup> Scholar<sup>™</sup> (2004 Edition)

*for Windows and Macintosh*

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# Getting Started with SciFinder® Scholar™ (2004 Edition)

Welcome to the 2004 Edition of SciFinder Scholar! 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 science-related topics.

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## SciFinder Scholar Features

Enhancements for SciFinder Scholar (2004 Edition) include:

- Limit structure searches “up front” by including or excluding particular substance classes
- Refine substance answer sets by:
  - Presence or absence of isotopically labeled atoms
  - Presence or absence of metals
  - Availability of specified properties
  - Reference availability
- Get reactions from a substance answer set
- Limit reaction searches “up front” by:
  - Patent/Non-patent literature
  - Publication Year
  - Number of Steps
  - Language
  - Reaction Classification
- View reactions in Compact, Standard, or the enhanced Full format
- Analyze reaction answer sets by:
  - Catalyst
  - Number of Steps in Reaction
  - Solvent
  - Product Yield
  - Author
  - Journal Name
  - Company/Organization
  - Language
  - Document Type
  - Publication Year

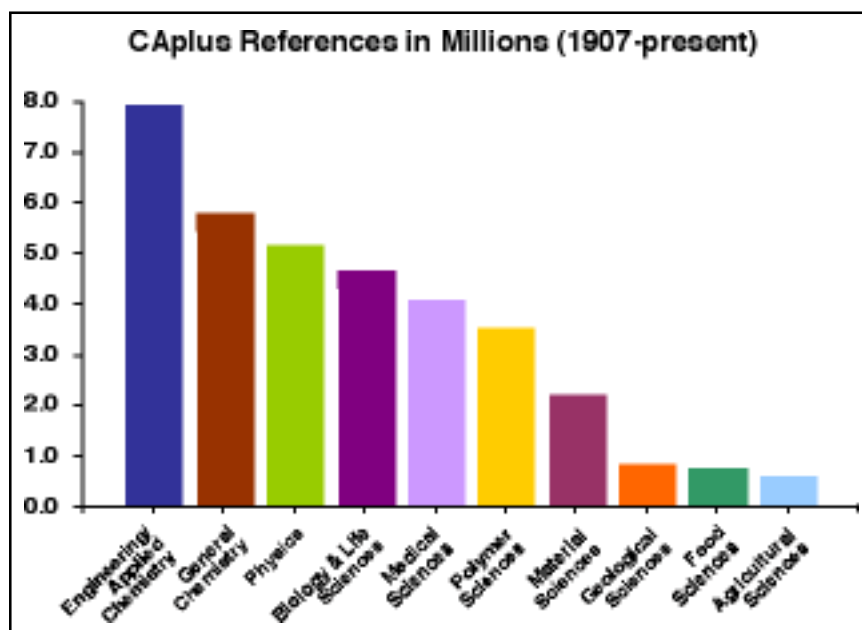
SciFinder Scholar also features:

- Exploring by Chemical Substance (including full reactions and substructures), Research Topic, Author Name, Document Identifier, and Company Name or Organization
- Sorting, analyzing, and refining reference and structure answer sets
- Refining reaction answer sets
- Citation searching and linking
- Linking from substance answer sets to detailed substance records, references, 3D models, commercial sources, regulatory information, and reactions
- Saving and printing results
- Accessing full-text documents via the ChemPort® Connection<sup>SM</sup>
- Linking to substance records, commercial sources, regulatory information, and 3D models
- 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 CPlus<sup>SM</sup> database contains over 23 million documents from more than 9000 journals and 150 countries, covering literature from 1907 to the present. Sources of the documents include journals, patents, conference proceedings, dissertations, technical reports, books, and more. Patents number over 4.1 million and originate from over 45 active patent-issuing authorities. CPlus covers a wide spectrum of science-related information, including chemistry, biology, engineering, and related sciences.



The MEDLINE database covers biomedical literature from more than 3900 journals and 70 countries. MEDLINE, which includes data from the former OLDMEDLINE database, contains more than 13 million biomedical citations from 1958 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, CAS's REGISTRY<sup>SM</sup> database provides you with access to more than 22 million organic and inorganic compounds and more than 32 million sequences. From these records, you may access structure diagrams, names, molecular formulas, properties, and more.

The CASREACT<sup>®</sup> database gives you access to reaction information for more than 7 million single- and multiple-step reactions from journals and patents from 1907 to the present. SciFinder Scholar 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<sup>®</sup> and CHEMLIST<sup>®</sup> databases. Chemical source information, including supplier addresses and pricing information, for over 6 million substances is derived from over 700 chemical catalogs and libraries. Over 230,000 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 <http://www.cas.org>.

