

Getting Started with SciFinder Scholar™ 2006

for Windows®

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Welcome to SciFinder Scholar 2006! 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 2006 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 CPlusSM records, or set a preference to omit duplicates automatically

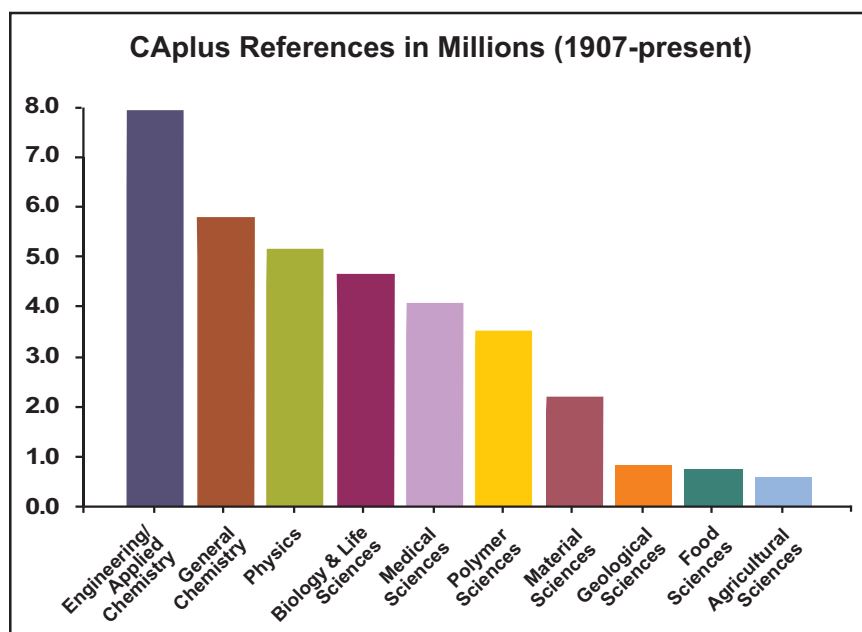
SciFinder Scholar also features:

- Exploring by Chemical Structure (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 answers to detailed records, references, 3D models, commercial sources, regulatory information, and reactions
- Saving and printing results
- Accessing full-text documents via the ChemPort® ConnectionSM
- 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 database contains over 25 million documents from nearly 9,500 journals and 150 countries, covering literature from 1907 to the present plus over 21,600 pre-1907 journal records. Sources of the documents include journals, patents, conference proceedings, dissertations, technical reports, books, and more. Patents originate from over 50 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 4,780 journals and 70 countries. MEDLINE, which includes data from the former OLDMEDLINE database, contains more than 15 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 vast literature sources, the CAS REGISTRYSM database provides you with access to more than 26 million organic and inorganic compounds and more than 56 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 9.2 million single- and multiple-step reactions from journals and patents from 1840 to the present. SciFinder Scholar displays reaction diagrams, including structures for reactants, reagents, products, and reaction conditions, as well as reference information.

For many substances, you can obtain chemical source and regulatory information from the CHEMCATS[®] and CHEMLIST[®] databases. Chemical source information, including supplier addresses and pricing information, for nearly 9 million substances is derived from over 900 chemical catalogs and libraries. Over 238,000 regulatory information records from 1979 to 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.

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 in which 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

Optional Features

Optional features for SciFinder Scholar are briefly described below. For details about the features, see the SciFinder Scholar online Help.

SciFinder Substructure Module

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

- Search your query structure 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

3D Structure Modeling

Discovery Studio™ Viewer products (DS ViewerPro or DS ViewerLite) from Accelrys may be used 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.

Hardware and Software Requirements

Computer: PC with at least a Pentium-class or equivalent processor

- Microsoft® Windows® 98, Me, 2000, XP, or NT 4.0
- Minimum of 32 MB (RAM) memory for Windows 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 70 MB of available hard disk space (not including pagefile memory), 80-85 MB recommended (minimum 150 MB needed for installation)

For the SciFinder Scholar Toolbar for Microsoft Internet Explorer, an additional 25 MB of available disk space is needed (75 MB needed for installation).

(This assumes Microsoft .NET software is already installed.)

- TCP/IP network-level connection to CAS via the Internet, Z39.50 application-level connection to CAS through port 210
Accessing full text via the ChemPort® ConnectionSM 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

Additional Software

Web Browser: Microsoft® Internet Explorer (MSIE), version 4 or higher, Netscape® Navigator or Communicator, version 4 or higher, or Mozilla Firefox™, version 1.0

A web browser is needed to access full text via ChemPort, online Help, and Internet resources within the Tools menu.

