SciFinder Scholar 2001 User Guide

for Windows and Macintosh

October 2001

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1 Getting Started

Welcome to the *SciFinder Scholar User Guide*. Chapter 1 provides information you need to get started:

- SciFinder Scholar features and content
- SciFinder Scholar web site addresses
- Optional features and modules
- Hardware and software requirements
- Technical support information
- Descriptions of the User Guide and Online Help

SciFinder Scholar Features

SciFinder Scholar, a desktop research tool used to locate and process information on a wide variety of chemical and science-related topics, has been enhanced to include:

- User Preferences kept for an individual session
- Property data for 4 million druglike substances
- Citation searching
- Get Substances from reference answer sets
- Links to eScience®, a dynamic web resource from CAS®
- Additional reaction information with coverage back through 1975

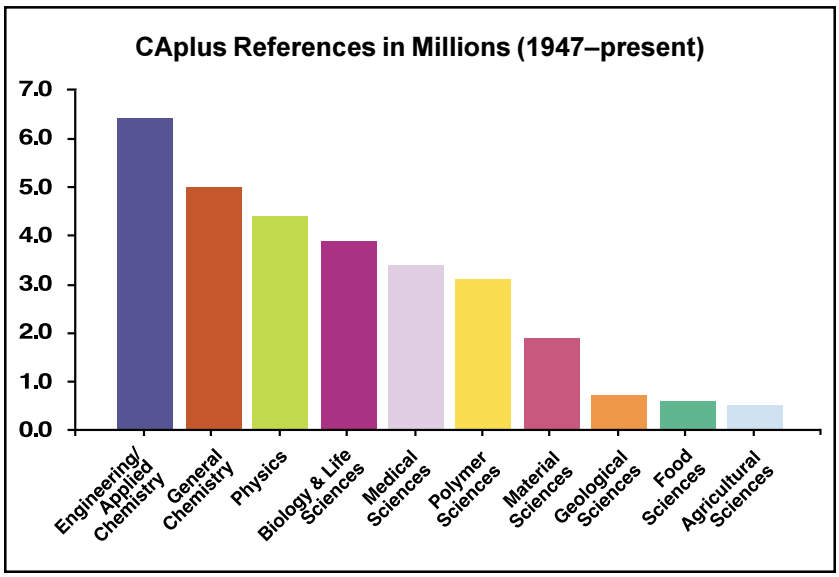
SciFinder Scholar also features:

- 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
- Citation linking
- Saving and printing results
- Accessing full-text documents via ChemPort℠
- 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

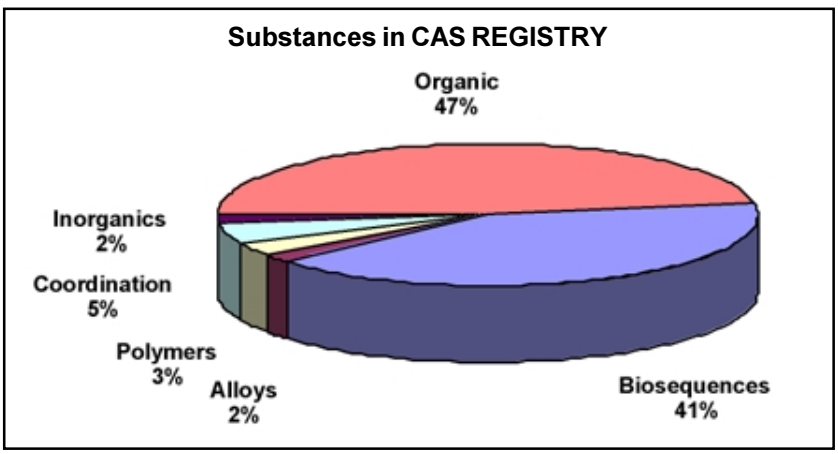
SciFinder Scholar retrieves information contained in databases produced by Chemical Abstracts Service® (CAS) as well as the MEDLINE® database of the National Library of Medicine. All records are in English.

The CAplus database contains over 19.6 million documents from more than 8000 journals and 150 countries, covering literature from 1947 to the present. Sources of the documents include journals, patents, conference proceedings, dissertations, technical reports, books and more. Patents number over 3 million and originate from 32 patent-issuing countries and organizations. CAplus covers a wide spectrum of science-related information, including chemistry, biochemistry, chemical 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 12 million biomedical citations from 1958 to the present. Beginning August 12, 2001, MEDLINE also contains IN-PROCESS records, the latest documents before they have been completely indexed for inclusion on MEDLINE.

In addition to the vast literature sources, CAS's REGISTRY database provides you with access to 32 million different specific chemical substances, including organic compounds, biosequences, coordination compounds, polymers, alloys, and tabular inorganics. From these records, you may access structure diagrams, names, molecular formulas, and more.



The CASREACT® database gives you access to reaction information for more than 5 million single- and multiple-step reactions from journals from 1975 to the present and patents from 1982 to the present. SciFinder Scholar displays the hit reactions, structures for reactants, reagents, and products, all reaction participants including solvents and catalysts, and 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 over 3,300,000 products is derived from over 700 chemical catalogs and libraries. Over 225,000 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 http://www.cas.org.

The information you can find with SciFinder Scholar includes:

- **Substance Information**
  - Chemical Names
  - CAS Registry Numbers®
  - Chemical Structure Diagrams for Substances
  - Chemical Structure Diagrams for Reactions
  - Biosequence Information
  - Property Data
  - Commercial Source Information from Chemical Substance Supplier Catalogs
  - Regulatory Information
  - A list of other publicly available databases available from CAS's STN International online service, where additional information related to the substance may be located

- **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 of the article or patent
  - Indexing
  - Supplementary Terms
  - Citations

SciFinder Scholar Web Sites

You can obtain more information about SciFinder Scholar by visiting the SciFinder Scholar web site at http://www.cas.org/SCIFINDER/SCHOLAR. At the site, you will find general information as well as be able to access SciFinder Scholar Solutions - a series of instructional tips to help make your exploration with SciFinder Scholar more productive.

For quick access to the web site from SciFinder Scholar, click the **Internet** button on the **Main Menu Toolbar**. Select **SciFinder Scholar** and click **OK**.

Optional Features

Optional features for SciFinder Scholar are briefly described below.

SciFinder Substructure Module

You have the option to purchase the SciFinder Substructure Module (SSM), which gives you the ability to draw a structure and search it as a substructure of a more complex structure. Substructure searching is discussed in Chapter 5. The module includes specific drawing features and tools that are used for drawing substructure queries. These features and tools are marked in this *User Guide* with 

to indicate that they may not be included in your package.

3D Structure Modeling

Windows users may use Molecular Simulations Inc. WebLab® ViewerPro™ or ViewerLite™ software along with SciFinder Scholar to view 3D structure models. WebLab Viewer products are a high-end molecular visualization applications that allow models to be manipulated for better understanding of 3D structure. WebLab Viewer software may be downloaded from the Internet. See *Linking to 3D Structure Models* in Chapter 8 for details.

SciFinder Scholar Requirements

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

Windows®

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

- Microsoft® Windows® 95, 98, Me, 2000, 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
- Minimum of 25 MB of available hard disk space (not including pagefile memory), 40-45 MB recommended
- TCP/IP network level connection to CAS via 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 compatible with Windows, minimum 800x600 screen resolution
Printer: High-quality graphics printer, e.g., laser or inkjet, recommended

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℠, Help messages, and web 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. Generally, the plug-in is installed automatically during the SciFinder Scholar 2001 installation. If this in not the case, an alternative installation procedure is available at the SciFinder download web site.
- Java and JavaScript must be enabled for on-line 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 version of this *User Guide* and other user documentation. Acrobat Reader is provided on the SciFinder Scholar 2001 CD-ROM, or can be downloaded at http://www.adobe.com/support/downloads/main.html.

WebLab ViewerPro or ViewerLite: Windows version 3.5 or higher. The WebLab Viewer products allow you to view 3D molecular models for structure results. ViewerLite may be downloaded free at http://www.accelrys.com/viewer/register/lite/viewerlite_reg.php. See *Linking to 3D Structure Models* in Chapter 8 for details.

Technical Support

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

About This User Guide

This *User Guide* introduces the features you can use to retrieve chemical and science-related information. Each chapter describes an individual feature of SciFinder Scholar and often includes an example to illustrate the feature.

The Preference options that allow you to customize your SciFinder Scholar sesson are described in the first appendix. Other appendixes offer additional information about particular features in SciFinder Scholar.

Throughout this guide, **boldface** type is used to indicate names of windows, buttons, pulldowns, and other features. *Italic* type is used for items that you should type or enter. *Italic* type is also used to indicate names of section and chapter headings when they are referred to in the text, and to indicate names of files on your hard drive.

Features marked with a SSM symbol are used for substructure searching via the SciFinder Substructure Module (SSM). These features may not be available in your package.

Features marked with a RXN symbol are used for reaction searching. If you use one of these features for a structure search, SciFinder Scholar will alert you that the feature is available only for reaction searches.

Features marked with both SSM and RXN symbols may be used for substructure searching and reaction searching.

A Portable Document Format (PDF) file containing this *User Guide* can be accessed by selecting **User Guide** from the **Help** menu.

Online Help

Help files that include troubleshooting information are provided in the **Help** menu (Windows) or the **SciFinder Help** menu (Macintosh) located on the **Main Menu**, or you may click the **Help** icon located on the **Main Menu Toolbar**. The main **SciFinder Help** window is displayed.

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

2

Overview

Once SciFinder Scholar is successfully installed (see your Site Administrator for details), you are ready to begin exploring and retrieving chemical and science-related information. If SciFinder Scholar does not appear to be installed properly, please contact your Site Administrator.

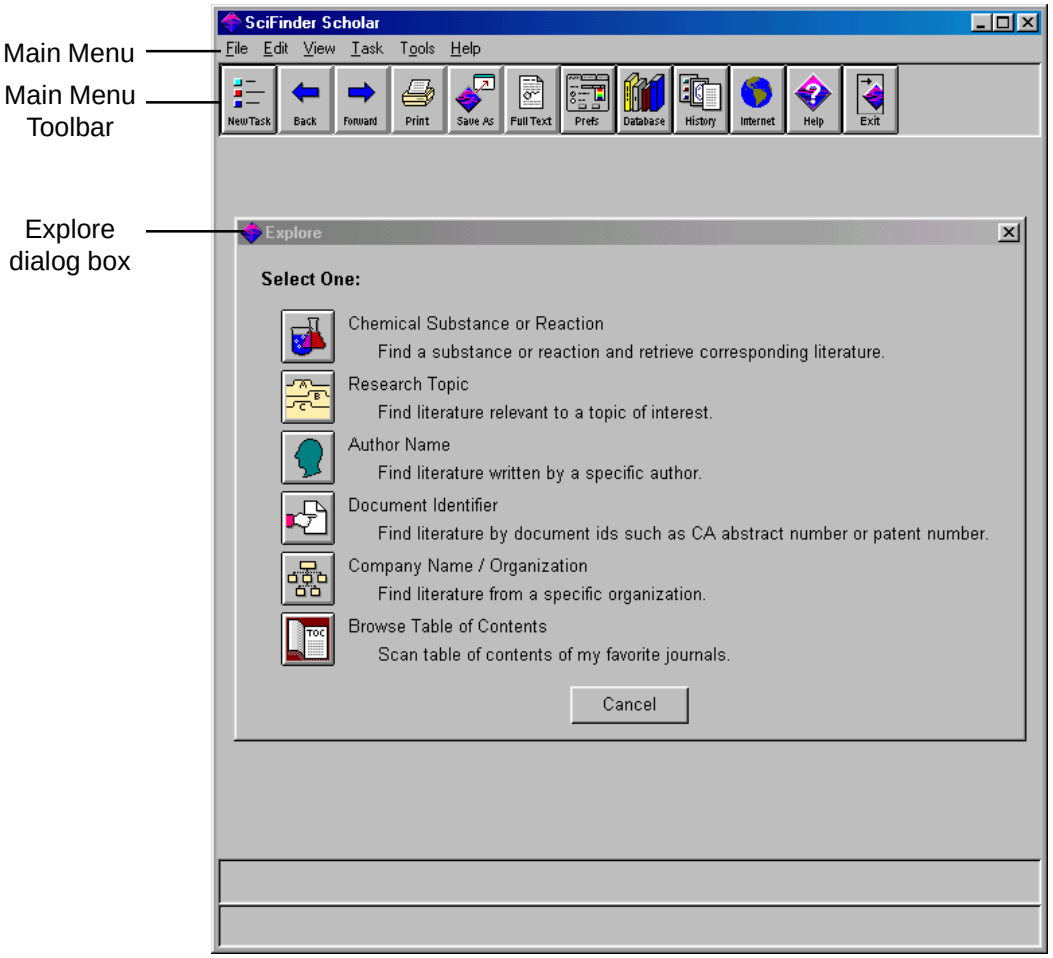
Chapter 2 introduces you to:

- Logging on to SciFinder Scholar
- **SciFinder Scholar** window and its menu and toolbar
- SciFinder Scholar tasks
  - Explore by Chemical Substance or Reaction
  - Explore by Research Topic
  - Explore by Author Name
  - Explore by Document Identifier
  - Explore by Company Name/Organization
  - Browse Table of Contents
- Saving and printing files
- Ending a task
- Exiting SciFinder Scholar

Starting SciFinder Scholar

To start SciFinder Scholar, open the SciFinder Scholar application from the **Start** menu (Windows) or double-click the **SciFinder Scholar icon** (Macintosh). The SciFinder Scholar splash screen is displayed, and you are connected to CAS.