The information you can find with 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, and solvents
- Document in which the reaction is referenced
- Additional reactions, references, substance details, commercial sources, and regulatory information for all reaction participants

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## Optional Features

Optional features for SciFinder Scholar are briefly described below. For more information, see the SciFinder Scholar online Help files.

### SciFinder Substructure Module

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

- Draw a structure query and search it as a substructure of a more complex structure
- Draw variables and R-groups, i.e., nodes that allow multiple substituents
- Prohibit substitution and ring fusion at particular nodes and bonds
- Limit your search “up front” to specified substance classes
- 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

### 3D Structure Modeling

Windows users may use Discovery Studio™ Viewer products (ViewerPro or ViewerLite) from Accelrys along with SciFinder Scholar to view 3D structure models. The Viewer products are high-end molecular visualization applications that allow models to be manipulated for better understanding of 3D structure.

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## Hardware and Software Requirements

### Windows®

**Computer:** An IBM® or compatible PC with at least a Pentium processor

- Microsoft® Windows® 95, 98, Me, 2000, XP, or NT 4.0
- Minimum of 32 MB (RAM) memory for Windows 95, 98, Me, or NT 4.0, 64 MB or higher recommended; Minimum of 64 MB memory for Windows 2000 or XP, 128 MB (RAM) or higher recommended for XP
- Minimum of 30 MB of available hard disk space (not including pagefile memory), 50 MB recommended
- 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:** SVGA color monitor; minimum 800x600 screen resolution, 1024x768 or higher recommended; minimum of 256 colors

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

### Macintosh®

**Computer:** An Apple® Macintosh® or compatible with a PowerPC processor

- System 7.6.1 or higher, Mac® OS 8.x, OS 9.x, or OS X (in OS 9 Classic mode)
- Minimum 15 MB (RAM) memory, 17 MB or higher recommended
- Minimum 30-40 MB of available hard disk space; this number will vary with different systems and may be larger for larger hard drives
- 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

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## Optional Software

**Internet Browser:** Netscape® Navigator or Communicator or Microsoft® Internet Explorer (MSIE), version 4.0 or higher. An Internet browser is needed to access full text via ChemPort, online Help, and Internet resources within the **Tools** menu.

- For Windows, a Netscape plug-in must be installed in the Netscape plug-ins folder for some of the features in ChemPort, e.g., Reference Linking. The plug-in is installed automatically during the SciFinder Scholar (2004 Edition) installation.
- Java™ and JavaScript must be enabled for online Help and some features within ChemPort.
- ActiveX must be enabled in MSIE for ChemPort Reference Linking.
- Cookies must be accepted for some features in ChemPort.

**Adobe® Acrobat® Reader™:** Version 4.0 or higher. The Reader is needed to access the PDF documents available via the CAS web site and ChemPort. Acrobat Reader can be downloaded at <http://www.adobe.com>.

**Discovery Studio™ ViewerPro or ViewerLite:** Windows version 3.5 or higher. Discovery Studio Viewer products from Accelrys are visualization tools that allow you to view 3D molecular models for structure results.

- DS ViewerPro may be obtained from Accelrys at [http://www.accelrys.com/dstudio/ds\\_viewer/](http://www.accelrys.com/dstudio/ds_viewer/).
- ViewerLite is no longer supported by Accelrys but may be obtained free of charge from CAS at <http://my.cas.org>. ViewerLite is provided "AS IS", without warranties of any kind.

## Starting SciFinder Scholar

The Site Administrator for your organization has access to installation information. Please work with the Site Administrator to install SciFinder Scholar (2004 Edition). Once it is installed properly, you can log on and begin searching.