- Plug-ins must be installed in the Netscape and Firefox plug-ins and components folders for some features in ChemPort, e.g., Reference Linking. The plug-ins are installed automatically during the SciFinder Scholar 2006 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® Reader®: Version 4.0 or higher

Adobe Reader is needed to display PDF documents available via the CAS web site and ChemPort. The Reader can be downloaded at 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 www.accelrys.com/products/dstudio/.
- DS ViewerLite is no longer supported by Accelrys but may be obtained free of charge from CAS at my.cas.org. DS ViewerLite is provided "AS IS", without warranties of any kind.

After installation of DS ViewerPro or DS ViewerLite, run the program once to ensure that it creates Windows Registry entries that will be used by SciFinder Scholar to display 3D models.

Starting SciFinder Scholar

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

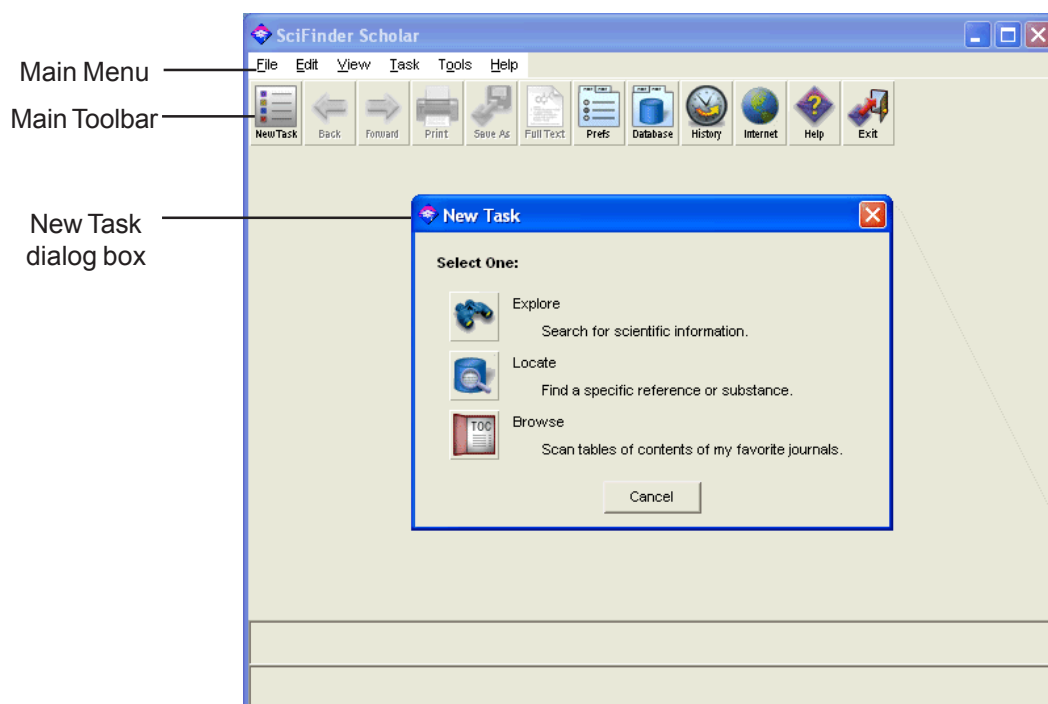
To start SciFinder Scholar:

1. Double-click the SciFinder Scholar icon created during installation. Or, select **Start > Programs > SciFinder Scholar 2006**.