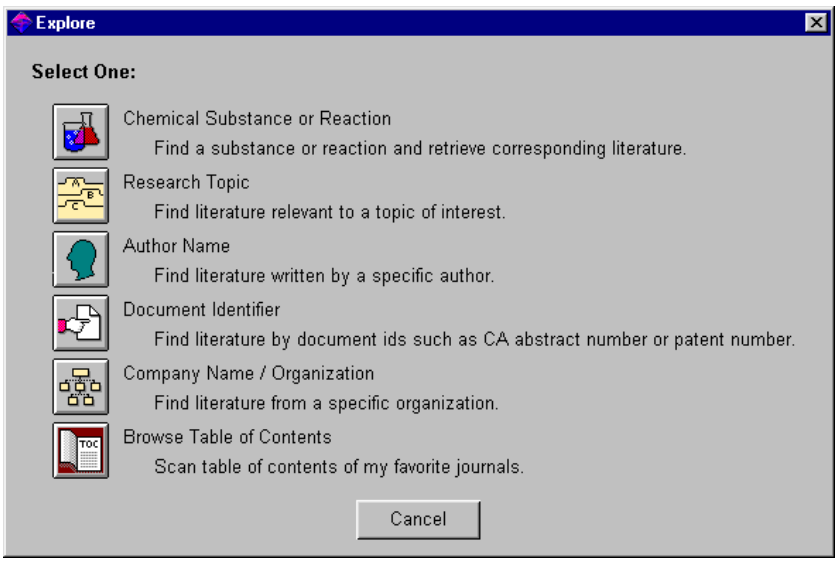
The **SciFinder Scholar** window is displayed. It contains the **Main Menu**, the **Main Menu Toolbar**, and the **Explore** dialog box.



Explore Dialog Box

Explore allows you to look for scientific information dating from 1947 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:

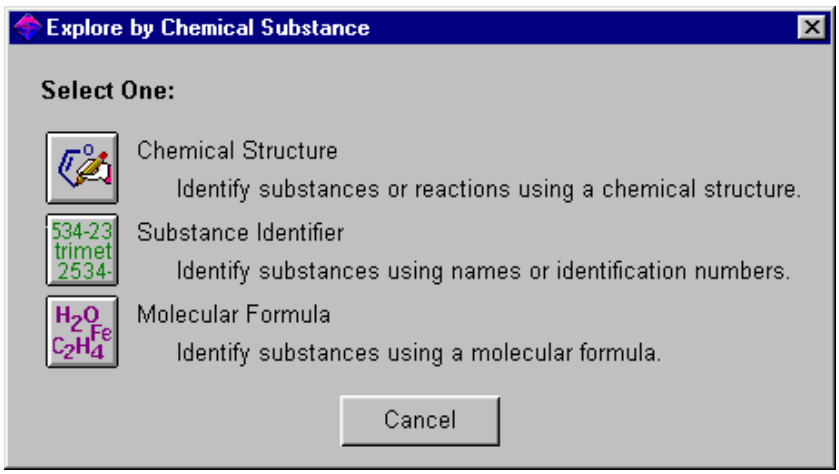
- Chemical Substance or Reaction
- Research Topic
- Author Name
- Document Identifier
- Company Name/Organization



Click the icon for the task you want to perform.

Explore by Chemical Substance or Reaction

Click the **Chemical Substance or Reaction** icon from the **Explore** dialog box to display the **Explore by Chemical Substance** dialog box.



SciFinder Scholar offers you three ways to retrieve chemical substances:

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

SciFinder Scholar offers one way to retrieve chemical reactions:

- Chemical Structure

For detailed information about Explore, refer to Chapters 3-6.

Browse Table of Contents

Browse Table of Contents allows you to scan a list of more than 1600 key scientific journals covered by the CAS databases. You can view the tables of contents and link to full-text options for selected journals.

For detailed information about Browse Table of Contents, refer to Chapter 9, *Browse Journal Tables of Contents*.

Main Menu

The following tables list the commands located on the SciFinder Scholar **Main Menu**. The menu items and their functions are given in the tables.

File Menu

The **File** menu provides basic window management commands.

Menu Item	Definition
New Task	Displays the **Explore** dialog box with the available options in SciFinder Scholar
Save As	Allows you to save an answer set in one of several formats, e.g., Rich Text Format. See the *Saving Files* section later in this chapter for more information.
Print Setup (Windows) or Page Setup (Macintosh)	Allows you to select parameters for printing
Print	Prints the displayed window
Full Text Options	Opens your web browser and links to ChemPort. This allows you to access the full document of selected references. For details, see *Accessing Full-Text Documents* in Chapter 8.
Exit SciFinder Scholar (Windows) or Quit (Macintosh)	Quits SciFinder Scholar and closes the application

Edit Menu

The **Edit** menu provides standard editing functions.

Menu Item	Definition
Cut	Removes a selected block of text and/or graphics and places it on the clipboard to be used or pasted in other applications
Copy	Copies a selected block of text and/or graphics to the clipboard to be used or pasted in other applications
Paste	Places the contents from the clipboard at the location of your cursor
Select All	Selects everything in the current window
Unselect All	Unselects anything selected

View Menu

The **View** menu provides options for displaying references, substances, or reactions in the **SciFinder Scholar** window. Options that are grayed out are not available for your current answer set. For example, Title Order is not applicable to substance answer sets.

Menu Item	Definition
Compact	*References*: Displays the title of the article or patent *Substances*: Displays the chemical structure
Standard	*References*: Displays the bibliographic information with the author names listed first *Substances*: Displays the chemical structure, CAS Registry Number, the approximate number of references citing the substance, and, if available, links to additional information
Summary	*References*: Displays the bibliographic information with the title listed first followed by the abstract, and, if applicable, patent family information *Substances*: Displays the chemical structure, CAS Registry Number, CA Index Name, the approximate number of references citing the substance, and, if available, links to additional information
Full	*References*: Displays the entire record, listing the bibliographic information (title first), followed by the abstract, and, if applicable, patent family information, indexing, supplementary terms, controlled terms, CAS Registry Numbers, chemical names, and citations *Substances*: Displays the entire record including the chemical structure, CAS Registry Number, chemical names, molecular formula, a list of STN files that contain information about the substance, property data, the approximate number of references citing the substance, and, if available, links to additional information
Accession Number Order	Displays results in the order they were accessed, i.e., the order they were added to the database
Similarity Order	Displays substance results grouped by similarity to each other
Title Order	Displays reference results alphabetically by title
Year, Title Order	Displays reference results alphabetically by title, placing titles from the same year together
Reverse Order	Displays results in the order opposite of the current display

Task Menu

The **Task** menu provides tools for the tasks available in SciFinder Scholar.

Menu Item	Definition
Explore	Displays the Explore options in SciFinder Scholar
Chemical Substance or Reaction	Displays an **Untitled** Structure Drawing window, the **Explore by Substance Identifier** dialog box, or the **Explore by Molecular Formula** dialog box
Research Topic	Displays the **Explore by Research Topic** dialog box
Author Name	Displays the **Explore by Author Name** dialog box
Document Id	Displays the **Explore by Document Identifier** dialog box
Company Name	Displays the **Explore by Company Name** dialog box
Browse Journals	Accesses the Browse Table of Contents feature

Tools Menu

The **Tools** menu provides the tools available for the tasks in SciFinder Scholar.

Menu Item	Definition
Analyze References	Allows you to create subsets of reference answer sets on the basis of specific criteria, e.g., Publication Year. Then you can select only answers that are appropriate to your research needs.
Analyze Substances	Allows you to evaluate answers on the basis of real-atom attachments, variable or R group composition, or precision
Refine	Allows you to specify additional search criteria for an existing answer set. This can reduce the number of answers and pinpoint results that better match your needs.
Keep	Allows you to retain the selected references, reactions, or substances and discards the others
Get Related	Allows you to retrieve citations or substances or extend your search with eScience
Task History	Displays the history of your current task
Back	Displays the previous screen
Forward	Displays the next screen
Edit Preferences	Opens the **Preference Editor**. Refer to Appendix A, *Preferences*, for details.
Database Settings	Opens the **Database** tab of the **Preference Editor**. Refer to Appendix A, *Preferences*, for details.
Statistics Monitor	Displays information about your server, port, memory, and file access speed
Internet	Opens your web browser and links to SciFinder Scholar, CAS, ChemPort, and other web sites

Help (Windows) or SciFinder Help (Macintosh) Menu

The **Help** (Windows) or **SciFinder Help** (Macintosh) menu provides access to help while you are using SciFinder Scholar.

Menu Item	Definition
SciFinder Scholar Help	Opens SciFinder Scholar's online Help file
Contents and Index	Opens SciFinder Scholar's online Help file
User Guide	Open the *SciFinder Scholar User Guide* in PDF format
Message of the Day	Allows you to view the message of the day from CAS administrators
About SciFinder Scholar	Contains copyright and version

Macintosh users may have an additional **Help** menu that is unrelated to SciFinder Scholar.

Main Menu Toolbar

The **Main Menu Toolbar** consists of buttons that take you quickly to the function of your choice.

Default Toolbar Buttons	Definition
New Task	Displays the **Explore** dialog box
Back	Displays the previous screen
Forward	Displays the next screen
Print	Prints the displayed window according to the setup defined in your Print Setup
Save As	Allows you to save an answer set in several different formats, e.g., Rich Text Format
Full Text	Opens your web browser and links you to ChemPort
Prefs	Opens the **Preferences Editor**, which allows you to customize your SciFinder Scholar session. See Appendix A, *Preferences*, for details.
Database	Opens the **Databases** tab of the **Preferences Editor**. See Appendix A, *Preferences*, for details.
History	Displays the history of your current session
Internet	Opens your web browser and links to SciFinder Scholar, CAS, ChemPort, or other web sites
Help	Opens the **SciFinder Scholar Help** window
Exit	Quits SciFinder Scholar and closes the application

Saving Files

Reference, substance, and reaction answer sets as well as other displays may be saved to a file on your computer by using the **Save As** command.

To save an item for the first time, select **Save As** from the **File** menu or click the **Save As** button on the **Main Menu Toolbar**. A **Save As** or **Save File As** dialog box is displayed.

1. Select a folder where you want the item to be saved.
2. Type a file name in the **File name** box.
3. Select a file type for saving the file, e.g., Rich Text Format (.rtf).
4. Click **Save**. The file is saved and you are returned to the previous window.

File Formats and Options

Reference and substance records can be saved in several different formats: Plain ASCII (.txt), Rich Text Format (.rtf), Quoted Format (.txt), Tagged Format (.txt), and Answer Keys (.txt). Reaction answer sets can be saved in Plain ASCII (.txt) and Rich Text (.rtf) formats only. For information on saving structure queries, see Appendix B.

Plain ASCII format gives a simple text representation of what you would see if you printed your results. Rich Text Format is similar, but preserves some of the formatting, color in some cases, and graphics if present. The **Options** button for both of these formats allows you to select the amount of information and all or selected answers.

Quoted format allows you to create the type of delimited file you want. Use the **Options** button to define the Quoted format to your needs. For example, a typical Comma Separated Values format would use double quotes for the Quote Character and a comma for the Delimiter. A tab-delimited file would replace the comma with a tab. Delimited files can be useful for importing into database programs such as Microsoft® Access, Lotus® Notes, and Excel.

Tagged format files are typically used for importing data into bibliographic database programs such as EndNote®, ProCite®, and Reference Manager®. The **Options** button allows you to choose all or selected answers. Import requires the use of a special file that defines the tags. The producer of your bibliographic database application should be able to provide you with this file. If you need additional help, please contact your Site Administrator.

Answer Keys can be used for input into the Explore by Document Identifier function and other query functions. The **Options** button allows you to customize this list.

Printing

Reference, substance, and reaction answer sets as well as other displays may be printed to your local printer. Select the records you want to print; otherwise, SciFinder Scholar will print the entire answer set.

To print an item, select **Print** from the **File** menu or click the **Print** button on the **Main Menu Toolbar**. The **Print** dialog box is displayed.

Choose from the options available. Then click **OK** (Windows) or **Print** (Macintosh). Your item is printed, and you are returned to the previous window.

Ending a Task

To end any task and begin a new task, select **New Task** from the **File** menu or click the **New Task** button on the **Main Menu Toolbar**.

Exiting SciFinder Scholar

To leave a SciFinder Scholar session, select **Exit SciFinder Scholar** (Windows) or **Quit** (Macintosh) from the **File** menu or click the **Exit** button on the **Main Menu Toolbar**.