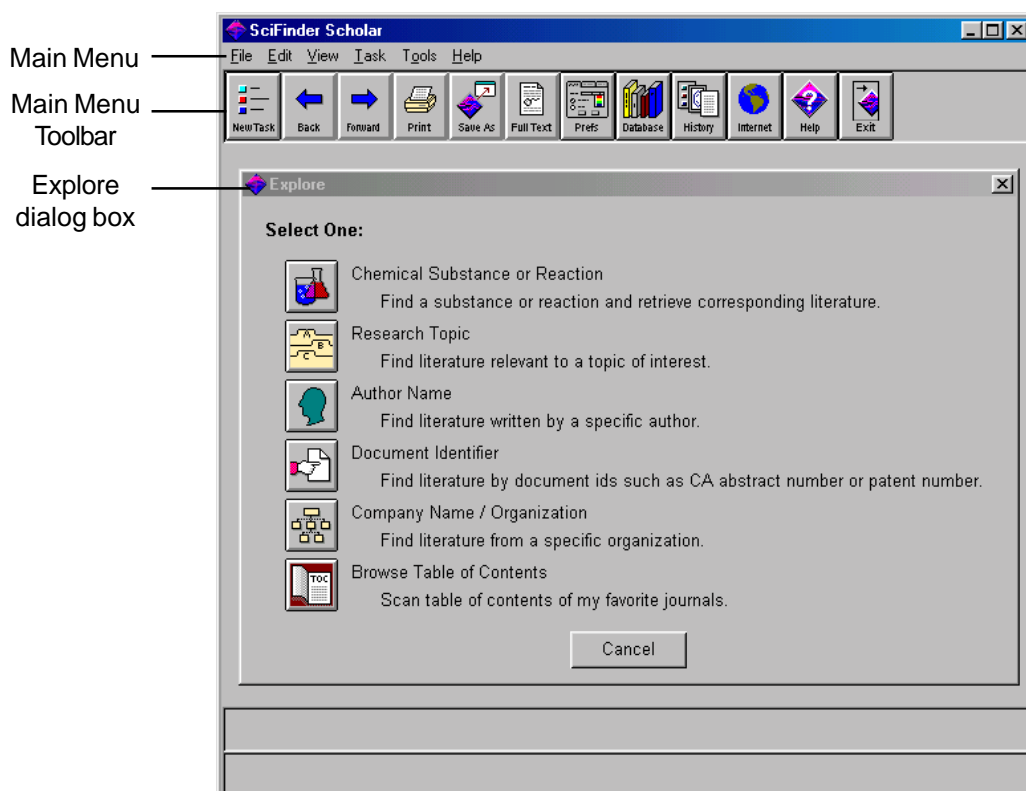
To start SciFinder Scholar:

1. Double-click the SciFinder Scholar icon created during installation. Or, Windows users may select **Start > Programs > SciFinder Scholar 2004 Edition**.

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 Menu Toolbar, and **Explore** dialog box.

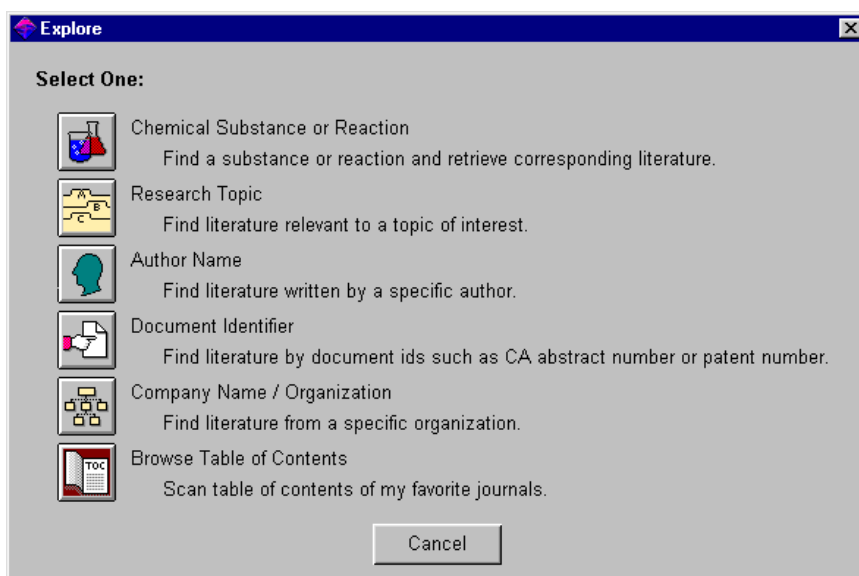


3. Select one of the options from the **Explore** dialog box.

## Explore

Explore allows you to look for scientific information dating from 1907 to present in the CAS databases as well as information dating from 1958 to present in the MEDLINE database. You may choose to explore by:

- Chemical Substance or Reaction (see page 13)
- Research Topic
- Author Name
- Document Identifier
- Company Name/Organization
- Browse Table of Contents (see page 14)