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

2. If you agree to the terms, click **Accept** to begin searching.

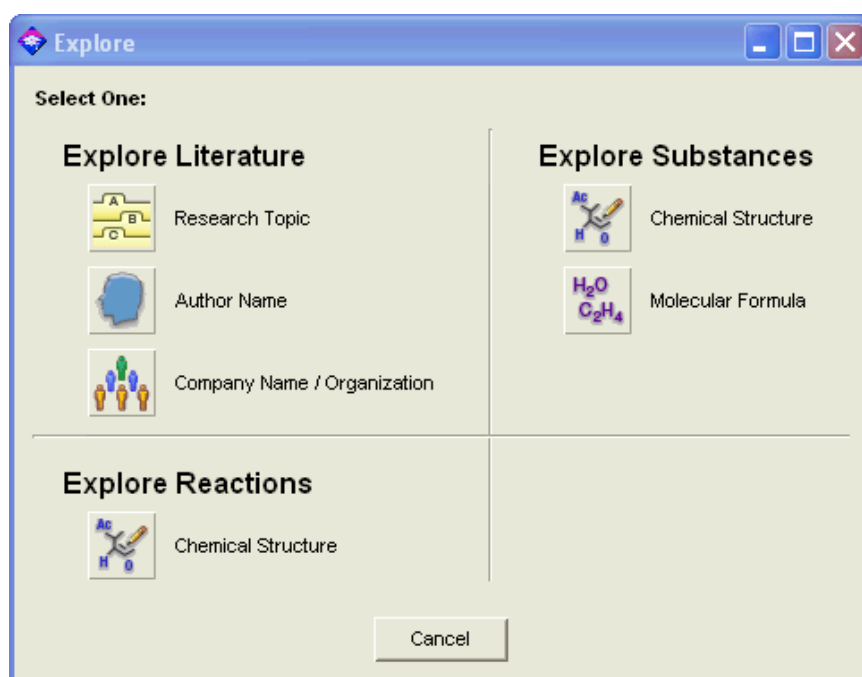
The main SciFinder Scholar window displays. It contains the Main Menu, Main Toolbar, and New Task dialog box.



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

Explore

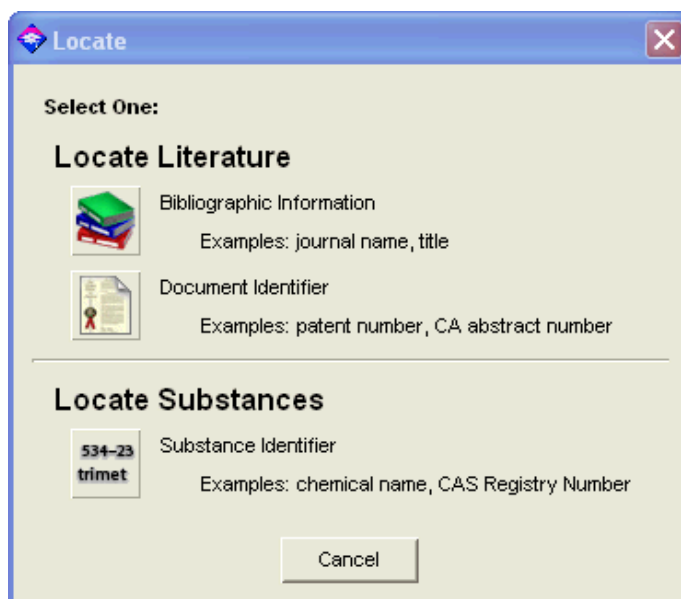
Explore allows you to retrieve scientific information in the CAS databases as well as the MEDLINE database.



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

Locate

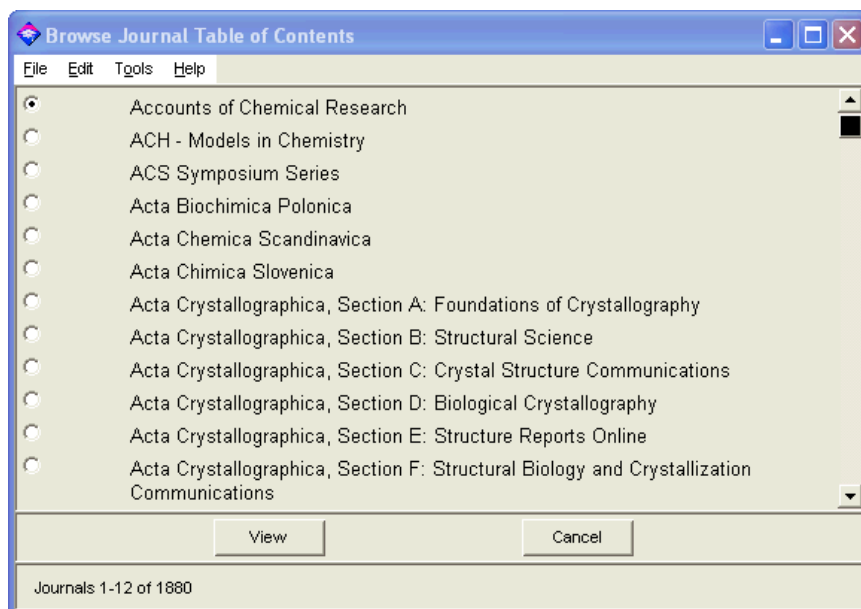
Locate allows you to quickly find a specific reference based on one or more pieces of bibliographic information or a document identifier. It also lets you search for specific substances by using a name or CAS Registry Number.



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 nearly 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 Scholar Help** from the **Help** menu.

Press <F1> to bring up context-specific helps.

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.