3 Exploring with SciFinder Scholar

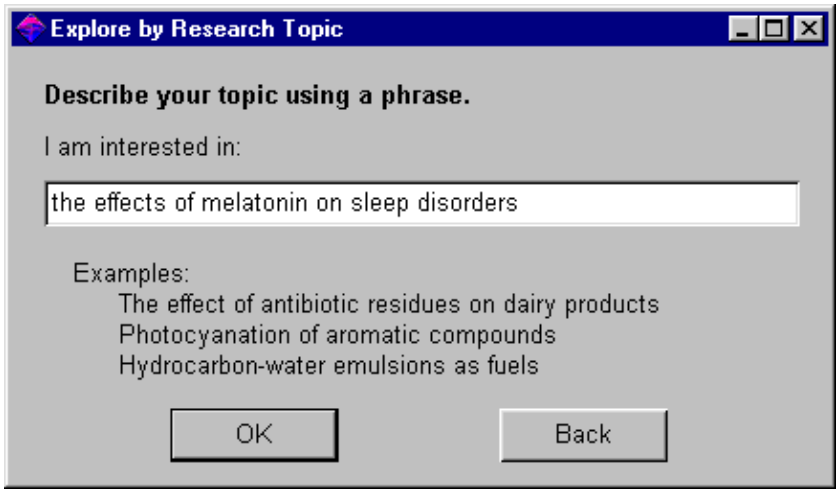
SciFinder Scholar offers several ways of exploring CAS and MEDLINE databases. Chapter 3 familiarizes you with some primary ways to explore and retrieve references with SciFinder Scholar. You may explore by:

- Research topic
- Author
- Document identifier, e.g., a patent number or accession number
- Company name or organization
- Substance identifier, e.g., CAS Registry Number or chemical name
- Molecular formula

Explore by Research Topic

Use Explore by Research Topic to find references for a research area of interest.

To explore by research topic, select **Research Topic** from the **Explore** dialog box. The **Explore by Research Topic** dialog box is displayed.

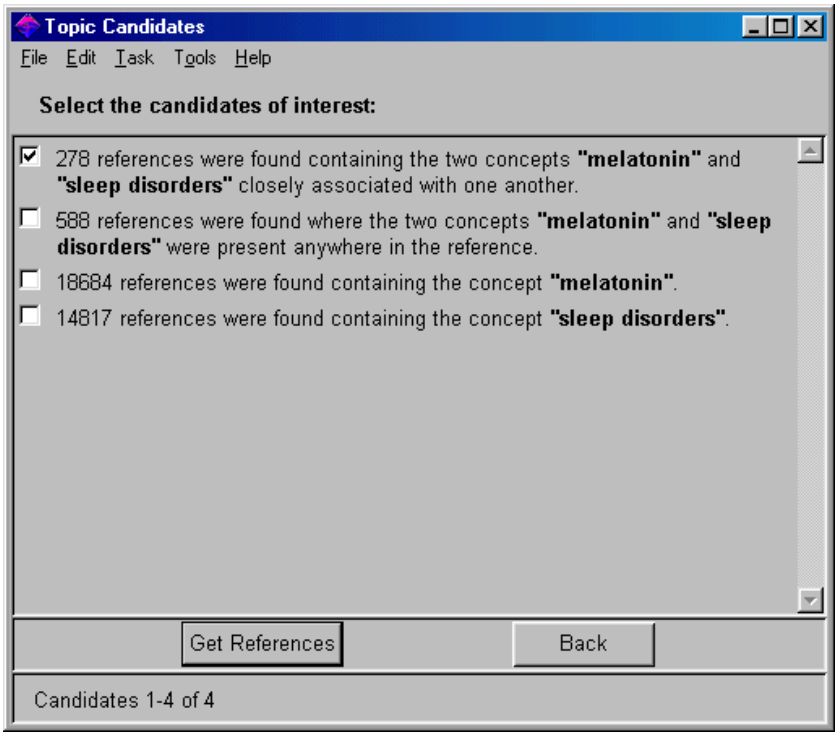


Type a phrase or a few words that describe your topic in the **I am interested in** box.

Enter the phrase as you would normally complete the sentence, “I am interested in...”, using prepositions, conjunctions, etc. Terms entered may be in upper- or lowercase, or both. The phrase may be any length, as words that do not fit in the box are scrolled forward. More details are given in the following section.

After you have entered your topic, click **OK**.

If candidates are found, they are displayed in the **Topic Candidates** dialog box.

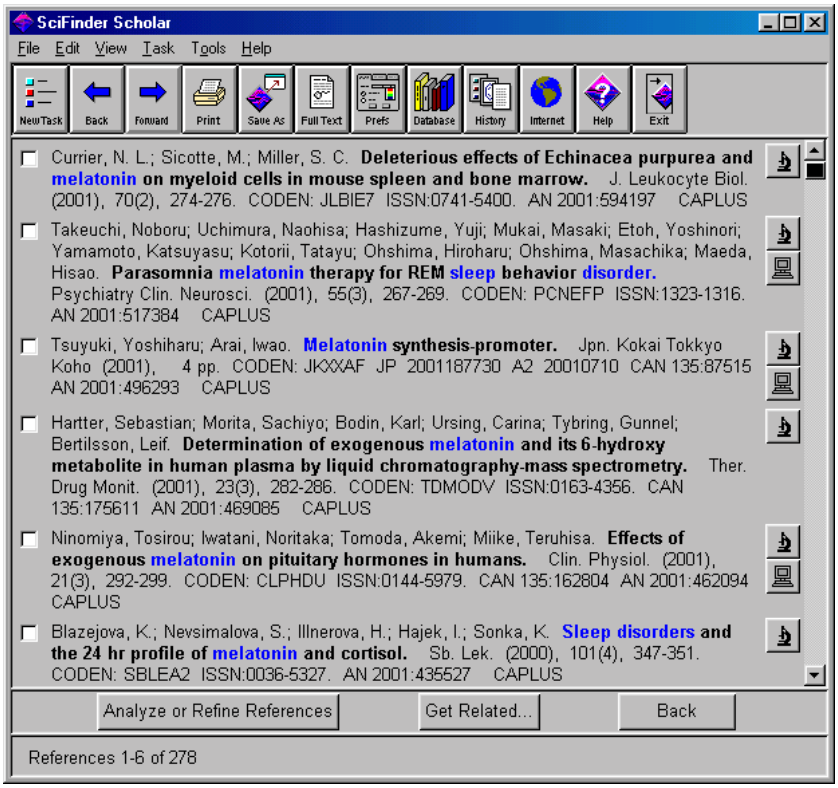


A list of candidates containing the terms in your research topic is displayed. SciFinder Scholar lists different views of search results that may be pertinent to your needs. The number of references is given for each candidate.

To modify your research topic, click **Back**. You are returned to the **Explore by Research Topic** dialog box.

To view references for one or more candidates listed, select those candidates by clicking the adjacent boxes. Then click **Get References**.

The references are displayed in the **SciFinder Scholar** window.



The terms you searched are highlighted. The title is displayed in bold.

References are displayed in the default format and order. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

How Explore by Research Topic Works

When SciFinder Scholar receives a phrase, it breaks out the main ideas or concepts. The relationship between the words in your phrase is determined by scanning for prepositions and other connective words. Noise words, such as *the* or *could*, are automatically eliminated.

For example, the following phrase:

I am interested in caves in Kentucky, but not Mammoth Cave

would be broken into three concepts by SciFinder Scholar: caves, Kentucky, and Mammoth Cave. SciFinder Scholar knows that caves and Kentucky are related to one another and that the concept Mammoth Cave is negated.

SciFinder Scholar's internal dictionary determines if any words or word combinations may benefit from special processing. Specifically, SciFinder Scholar adds these embellishments to words found in its dictionary:

- **synonyms** - enter *cancer* and SciFinder Scholar also looks for *neoplasm* and *carcinoma,* along with dozens of other terms
- **other word forms** - enter *freeze* and SciFinder Scholar also looks for *froze, frozen, freezing*, etc.
- **abbreviations** - enter *chem* and SciFinder Scholar also looks for *chemical*
- **American and British spellings** - enter *color* and SciFinder Scholar also looks for *colour*

As SciFinder Scholar processes the phrase, it determines if any of the words or word combinations are chemical substances. If a substance is identified, SciFinder Scholar finds its CAS Registry Number and includes it in the search.

Any remaining terms go through additional processing to remove suffixes. The terms may be truncated, i.e., shortened to meaningful stems. For example, the term *adjustment* may be processed so that *adjust, adjusted,* and *adjustable* are retrieved. In some cases, this truncation may result in imprecise retrievals.

Tips for Using Explore by Research Topic

The following tips may help you retrieve more precise results.

- **Use a simple English phrase** - Enter phrases as you would normally say or write them, including prepositions, conjunctions, etc. SciFinder Scholar does not look for or understand computer command languages, e.g., Boolean operators, parentheses for grouping, truncation symbols, etc.

- **Specify two or three concepts** - Combine two or three concepts with prepositions, e.g., *I am interested in wastewater treatment at Walt Disney World*

- **Use prepositions instead of OR and AND where possible** - Prepositions may be more exact than OR or AND, e.g., *I am interested in the effects of human growth hormone on fetal development* is more precise than *I am interested in human growth hormone and fetal development.*

- **Distribute your modifiers** - Distribute modifiers across all words to which they apply, e.g., *black dragons and black magic* instead of *black dragons and magic.*

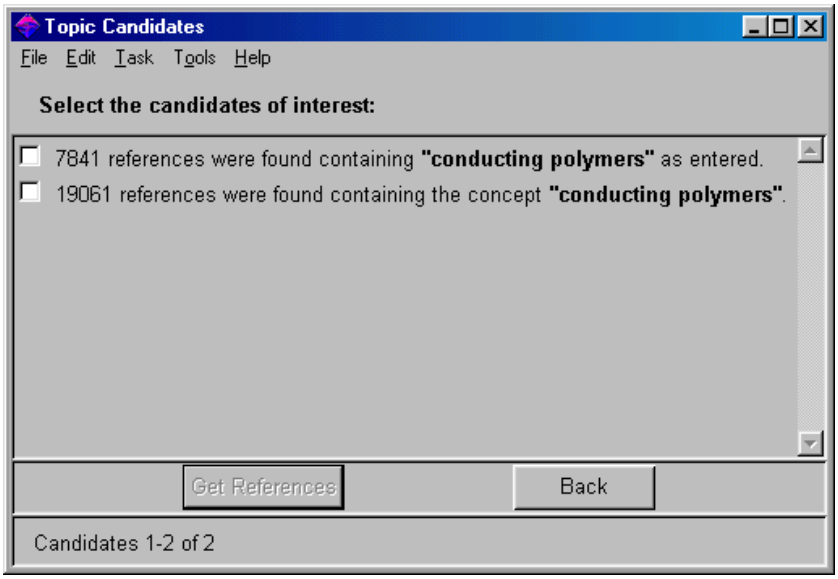
- **Use negation to eliminate "junk"** - SciFinder Scholar understands negative words such as *not* and *except*. If there are areas related to your topic that you are not interested in, remove them by negating items from the topic.

- **Use your own synonyms** - Place synonyms in parentheses next to the related concept, e.g., *I am interested in topical treatments for poison ivy (Rhus radiacans).*

- **Try rephrasing** - Rephrase your question in a different way, e.g., use synonyms, enter different adjectives, and add different spellings, to produce additional or better results.

Exact Phrase Candidate

When the topic you enter is relatively short, e.g., one to three words, SciFinder may find exact matches for the word(s) entered. For example, enter the topic *conducting polymers*.



In this case, the first candidate is the exact phrase candidate, indicated by the wording "*X* references were found containing **"conducting polymers"** as entered."

The exact phrase candidate includes documents in which the input word or phrase is found as an exact match. In this case, *conducting* and *polymers* must appear together in that order.

The exact phrase search does not incorporate the smarts described in *How Explore by Research Topic Works*. Therefore, it is more precise than the other candidates. If no exact matches are found, the exact phrase candidate does not appear.

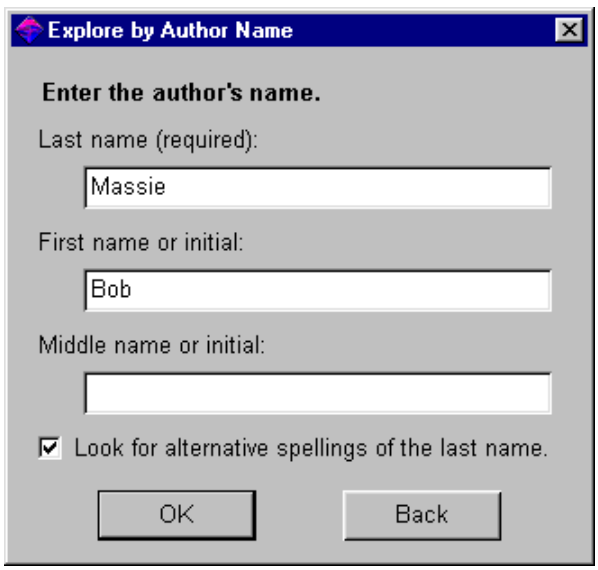
Explore by Author Name

Use Explore by Author Name to obtain references written by authors of interest, regardless of whether or not you know the exact name under which the author published.

With this Explore option, simply enter as much of the author's name as you know. SciFinder Scholar finds references written by authors with:

- Name as entered
- Similar sounding last names
- Nicknames and common spelling alternatives to the first name

To explore by author, select **Author Name** from the **Explore** dialog box. The **Explore by Author Name** dialog box is displayed.

