Getting Started with SciFinder Scholar[™] 2007

for Windows®

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Getting Started with SciFinder Scholar[™] 2007

Welcome to SciFinder Scholar 2007! 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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This document describes SciFinder Scholar for Windows. For Mac OS X version of this document, visit the SciFinder Scholar Support Information at www.cas.org.

SciFinder Scholar Features

Enhancements for SciFinder Scholar 2007 include:

- Combine two answer sets of the same kind: reference, substance, or reaction
- Access journal titles
 - View full journal titles in Analyze by Journal Name histograms
 - Include abbreviated and full journal titles in Tagged and Quoted Save As formats
- Explore or Refine from a substance display by inserting a copied structure directly into the Structure Drawing window
- Export commercial source information to Microsoft Excel[®]
- Print substance records in grid format

SciFinder Scholar also features:

- Exploring by Chemical Structure (including substructures, with SSM), Reaction Structure, Research Topic, Author Name, Company Name or Organization, and more.
- Removal of duplicate references
- 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 **CAplusSM** database includes more than 27 million document records from nearly 9,500 journals and 150 countries from the late 19th century to the present. Document sources include journals, patents, conference proceedings, research disclosures, books, dissertations, technical reports, and more. The more than 5 million patent records are from over 50 active patent-issuing authorities. CAplus covers a broad spectrum of scientific and technical information from chemistry, biology, physics, engineering, and related sciences.

The **MEDLINE** database, which also includes OLDMEDLINE, covers biomedical literature from more than 4,780 journals and 70 countries. The database includes more than 16 million biomedical document records from 1950 to the present. MEDLINE also includes IN-PROCESS records, which have not been completely indexed, covering the most current documents in MEDLINE.

The **CAS REGISTRYSM** database provides you with access to more than 31 million searchable structures along with over 58 million biosequences. For these records, you may access structure diagrams, names, molecular formulas, properties, and more.

The **CASREACT**[®] database provides access to more than 13 million single and multistep organic reactions from 1840 to the present. SciFinder displays reactions including the reactants, reagents, products, catalysts, solvents, reaction conditions, and reference information.

For more than 13 million substances, you may obtain chemical source information from the **CHEMCATS**[®] database. Chemical source information, including supplier addresses, is derived from more than 900 chemical catalogs and libraries. Regulatory information for more than 245,000 substances from 1979 to the present is available from the **CHEMLIST**[®] database, including substance identity information, inventory status, sources of information, and compliance information.

For more information about the databases and their content, visit <u>www.cas.org</u>.

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
- Documents in which the reaction is referenced
- Additional reactions, references, substance details, commercial sources, and regulatory information for all reaction participants
- 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

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[™] visualization products from Accelrys may be used along with SciFinder Scholar to view 3D structure models. These molecular visualization applications allow models to be manipulated for better understanding of 3D structure.

Hardware and Software Requirements

Computer: PC with at least a 450 MHz Pentium-class or equivalent processor

Operating System: Microsoft[®] Windows[®] 2000 (SP3 or higher), XP (SP1 or SP2), or Vista

Memory: 256 MB RAM

Available Hard Disk Space: 50 MB (not including pagefile memory); 90 MB for installation.

For the SciFinder Scholar Toolbar, an additional 25 MB is needed; 75 MB for installation. This assumes Microsoft .NET software is already installed.

Connection: 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; 1024x768 screen resolution; 16 bit (64,000) colors

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

Additional Software

Web Browser: Microsoft[®] Internet Explorer (MSIE), version 5 or higher, Netscape[®], version 7 or higher, or Mozilla Firefox[™], version 1.0 or higher

A web browser is needed to access full text, 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 2007 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 5.0 or higher

Adobe Reader is needed to display PDF documents available via the CAS web site and ChemPort. The Reader can be downloaded at <u>www.adobe.com</u>.

Microsoft® Excel®: Excel 97,2000, 2002, 2003, or 2007

Excel is neeeded for the Export CHEMCATS[®] data to Microsoft[®] Excel[®] feature.

Discovery Studio[™] Visualizer and ViewerLite

Discovery Studio[™] visualization products from Accelrys are tools that allow you to view 3D molecular models for structure results.

- DS Visualizer may be obtained from Accelrys at www.accelrys.com/products/downloads/ds_visualizer/.
- SciFinder Scholar is compatible with Discovery Studio Visualizer up to version 1.5.
- ViewerLite is no longer supported by Accelrys, Inc. but, for a limited time, may be downloaded free of charge by SciFinder Scholar customers. ViewerLite is provided "AS IS", without warranties of any kind.

A software patch is available that corrects the viewing of 3D models with ViewerLite version 5.0. After downloading and unzipping the patch, read the *MDMReadme.txt* file for instructions.

Starting SciFinder Scholar

The Site Admininistrator for your organization has access to installation information. Please work with your Site Administrator to install SciFinder Scholar 2007. Once it is installed properly, you can log on and begin searching.

To start SciFinder Scholar:

 Double-click the SciFinder Scholar icon created during installation. Or, select Start > Programs > SciFinder Scholar 2007.

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

2. If you agree to the terms, click Accept.

A "Message of the Day" window opens. Click **OK** to proceed.

You are now ready 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 2,000 key scientific journals covered by the CAS databases. You can view the tables of contents and link to full-text options for selected journals.

🧇 В	rowse Journal Table of Contents	
<u>F</u> ile	<u>E</u> dit T <u>o</u> ols <u>H</u> elp	
0	Accounts of Chemical Research	_
0	ACH - Models in Chemistry	
0	ACS Chemical Biology	
0	ACS Symposium Series	
0	Acta Biochimica Polonica	
0	Acta Chemica Scandinavica	
0	Acta Chimica Slovenica	
0	Acta Crystallographica, Section A: Foundations of Crystallography	
0	Acta Crystallographica, Section B: Structural Science	
0	Acta Crystallographica, Section C: Crystal Structure Communications	
0	Acta Crystallographica, Section D: Biological Crystallography	
0	Acta Crystallographica, Section E: Structure Reports Online	
0	Acta Crystallographica, Section F: Structural Biology and Crystallization	-
	View Cancel	
Jou	rnals 1-13 of 1991	

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 helps.

SciFinder Scholar Web Sites

For more information about SciFinder Scholar, visit <u>www.cas.org</u>. SciFinder Scholar resources provide easy-to-follow examples and tips to help make your exploration with SciFinder 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

For questions, technical assistance, or suggestions concerning SciFinder Scholar, please contact your Site Administrator.