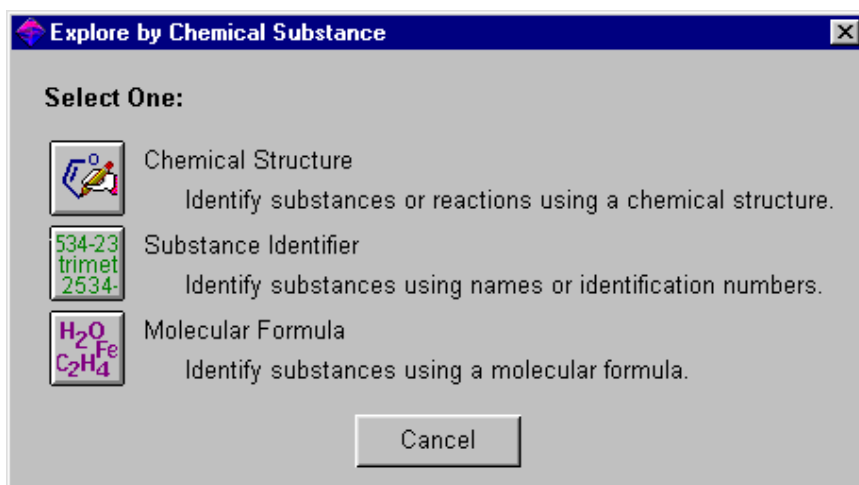
Click the icon for the task you want to perform. SciFinder Scholar prompts you for the appropriate information to conduct your search. For more details about the Explore feature, see the SciFinder Scholar online Help files.

## Explore by Chemical Substance or Reaction

SciFinder Scholar offers you three ways to retrieve chemical substances and reactions:

- Chemical Structure
- Substance Identifier, e.g., a CAS Registry Number
- Molecular Formula

To access the Explore by Chemical Substance options, click the **Chemical Substance or Reaction** icon from the **Explore** dialog box.

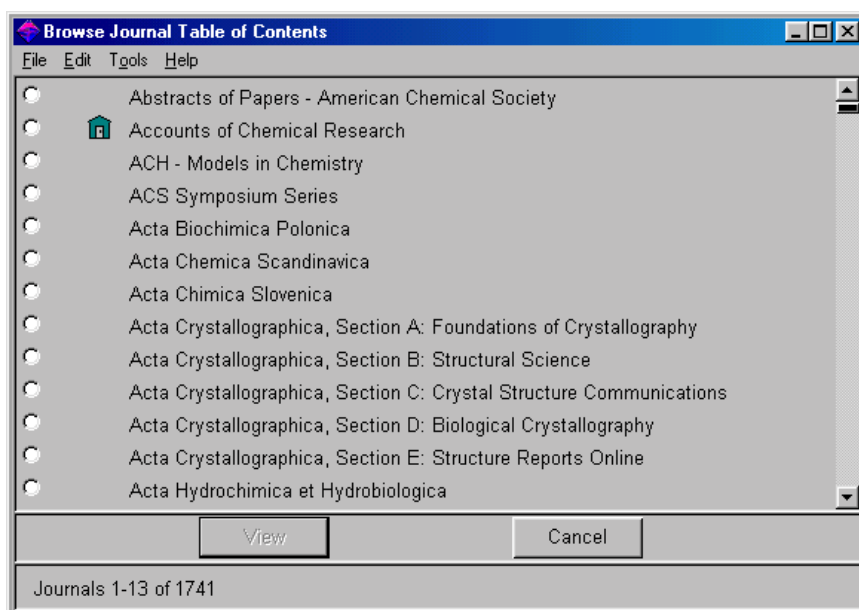


Click the icon for the task you want to perform. SciFinder Scholar prompts you for the appropriate information to conduct your search. For more details about Explore by Chemical Substance or Reaction, see the SciFinder Scholar online Help files.

## Browse Table of Contents

Browse Table of Contents allows you to scan a list of more than 1700 key scientific journals covered by the CAS databases. You can view the tables of contents and link to full-text options for selected journals. If your SciFinder Scholar Site Administrator has set up a list of in-house journals, a **house** icon displays next to those journals.

To access Browse Table of Contents, click the **Browse Table of Contents** icon from the **Explore** dialog box.



Select a journal. Then click **View** to begin browsing tables of contents for the journal. For more details about Browse Table of Contents, see the SciFinder Scholar online Help files.

## SciFinder Scholar Help and Resources

### SciFinder Scholar Online Help Files

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

To access the Help files, click the **Help** button located on the Main Menu Toolbar. Or, select **SciFinder Scholar Help** from the **Help** menu (Windows) or **SciFinder Help** menu (Macintosh). The main SciFinder Scholar Help window is displayed.

In Windows, pressing <F1> brings up context-specific helps.

### SciFinder Scholar Web Sites

For more information about SciFinder Scholar, visit <http://www.cas.org/SCIFINDER/SCHOLAR>. Click the **SciFinder Scholar Resources** link to access easy-to-follow search examples and SciFinder Scholar Solutions - a series of instructional 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 Menu 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.