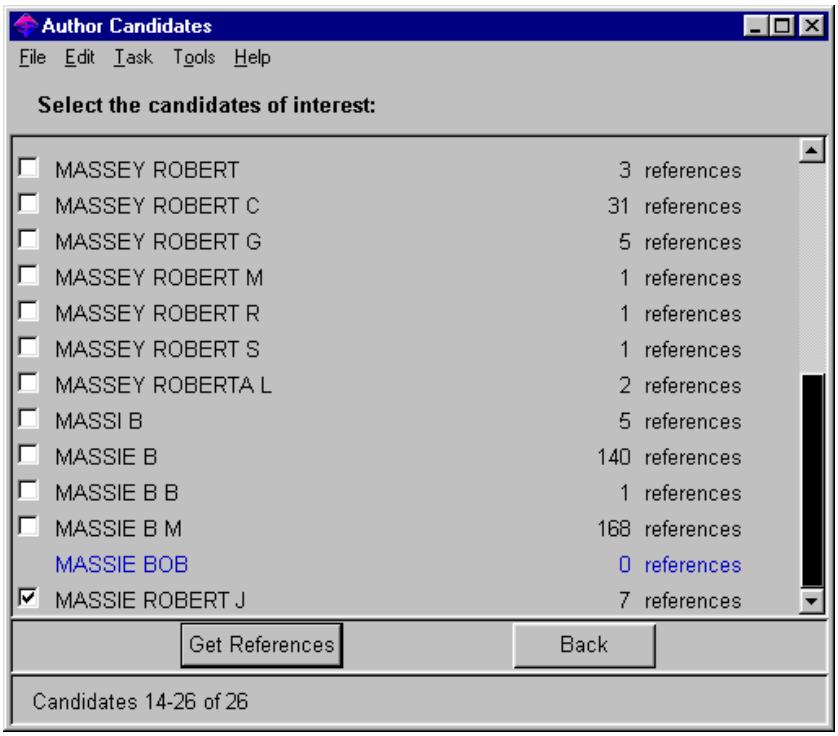


Type a last name in the **Last name (required)** box. You *must* type a last name for all author searches.

Optionally, type a first name or initial and a middle name or initial in the respective boxes. Entering this additional information typically eliminates unwanted references to provide a more precise list of candidates.

Accept the default or deselect the **Look for alternate spellings of the last name** option by clicking its box. This unique feature, when selected, returns results that include alternate spellings of an author's last name, e.g., ROBINS, ROBBINS, ROBENS.

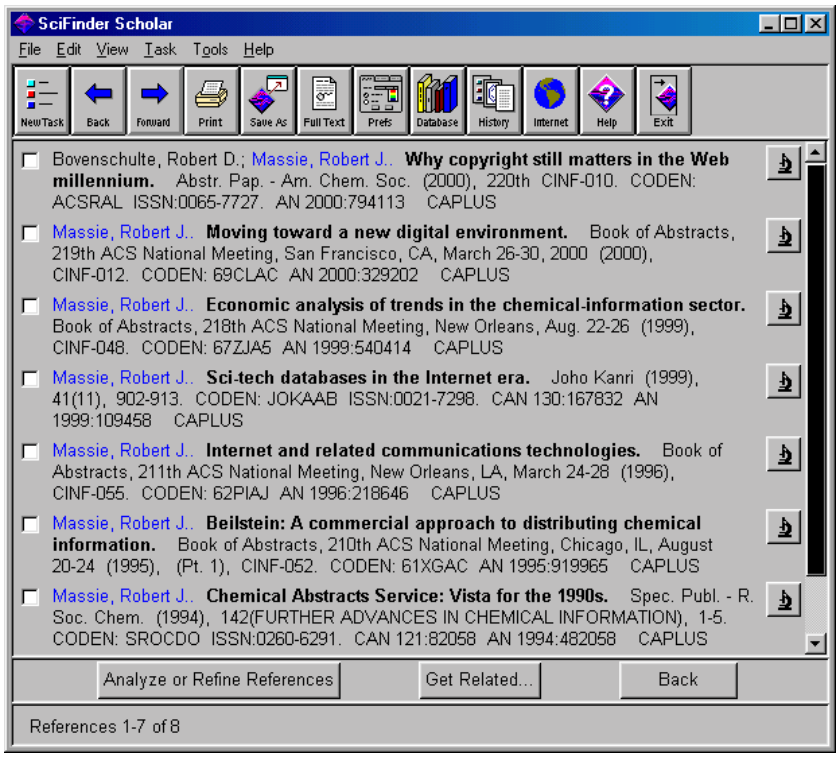
For this example, enter the author name *Bob Massie* into the **Explore by Author Name** dialog box. Then click **OK**. An **Author Candidates** dialog box is displayed.



The window contains an alphabetical list of candidates that match your author, including alternate spellings of the author's last name, if this option was selected. Various forms of the first and middle names are offered as candidates as well. The entered name is highlighted, and the number of references for each candidate is given.

Select author name(s) of interest by clicking in the box next to the name(s).

After you have chosen the author names, click **Get References**. SciFinder Scholar lists the references for the candidates you selected in the **SciFinder Scholar** window.



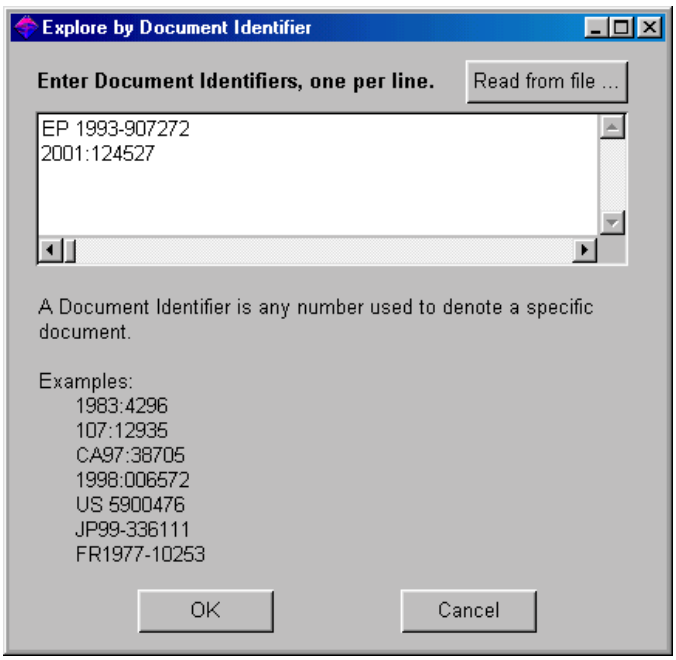
The author names that match the one you entered are highlighted. The titles are in bold.

References are displayed in the default format and order. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Explore by Document Identifier

Use Explore by Document Identifier to obtain references for specific accession numbers and patent numbers, including patent application and priority application numbers. Records are retrieved for all patent family members that have records in CAplus.

To explore by document identifier, select **Document Id** from the **Explore** dialog box. The **Explore by Document Identifier** dialog box is displayed.

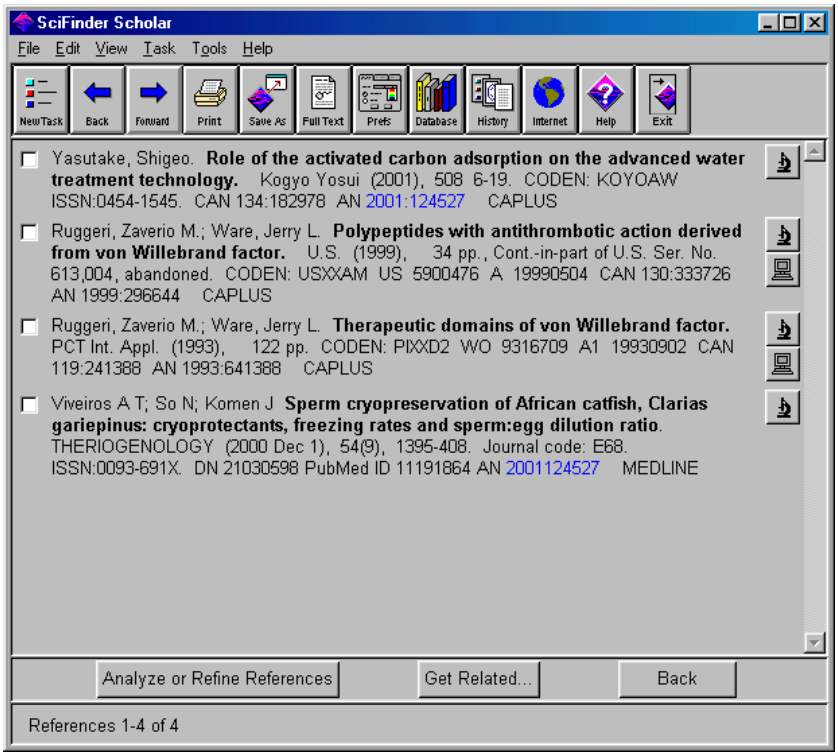


Enter document identifiers, one on each line.

Document identifiers from a text file, such as a file created from Save As using the Answer Keys option (see Chapter 2 for details), may be read directly into the entry box. Click the **Read from file** button to select a file.

Click **OK**. If no accession numbers or patent numbers you enter are found, SciFinder Scholar displays a **SciFinder Scholar Alert!** dialog box. Click **OK** and correct your entries. Then click **OK** again.

SciFinder Scholar displays the references in the **SciFinder Scholar** window.



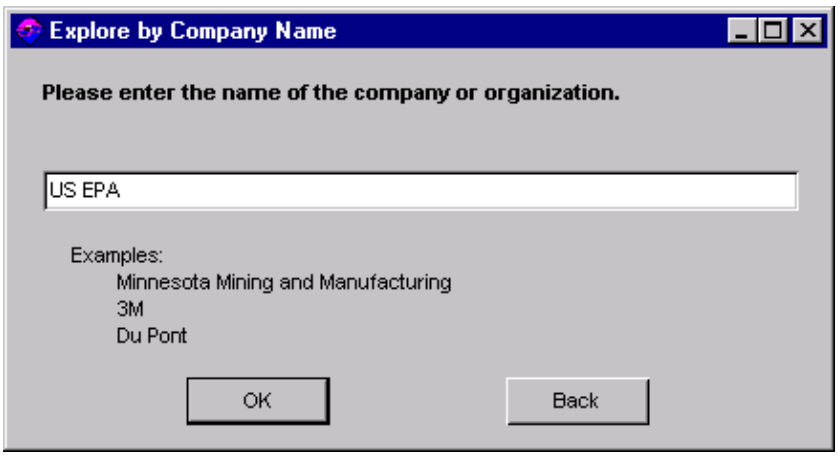
The document identifiers that match the ones you typed are highlighted. The titles are in bold. In this example, two references were retrieved with the accession number entered. Plus, two references were retrieved from the patent family containing the application number entered.

References are displayed in the default format and order. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Explore by Company Name/ Organization

Use Explore by Company Name/Organization to find references published by a company, university, or other organization of interest.

To explore by company name or organization, select **Company Name/ Organization** from the **Explore** dialog box. The **Explore by Company Name** dialog box is displayed.



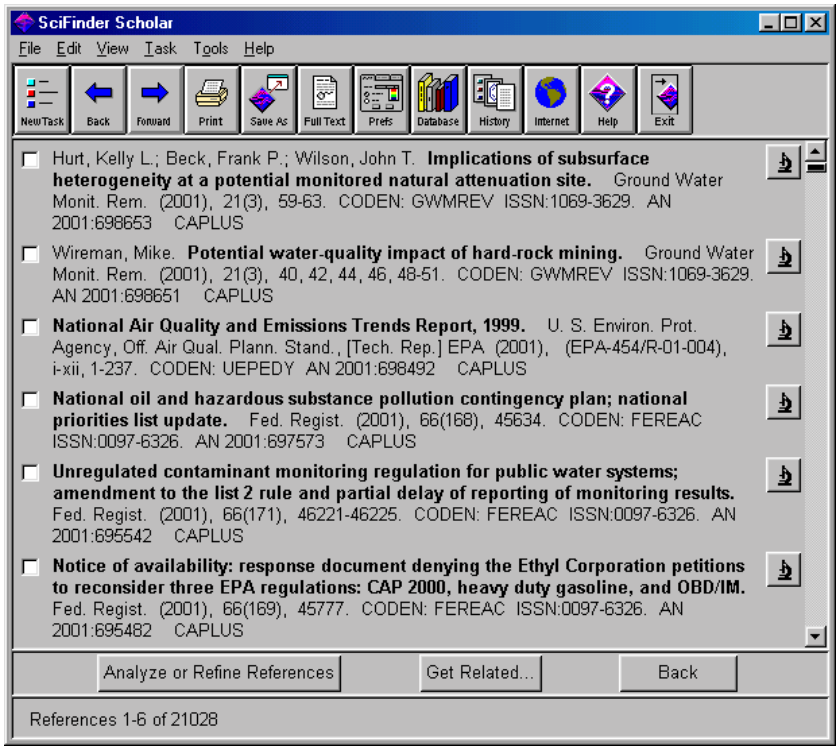
Enter the name of a single company or organization. You may enter your terms in capital or lowercase, and the order of the terms does not matter. You may not use Boolean operators, such as “and” or “or,” to join together multiple companies or organizations.

SciFinder Scholar finds answers that contain all of the words entered. In general, entering more terms will retrieve fewer results. For example, entering *University of North Carolina at Chapel Hill* will retrieve fewer references than entering *North Carolina*.

SciFinder Scholar uses an internal dictionary of company and organization synonyms to increase recall of documents from many large organizations. This dictionary attempts to identify spelling variations, acronyms, and abbreviations. However, the current dictionary does not include most mergers or acquisitions. For example, a search for *Novartis* will retrieve only references that list some variation of Novartis as the source of the document. References from Ciba-Geigy and Sandoz, the companies that merged to form Novartis, will not be retrieved.

Click **OK**.

References that list your search term as the source of the document are displayed in the **SciFinder Scholar** window.



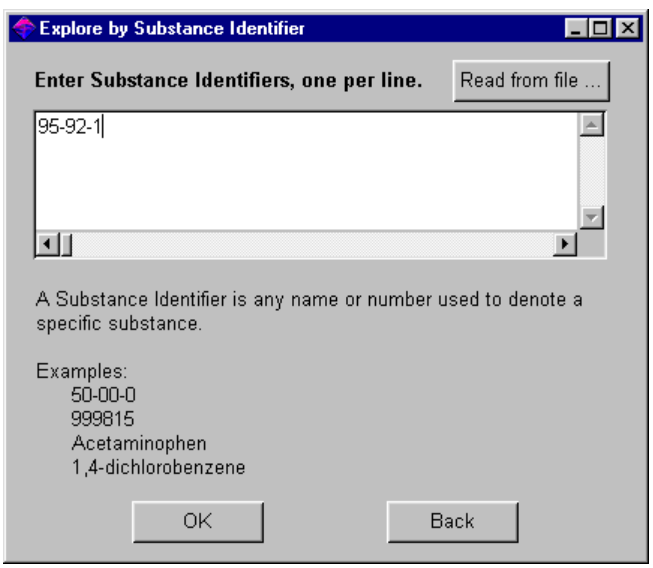
References are displayed in the default format and order. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Explore by Substance Identifier

Use Explore by Substance Identifier to:

- Find CAS Registry Numbers, chemical names, molecular formulas, etc.
- Verify CAS Registry Numbers
- Identify commercial sources
- Retrieve regulatory compliance data
- Obtain references

To explore by substance identifier, select **Chemical Substance or Reaction** from the **Explore** window. Finally, select **Substance Identifier**. The **Explore by Substance Identifier** dialog box is displayed.



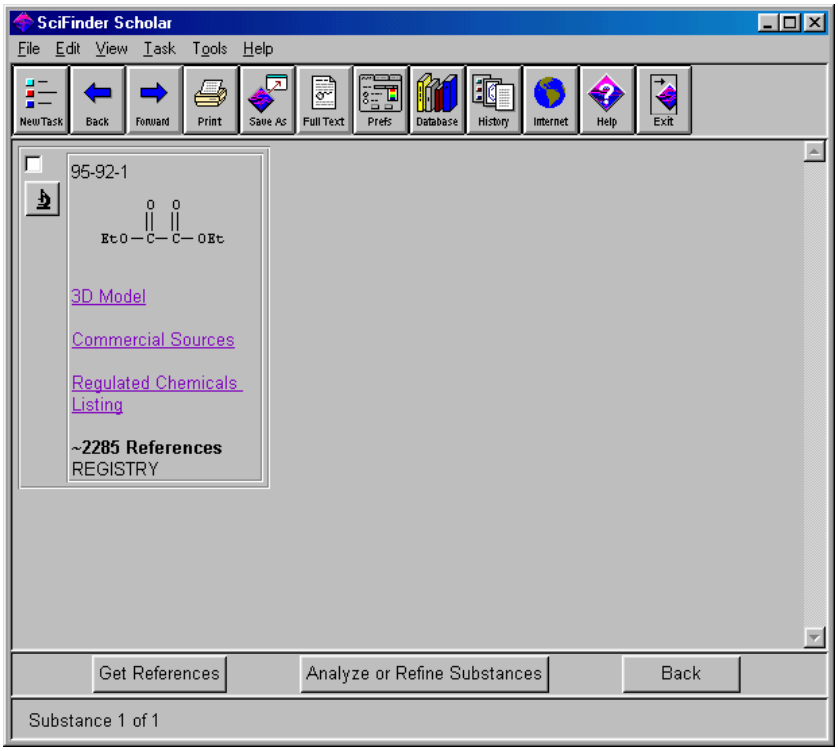
Enter a chemical name, common name, trade name, acronym, or CAS Registry Number for a chemical substance. To enter more than one identifier, or identifiers for different substances, type each item on a separate line.

Names entered are case-insensitive and may include spaces and/or punctuation.

CAS Registry Numbers may be entered with or without hyphens. You may also add leading zeros while maintaining the 5-10 digit range.

Substance identifiers from a text file, such as a file created from Save As using the Answer Keys option (see Chapter 2 for details), may be read directly into the entry box. Click the **Read from file** button to select a file.

Click **OK** to retrieve substances that have the identifiers you entered. SciFinder Scholar looks for substances that match your entries. If substances are found, they are displayed in the **SciFinder Scholar** window.



Substances are displayed in the default format and order. To change the display, select from options in the **View** menu. Or, change the defaults in the **Display** tab of the **Preference Editor**. See Appendix A for details.

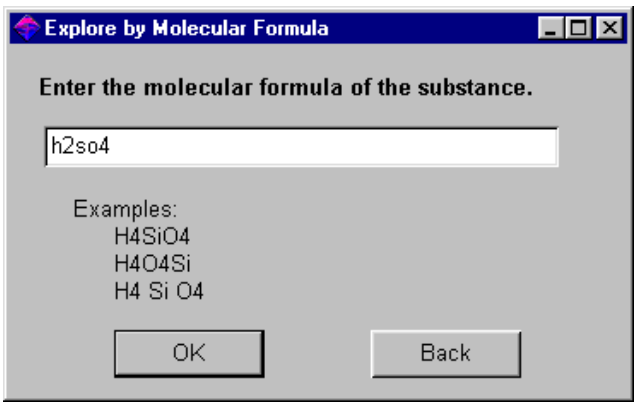
To retrieve references for the substance(s) displayed, click **Get References**. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Explore by Molecular Formula

Use Explore by Molecular Formula to find substances with a particular molecular formula and to:

- Find CAS Registry Numbers, chemical names, etc.
- Identify commercial sources
- Retrieve regulatory compliance data
- Obtain references

To explore by molecular formula, select **Chemical Substance or Reaction** from the **Explore** dialog box. Then select **Molecular Formula**. The **Explore by Molecular Formula** dialog box is displayed.



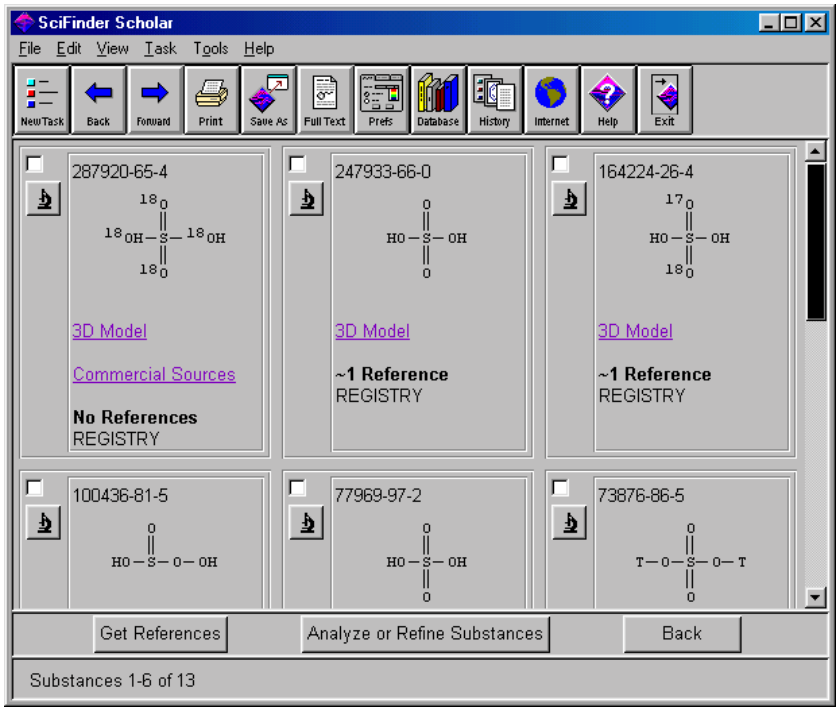
Type a valid molecular formula, with atoms arranged in any order, e.g., h2so4. You may also enter molecular formulas for multicomponent substances. Polymers, mixtures, and salts are represented by dot-disconnected formulas, e.g., c10h5n.hcl.

Molecular formulas entered are case-insensitive. However, you must type some molecular formulas in their proper case to eliminate ambiguity, e.g., H4SiO4, where entering “si” could imply either silicon or sulfur and iodine. Formulas may include spaces between elements, e.g., c6 h6.

After entering a molecular formula, click **OK**.

If the molecular formula entered cannot be recognized or found by SciFinder Scholar, a **SciFinder Scholar Alert!** dialog box is displayed. Click **OK**. The **Explore by Molecular Formula** dialog box is redisplayed. Retype the molecular formula and click **OK**.

If substances are found, they are displayed the results in the **SciFinder Scholar** window.



Substances are displayed in the default format and order. To change the display, select from options in the **View** menu. Or, change the defaults in the **Display** tab of the **Preference Editor**. See Appenidx A for details.

To retrieve references for the substance(s) displayed, click **Get References**. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Ending Your Explore Session

To end your session, select **New Task** from the **File** menu or click the **New Task** button on the **Main Menu Toolbar**.

To exit SciFinder Scholar, select **Exit SciFinder Scholar** from the **File** menu or click **Exit** on the **Main Menu Toolbar**.

4 Exploring by Exact Chemical Structure

SciFinder Scholar's exact structure searching capability allows you to draw chemical structures and retrieve exact or related structure candidates, which may include:

- The structure exactly as you have drawn it
- Stereoisomers
- Tautomers (including keto-enol)
- Coordination compounds
- Charged compounds
- Radicals or radical ions
- Isotopes
- Polymers in which the structure is a monomer

Substance answers provide:

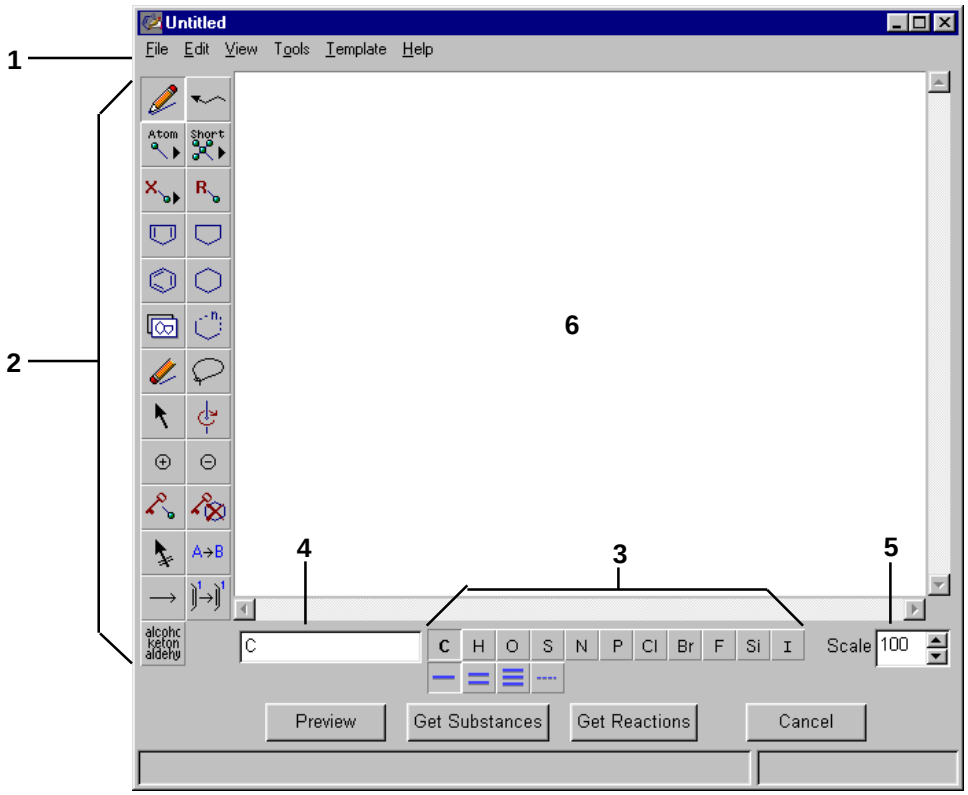
- substance identification information
- commercial sources and regulatory information
- bibliographic references and abstracts

Chapter 4 introduces structure searching with SciFinder Scholar. You will become familiar with:

- Structure Drawing window
- Structure Drawing Menu
- Structure Drawing tool palettes
- Exact structure searches
- Performing an exact structure search
- Viewing substance details
- Refining your structure query
- Retrieving references for your substance

Accessing Explore by Chemical Structure

To access this feature, click the **Chemical Substance or Reaction** icon in the **Explore** window. Then click **Chemical Structure**. An **Untitled** Structure Drawing window is displayed.



The Structure Drawing window includes:

1 Structure Drawing Menu
2 Vertical Tool Palette containing drawing tools
3 Horizontal Tool Palette containing the Common Atoms and Bonds
4 Current Atom box
5 Scaling Factor box
6 Blank screen for Structure Drawing

Structure Drawing Menu

The **Structure Drawing Menu** provides the tools necessary to create a structure.

File Menu

The **File** menu provides basic structure and window management commands.

Menu Item	Definition
New	Opens a new **Untitled** Structure Drawing window
Open	Opens an existing structure that was previously saved
Close	Closes the current Structure Drawing window and displays the **Explore** window
Save	Saves the structure in the Structure Drawing window to the file that is currently open (there are no dialog boxes)
Save As	Allows you to save a structure in an alternate format, e.g., MDL molfile, or with a different name
Revert	Discards all changes to the current structure and reverts to the last saved structure
Get Substances	Searches for substances matching the drawn structure, including tautomers, ions, etc.
Get Reactions RXN	Searches for reactions that contain your structure query
Preview SSM	Allows you to estimate the number of answers and review sample answers for a substructure search
Print Setup (Windows) or Page Setup (Macintosh)	Selects print settings for structures to be printed
Print	Prints the current structure
Exit SciFinder Scholar (Windows) or Quit (Macintosh)	Quits SciFinder Scholar and closes the application

Edit Menu

The **Edit** menu provides standard and SciFinder Scholar-specific editing features.

Menu Item	Definition
Undo	Erases the last edit function and restores the item to its previous condition. Multiple **Undo** functions are permitted.
Redo	Restores the item that you "undid" when you used the **Undo** command
Cut	Removes a selected block of text and/or a structure and places it on the clipboard to be used or pasted in other applications
Copy	Copies a selected block of text and/or a structure to the clipboard to be used or pasted in other applications
Paste	Places the contents from the clipboard at the location of your cursor
Clear	Removes a selected block of text or graphics
Select All	Selects everything in the Structure Drawing window
Unselect All	Unselects anything selected
Clear All	Clears the entire Structure Drawing window
Repaint	Forces a screen update
Delete All Mappings 	Removes all mappings that you applied with the **Reaction Mapping** tool

View Menu

The **View** menu provides options for customizing the display of atoms and bonds in a structure drawing. These options work as toggle switches. When you select an option, a check mark appears next to it. To deselect an option, select it again and the check mark disappears.

Menu Item	Definition
Dot Atoms	Toggles the display of carbon atoms as dots or angles. The default is angles.
Position Numbers	Toggles the display of position numbers on or off. The default is off.
Status Bar	Toggles the display of the status bar that displays the molecular formula and formula weight of the current structure. The default is on.

Dot Atoms and **Position Numbers** cannot be set at the same time. Selecting one option deselects the other.

You may set defaults for your session in the **Drawing** tab of the **Preference Editor**.

Tools Menu

The **Tools** menu provides options to help you draw your structure, including tools to edit your Preferences. The first three options work as toggle switches. When you select **Valency Checking**, **Fix Drawing Angles**, or **Fix Drawing Length**, a check mark appears next to the option. To deselect an option, select it again and the check mark disappears. Session defaults for these options may be changed in the **Drawing** tab of the **Preference Editor**.

Menu Item	Definition
Valency Checking	Checks valencies as you draw and displays a warning when valency problems may exist
Fix Drawing Angles	Toggles bond angles as fixed or variable. The default uses variable angles. The fixed angle applies only to individually drawn bond angles, not to chains or rings made with tools or templates.
Fix Drawing Length	Toggles drawing bonds as fixed or variable lengths. The default displays variable bond lengths. The fixed length applies to chains and rings as well as to individually drawn bonds.
Check Overlaps	Checks if any nodes or bonds overlap and displays a message if any do
Unlock All Positions 	Unlocks all nodes in the Structure Drawing window that you have locked with the **Lock Out Substitution** tool or the **Lock All Positions** option
Lock All Positions 	Locks out from substitution all nodes in the Structure Drawing window
Reverse Shortcut	Displays a selected shortcut in the opposite orientation
Flip Horizontal	Flips selected structure(s) or fragment(s) around the vertical axis, creating a mirror image
Flip Vertical	Flips selected structure(s) or fragment(s) around the horizontal axis, creating a mirror image
Fuse Fragments	Joins two fragments at selected nodes or bonds
Edit Preferences	Opens the **Preference Editor**. Refer to Appendix A, *Preferences*, for details.
Database Settings	Opens the **Databases** tab of the **Preference Editor**. Refer to Appendix A, *Preferences*, for details.

Template Menu

The **Template** menu provides templates of predefined structures. Templates may be selected and then placed into your Structure Drawing window.

Menu Item	Definition
Monocarbocyclic	Displays structure templates of single rings containing only carbon atoms
Bicarbocyclic	Displays structure templates of bicyclo rings containing all carbon atoms
Polycarbocyclic	Displays structure templates of multi-ring systems containing all carbon atoms
N-containing	Displays structure templates of rings with one or more nitrogens
O-containing	Displays structure templates of rings with one or more oxygens
S-containing	Displays structure templates of rings with one or more sulfurs
NOS-containing	Displays structure templates of rings with one or more nitrogens, oxygens, and sulfurs
Alkaloid	Displays alkaloid structure templates
Amino Acid	Displays amino acid structure templates
Carbohydrate	Displays carbohydrate structure templates
Nucleic Acid	Displays nucleic acid structure templates
Steroid	Displays steroid structure templates
Coordination	Displays templates of a specific metal with different coordination configurations
Misc.	Displays a variety of structure templates

Help (Windows) or SciFinder Help (Macintosh) Menu

The **Help** (Windows) or **SciFinder Help** (Macintosh) menu provides assistance for using SciFinder Scholar.

Menu Item	Definition
SciFinder Scholar Help	Opens SciFinder Scholar's online Help file
Contents and Index	Opens SciFinder Scholar's online Help file
User Guide	Open the *SciFinder Scholar User Guide* in PDF format
Message of the Day	Allows you to view the message of the day from CAS administrators
About SciFinder Scholar	Contains copyright and version

Macintosh users may have an additional **Help** menu that is unrelated to SciFinder Scholar.

Vertical Tool Palette

The **Vertical Tool Palette** contains tools to draw and modify your structure. To use a tool, click its icon. When the cursor is placed in the Structure Drawing window, it changes to resemble the tool you selected.

Pencil tool

Chain tool

Atom Menu tool

Short Menu tool

X Menu tool*

R Group tool*

Cyclopentadiene tool

Cyclopentane tool

Benzene tool

Cyclohexane tool

Template tool

3-15 Member Ring tool

Eraser tool

Lasso tool

Selection tool

Rotation tool

Positive Charge tool

Negative Charge tool

Lock Out Substitution tool*

Lock Out Rings tool*

Reaction Site Marking tool**

Reaction Role tool**

Reaction Arrow tool**

Reaction Mapping tool**

Functional Groups tool**

*****Valid only for substructure or reaction searching.
**Valid only for reaction searching.

Pencil Tool

The **Pencil** tool is used to place or change nodes or bonds. Nodes can be atoms, shortcuts, or variables. Click the **Pencil** tool icon to activate the tool and draw nodes and bonds with the current atom/bond type. When you click the **Pencil** tool icon, the cursor changes to resemble a pencil.

To draw one node bonded to another node:

1. Place the pencil where you want the first node to appear.
2. Press and hold the mouse button and drag the cursor to the point where you want the second node. Release the mouse button.

When the nodes are carbons (the default atom), the atomic symbol, C, is not displayed. The C atom symbol is displayed only when it stands alone. To verify the placement of all carbons, select **Dot Atoms** from the **View** menu.

Nodes and bonds can be applied by using the **Horizontal Tool Palette**, **Atom**, **Short**, and **X Menu** tools, or the **Current Atom** box. (See the corresponding sections for these items later in this chapter.)

- Choose a node and/or bond to apply. Click the **Pencil** tool in the Structure Drawing window to draw the node. Click and drag the **Pencil** tool to draw the bond with nodes on both ends.

- Similarly, you may replace an existing node or bond. Choose a node or bond to apply. Place the tip of the **Pencil** tool over the node or bond to be replaced. It becomes highlighted. Click the mouse button and the existing node or bond is replaced.

Chain Tool

The **Chain** tool is used to draw chains of lengths ranging from 1 to 30 atoms. When you click the **Chain** tool icon, the cursor changes to a chain.

To draw a chain, place the chain arrowhead where you want it to appear. Press your mouse button and drag the cursor to the desired length. A number indicating the chain length appears as you drag the tool to let you see how many atoms are in the chain you are drawing.

Release the mouse button when you have drawn your chain to the appropriate length. The number no longer displays.

To reverse the orientation of the attachment of a chain, press and hold the **<Shift>** key while drawing the chain.

Atom Menu Tool

The **Atom Menu** tool is used to select an atom to insert into your structure. The atom you select is the new default for the current SciFinder Scholar session and remains the default until you select a new atom, shortcut, variable, R group or functional group. When this tool is selected, the cursor automatically changes to the **Pencil** tool.

To use the **Atom Menu** tool, click its icon and hold. An atom menu portraying the Periodic Table is displayed. Only those atoms that are available for structure searching with SciFinder Scholar are shown in the Periodic Table.

To select an atom, drag the cursor to the atom you want to use. When the atom you want is highlighted, release the mouse button. This atom is placed in the **Current Atom** box on the **Horizontal Tool Palette**.

Position the **Pencil** tool in your Structure Drawing window or on an existing node and click. The new atom is inserted into your drawing.

Short Menu Tool

The **Short Menu (Shortcuts)** tool is used to select a shortcut to insert into the structure. The shortcut you select is the new default for the current SciFinder Scholar session and remains the default until you select a new atom, shortcut, variable, R group, or functional group. When this tool is selected, the cursor automatically changes to the **Pencil** tool.

To use the **Short Menu** tool, click its icon and hold. A shortcut menu is displayed.

To select a shortcut, drag the cursor to the shortcut you want to use. When the shortcut you want becomes highlighted, release the mouse button. The selected shortcut is placed in the **Current Atom** box on the **Horizontal Tool Palette**.

Position the **Pencil** tool in your Structure Drawing window or on an existing node and click. The shortcut is inserted into your drawing.

After placing a shortcut, you may choose to reverse its orientation, e.g., MeO to OMe. To do so, select the shortcut with the **Selection** tool (refer to its section later in this chapter for details). Select **Reverse Shortcut** from the **Tools** menu.

Terminal shortcuts are by definition locked, i.e., shortcuts will not contain any substitutions in the answer set. Shortcuts cannot be unlocked with the **Lock Out Substitution** tool discussed later in this chapter.

X Menu Tool

SSM

RXN

The **X Menu (Variables)** tool is used to select a fixed variable to insert into a *substructure (or reaction structure) query*. The variable you select is now the new default and remains the default until you select a new atom, shortcut, variable, R group, or functional group. When this tool is selected, the cursor automatically changes to the **Pencil** tool.

To use the **X Menu** tool, click its icon and continue to press the mouse button. A menu of available variables is displayed.

Drag the cursor to the variable you want to use. When the variable you want becomes highlighted, release the mouse button. The variable you select is placed in the **Current Atom** box on the **Horizontal Tool Palette**.

Position the **Pencil** tool in an area of your Structure Drawing window or on an existing node and click. The new variable is inserted into your drawing.

When Ak is drawn, it is surrounded by a box, i.e., locked. With Ak in the locked state, answers will be retrieved in which Ak is any linear or branched, saturated or unsaturated carbon chain with no substitution on the carbon nodes. To unlock Ak, click the **Lock Out Substitution** tool. Then place the cursor over the Ak to highlight it and click. The box is removed. With Ak in the unlocked state, retrieved answers may contain carbon chains that are substituted with any atom. For more details on locking, see the *Lock Out Substitution Tool* section later in this chapter.

R Group Tool

SSM

RXN

The **R Group** tool is used to create R groups to insert into a *substructure query*. R groups are used to define two or more values (maximum of 20) that may occur at the position.

To use the **R Group** tool, click its icon. The **R-group Definitions** dialog box appears near the bottom of the screen with R1 highlighted. R1 becomes the new default for the current SciFinder Scholar session and remains the default until you select a new atom, shortcut, variable, R group, or functional group.

To define R1, click the **Atom**, **Short**, and/or **X menu** button within the **R-group Definitions** dialog box and choose atoms, shortcuts, and/or variables that are allowed values for R. Or, type the atoms, shortcuts, and/or variables into the R1 box, separated by commas.

To define additional R groups, move the cursor to the R2, R3, etc., boxes. You may define up to 10 R groups.

To place an R group in a structure, click the appropriate R group in the **R-group Definitions** dialog box and use the **Pencil** tool to add it to your structure.

Cyclopentadiene Tool

The **Cyclopentadiene** tool is used to draw cyclopentadiene rings.

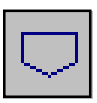
To use the **Cyclopentadiene** tool, click its icon. The cursor automatically changes to resemble a cyclopentadiene ring.

To place a cyclopentadiene ring, position the cursor in your Structure Drawing window and click.

To fuse a cyclopentadiene ring to an existing node or bond, point the tip of the **Cyclopentadiene** tool on a node or bond until it is highlighted and click.

Cyclopentadiene rings may be oriented around a node by continuing to press your mouse button while rotating the mouse. Release your mouse button when the ring is oriented correctly.

Cyclopentane Tool



The **Cyclopentane** tool is used to draw cyclopentane rings in your structure.

To use the **Cyclopentane** tool, click its icon. The cursor changes to resemble a cyclopentane ring.

To place a cyclopentane ring, position the cursor in your Structure Drawing window and click.

To fuse a cyclopentane ring to an existing node or bond, point the tip of the **Cyclopentane** tool on the node or bond until it becomes highlighted and click.

Cyclopentane rings may be oriented around a node by continuing to press your mouse button while rotating the mouse. Release your mouse button when the ring is oriented correctly.

Benzene Tool

The **Benzene** tool is used to draw benzene rings.

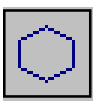
To use the **Benzene** tool, click its icon. The cursor changes to resemble a benzene ring.

To place a benzene ring, position the cursor in your Structure Drawing window and click.

To fuse a benzene ring to an existing node or bond, point the tip of the **Benzene** tool on the node or bond until it becomes highlighted and click.

Rings may be oriented around a node by continuing to press your mouse button while rotating the mouse. Release your mouse button when the ring is oriented correctly.

Cyclohexane Tool



The **Cyclohexane** tool is used to draw cyclohexane rings.

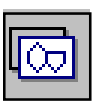
To use a **Cyclohexane** tool, click its icon. The cursor changes to resemble a cyclohexane ring.

To place a cyclohexane ring, position the cursor tip in your Structure Drawing window and click.

To fuse a cyclohexane ring to a node or bond, point the tip of the **Cyclohexane** tool on a node or bond until it becomes highlighted and click.

Rings may be oriented around a node by continuing to press your mouse button while rotating the mouse. Release your mouse button when the ring is oriented correctly.

Template Tool



The **Template** tool is used to place a template that you have selected from the **Template** menu. This tool is available *only* after you have selected a template from the **Template** menu.

To use this tool, select a structure template from the **Template** menu located on the **Structure Drawing Menu**. SciFinder Scholar displays structures conforming to your selection. Click the structure template that you want to use. You are returned to the Structure Drawing window.

Position the cursor tip in the Structure Drawing window and click. The template structure appears in the Structure Drawing window.

You may *not* attach a template structure to an existing node or bond.

3-15 Member Ring Tool

The **3-15 Member Ring** tool is used to draw 3-15 member rings and ring systems. When you click this icon, the **Ring Tool** dialog box is displayed.

Accept the default ring size, *6*, or type a number between 3 and 15. Click **OK**. Your cursor changes to resemble the **3-15 Member Ring** tool icon.

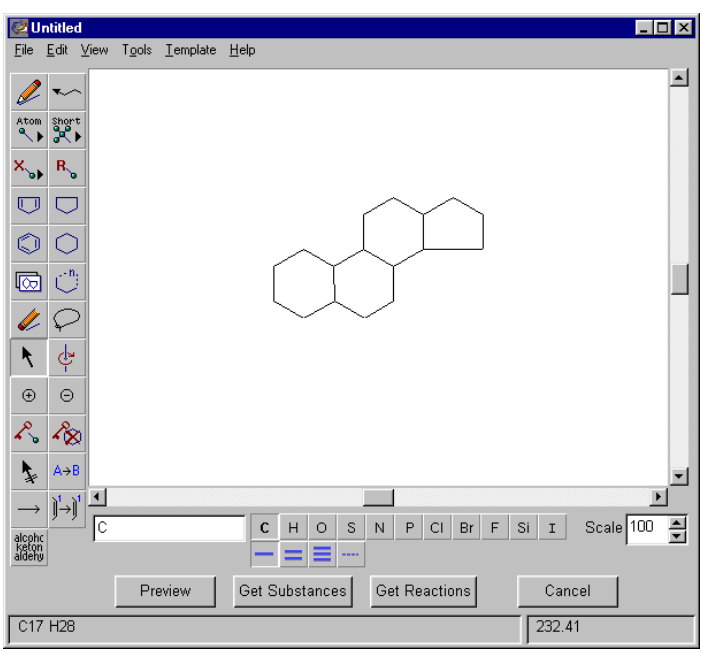
To place a ring, position the cursor tip in your Structure Drawing window and click.

You may attach a 3-15 member ring to an existing node or bond. Position the tip of the **3-15 Member Ring** tool on the node or bond until it becomes highlighted and click.

Rings may be oriented around a node by continuing to press your mouse button while rotating the mouse. Release your mouse button when the ring is oriented correctly.

Fused ring systems that consist of 4-, 5-, or 6-member rings may also be drawn in one step by clicking the **3-15 Member Ring** tool icon. Type a ring system in the **Ring Tool** dialog box. Control the direction of fusion by typing a *U* (Up) or a *D* (Down). The initial default direction is from left to right. After changing a direction, the fusion continues in the new direction until you change it.

For example, type *66U6D5* to draw a steroid ring system. Place your cursor in the Structure Drawing window and click.



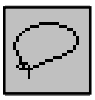
Eraser Tool

The **Eraser** tool is used to delete a node or bond from your structure. When you click the **Eraser** tool icon, the cursor changes to resemble a pencil eraser.

To delete a node, position the tip of the eraser on a node. The node is highlighted. Click and the node and any bonds attached to it are removed.

To remove a bond, place the eraser in the middle of the bond. The bond is highlighted. Click to remove the bond. Terminal nodes at either end of the bond are removed, but nonterminal nodes are not.

Lasso Tool



The **Lasso** tool is used to select a structure. Once selected, you may move it on your screen, cut, copy, or delete it. If a shortcut is selected, you may reverse it if applicable.

To lasso (select) an object, click the **Lasso** tool icon. The cursor changes to resemble a lasso. Then, press and hold your mouse button and drag the lasso cursor around the structure. A line (lasso) appears around the structure fragment as you drag the cursor. Release the mouse button when the entire fragment is enclosed.

To move the lassoed structure fragment, place the lasso cursor inside the lassoed area. The cursor changes to a hand. Press and hold your mouse button while dragging to a new location. Release the button and the selected fragment is relocated to the new location.

To remove the lassoed structure fragment, select **Cut** or **Clear** from the **Edit** menu or press your **<Delete>** key. The selected fragment is removed from the structure. If you select **Cut**, the structure fragment is removed and placed on your clipboard.

To place a copy of the structure fragment on your clipboard, select **Copy** from the **Edit** menu. The selected fragment is now in the structure and on your clipboard.

To lasso a single node, align the point of the Lasso tail on the node and click. The node is enclosed in a box.

Selection Tool

The **Selection** tool is used to select individual nodes, bonds, structure fragments, or entire structures. Selected items may be moved, cut, copied, or deleted. Selected shortcuts may be reversed, if applicable.

To select an item, click the **Selection** tool icon. The cursor changes to resemble an arrow. Place the arrow tip on a single node or bond and click. The item becomes highlighted.

To select more than one node or bond, press and hold the **<Shift>** key while you click each item that you want to select. Release the shift key and the mouse button. All of the items you clicked are highlighted.

To select several nodes and bonds quickly, click and hold the mouse button while you drag the cursor to draw a box around the area containing the nodes and bonds. Release the mouse button. All items within the box you drew are highlighted.

To select an entire structure, double-click any node or bond in the structure. The entire structure becomes highlighted.

To move a segment of a structure, select one or more nodes or bonds. Place the tip of the arrow cursor on a highlighted node or bond and press and hold your mouse button. Drag the node or bond to a new orientation and release your mouse button. All selected nodes or bonds will move in concert.

To move an entire structure, select the structure. Place the tip of the arrow cursor on any part of the structure and press your mouse button. Drag the structure to a new location and then release your mouse button.

To cut a selected item, select **Cut** from the **Edit** menu. The item is removed from the Structure Drawing window and placed on the clipboard.

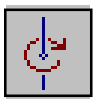
To copy a selected item, select **Copy** from the **Edit** menu. A copy of the item is placed on the clipboard for pasting.

To delete a selected item, press the **<Delete>** key.

To reverse a shortcut, e.g., change MeO to OMe, click the shortcut to highlight it. Then select **Reverse Shortcut** from the **Tools** menu.

To deselect highlighted nodes, bonds, or structures, click in an open area of the Structure Drawing window.

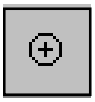
Rotation Tool



The **Rotation** tool is used to rotate a structure fragment either clockwise or counterclockwise around the axis of a node you select.

To rotate a structure or structure fragment, click the **Rotation** tool icon. The cursor changes to resemble the icon. Then click the node around which you want to rotate and continue to press your mouse button as you move the mouse. The fragment rotates as you move the mouse. When the object is at the orientation that you want, release your mouse button.

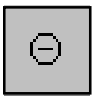
Positive Charge Tool



The **Positive Charge** tool is used to place a positive (1+) charge on a node. When you select this tool, the cursor changes to resemble the positive charge icon.

To insert a positive charge, click the **Positive Charge** tool icon. Then place the cursor tip on a node. The node becomes highlighted. Click and a positive charge is placed on that node. To increase the charge, continue to click.

Negative Charge Tool



To reduce the charge, use the **Negative Charge** tool.

The **Negative Charge** tool is used to place a negative (1-) charge on a node. When you select this tool, the cursor resembles the negative charge icon.

To insert a negative charge, click the **Negative Charge** tool icon. Then place the cursor tip on a node. The node becomes highlighted. Click and a negative charge is placed on that node. To decrease the charge, continue to click.

To increase the charge, use the **Positive Charge** tool.

Lock Out Substitution Tool

SSM

RXN

The Lock Out Substitution tool is used in *substructure searching* to block additional substitution at a particular node.

To lock a node, click the Lock Out Substitution tool icon. The cursor changes to resemble that icon.

Place the tip of the key in the cursor over a node until it is highlighted. Click and a box appears around that node. You may lock any number of nodes within a structure.

Terminal shortcuts from the Short Menu, with the exception of Ak, are by definition locked, i.e., you cannot mark them with a box.

Lock Out Rings Tool

SSM

RXN

The **Lock Out Rings** tool is used in *substructure and reaction searching* to isolate rings from additional fusion and to prevent bonds in a chain system from being part of a ring.

To isolate a ring and/or chain system, click the **Lock Out Rings** tool icon. The cursor changes to resemble that icon.

Place the tip of the key in the cursor on any segment of a ring or chain system until it becomes highlighted. Click and the entire ring or chain system becomes bold. You may lock out any number of ring or chain systems in your reaction structure.

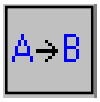
Reaction Site Marking Tool

The **Reaction Site Marking** tool is used to mark a bond in a *reaction structure* that must be modified in the reaction. When you click this icon, the cursor changes to resemble the **Reaction Site Marking** tool.

To mark a bond, click the **Reaction Site Marking** tool icon. Place the cursor tip on the bond that you want to mark until it is highlighted and click. A double line is placed perpendicular to the bond to identify the marked bond.

You may mark as many bonds as you like in the reaction structure. However, marking bonds creates a very specific query and may result in a smaller answer set than one in which bonds are not marked.

Reaction Role Tool



The **Reaction Role** tool is used for *reaction searches* to identify structures as Reactant/Reagent, Product, or Any Role.

To assign a role, click the **Reaction Role** tool icon. Place the cursor on the structure and click. A **Reaction Roles** dialog box is displayed. Choose a role for the structure and click **OK**. A role label appears below the structure.

To replace a role, click the **Reaction Role** tool icon and position the cursor on the structure or the role label. Click and the **Reaction Roles** dialog box is displayed. Choose a different role and click **OK**. The previously assigned role is overridden, and the new role appears below the structure.

To have reaction roles assigned automatically, use the **Reaction Arrow** tool described in the next section. If you attempt a reaction search and any part of your reaction has not been assigned a role, the **Unspecified Roles** dialog box appears, where you may choose to assign “Any Role” to the structure or return to the Structure Drawing window by clicking **Cancel**.

Reaction Arrow Tool

The **Reaction Arrow** tool is used for *reaction searches* and provides automatic assignment of roles for structures in the Structure Drawing window.

To draw an arrow, click the **Reaction Arrow** tool icon. The cursor changes to resemble a horizontal arrow. Position the cursor where you would like to draw the arrow. Click and drag the cursor in the direction of the reaction.

If there are structures present in the Structure Drawing window, roles are automatically assigned to them depending on their spatial relationship to the arrow. To redo the automatic role assignment, draw another arrow; the original arrow is replaced. To override the automatic role assignment, use the **Reaction Role** tool described in the previous section.

Reaction Mapping Tool

The **Reaction Mapping** tool allows you to specify reactant/product atom pairs in *reaction structures*. Reactant/product atom pairs are labeled with the same number, starting with 1.

To specify an atom pair, first draw both the reactant and the product. Click the **Reaction Mapping** tool icon. The cursor changes to resemble that icon. Place the cursor tip on the desired reactant node until it is highlighted and click. A number appears next to that reactant node. Then click the corresponding product node. The same number appears next to that product node.

To change or remove an atom pair label, use the **Eraser** tool and click the number. Both occurrences of that number are removed, and all occurrences of higher numbers drop down by one.

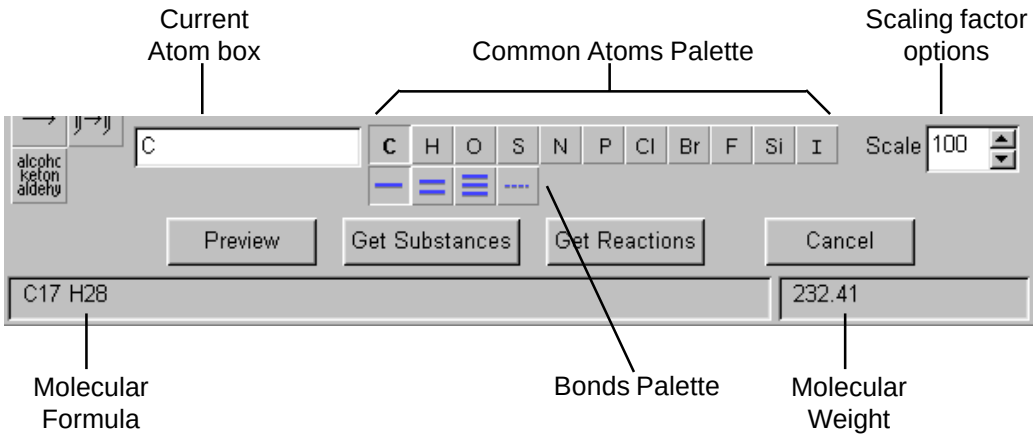
You may create any number of atom pairs. However, specifying atom pairs creates a very specific query and may result in a smaller answer set than one in which pairs are not marked.

Functional Groups Tool

The **Functional Groups** tool allows you to draw reactions that contain functional group terms. Functional group terms may be assigned roles with the **Reaction Role** tool or **Reaction Arrow** tool. For details about the use of functional group terms, see *Exploring Reactions by Functional Groups* in Chapter 6.

Horizontal Tool Palette

The **Horizontal Tool Palette** contains the common atoms and bonds that are used in structure drawing, along with the molecular formula and formula weight of the current structure drawing.



Current Atom Box

The **Current Atom** box displays the symbol of the current atom, shortcut, variable, R group, or functional group being used. This symbol is inserted when you draw with the **Pencil** tool. The default atom is carbon, *C*.

You may change the current atom by highlighting or deleting the current entry and typing another valid atom, shortcut, or variable. The **Current Atom** box is case-insensitive.

If an invalid node symbol is typed, a dialog box is displayed when you click in the Structure Drawing window or when you press **<Enter>**. Click **OK**. You are returned to the Structure Drawing window. Retype a valid atom, shortcut, or variable or make a selection from the **Atom**, **Short**, or **X Menu** tool.

To change an existing atom:

1. Place the desired atom in the **Current Atom** box by using the **Common Atoms Palette** (see next page) or **Atom**, **Short**, or **X Menu** tools, or by typing it into the **Current Atom** box.

2. Position the tip of the **Pencil** tool on the node that you want to change. It becomes highlighted. Then click the mouse button to change it to the item in the **Current Atom** box.

Common Atoms Palette

The **Common Atoms Palette**, to the right of the **Current Atom** box, displays the most frequently used atoms.

Click a different atom icon. This atom now becomes the default and is displayed in the **Current Atom** box.

Bonds Palette

The **Bonds Palette** represents the bonds that may be used in your SciFinder Scholar structure drawing. The bonds include single, double, triple, and unspecified. The default is the single bond.

Click a different bond icon. This bond now becomes the default and is highlighted.

Use the unspecified bond if you are willing to have any bond value, i.e., single, double, or triple, retrieved.

To change an existing bond:

1. Click the desired bond from the **Bonds Palette**.
2. Position the tip of the **Pencil** tool on the bond that you want to change. It becomes highlighted. Click the mouse button and the bond changes to the current bond.

Scaling Factor Box

The **Scaling Factor** box indicates the scaling factor for viewing the structure that you are currently drawing. 100% is the default.

To adjust this factor, highlight the current scaling factor, type a new scaling factor, and press **<Enter>**. Or, click the up or down arrow. The scaling factor takes affect immediately.

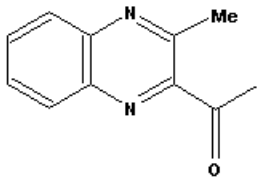
The scaling factor range is from 25% to 400%.

Molecular Formula/ Formula Weight

The molecular formula and the formula weight of the current structure drawing are displayed at the bottom of the **Horizontal Tool Palette**.

Drawing a Structure

Follow these steps to build the substance shown here:

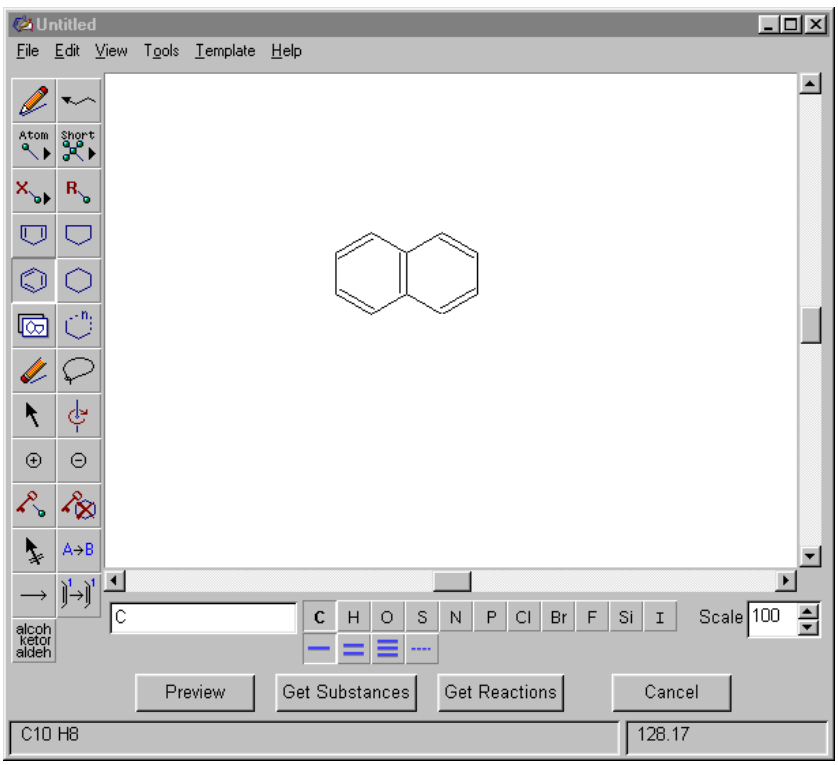


1. Click **Chemical Substance or Reaction** in the **Explore** window. Then click **Chemical Structure**. An **Untitled** Structure Drawing window is displayed.

2. Select the **Benzene** tool icon from the **Vertical Tool Palette**.

   Place the ring cursor arrowhead just left of the center in your Structure Drawing window. This centers your drawing. Click to place the benzene ring.

   Place the ring cursor arrowhead on the middle of the right-most vertical bond of the ring. The bond is highlighted when the cursor touches it. Click to fuse another ring. Two fused benzene rings are now in the structure window. Atoms in each ring are carbon.

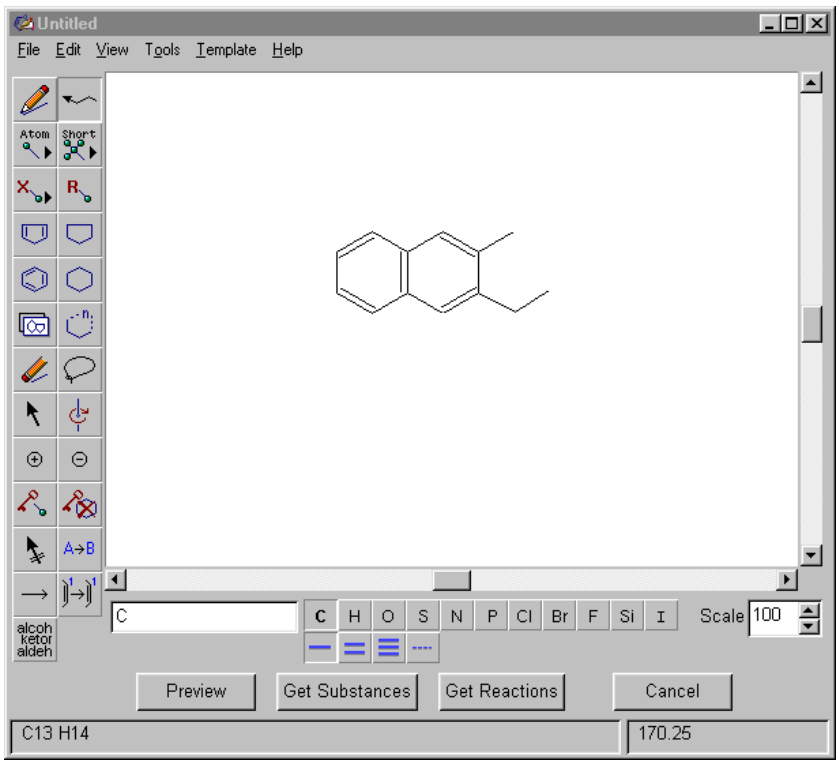


You may also fuse the second ring by placing the ring cursor arrowhead on a node on the right side of the existing ring. Click and hold your mouse button as you rotate the new ring. Release your mouse button when the two rings are fused.

3. Click the **Chain** tool icon.

   Place the chain arrowhead on the upper right node of the right-most ring. The node is highlighted when your arrowhead touches it. Click and drag the cursor away from the ring until you see a chain length of 1. Release the mouse button. A chain of one carbon atom is attached by a single bond to the ring.

   Then place the chain arrowhead on the lower right node of the right-most ring. Press and hold the **<Shift>** key as you click and drag the chain tool cursor away from the ring until you have drawn a chain length of 2. Pressing the **<Shift>** key while placing a chain reverses its orientation.



4. Click the **double bond** icon from the **Horizontal Tool Palette**. The cursor automatically changes to the **Pencil** tool.

   Place the pencil tip on the middle node of the 2-atom chain. Press and hold the mouse button as you drag the pencil straight down until a chain length of 1 is drawn. Release the mouse button. A double bond is drawn between the 2 carbon atoms.

   You may also attach a carbon by a single bond to the middle node of the 2-atom chain using the method described in step 3. Then click the **double bond** icon and place the pencil tip on the single bond and click. The bond changes to a double bond.

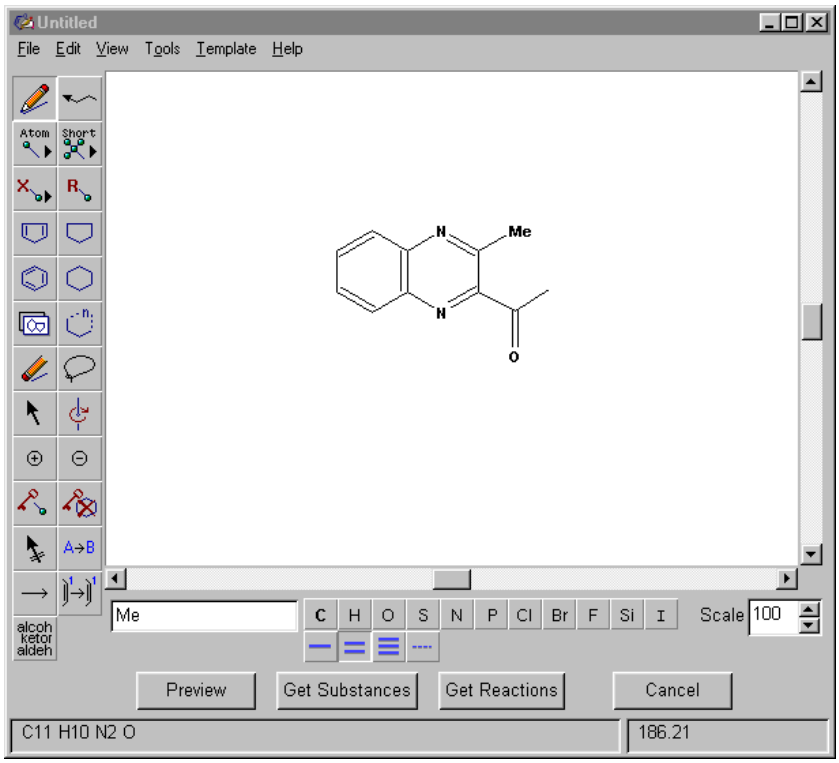
   A third method is to simply draw a second single bond between the two atoms. The result will be a double bond.

5. Click the **N atom** icon (nitrogen atom) on the **Horizontal Tool Palette**. Place the pencil tip on the top carbon in the right-most ring and click. The carbon is replaced with a nitrogen atom. Repeat the process for the bottom carbon in the same ring.

   Click the **O atom** icon (oxygen atom) on the **Horizontal Tool Palette**. Place the pencil tip on the bottom node of the double bonded chain and click. The carbon is replaced with an oxygen atom.

6. Click in the **Current Atom** box and highlight or delete the current atom (it should be oxygen, O). Type the symbol for methyl, *Me*. Me becomes the new atom default. Position the pencil tip on the top, right-most node of the 1-atom chain and click. The carbon is replaced with Me.

   You may also select the Me shortcut by clicking the **Short Menu** tool on the **Vertical Tool Palette**. Refer to the *Short Menu Tool* section earlier in this chapter for details.



Saving and Reusing Structures

Structures drawn in SciFinder Scholar may be saved for later use in SciFinder Scholar or other applications. For details about saving structure drawings and exporting structures to other applications, see Appendix B, *Importing and Exporting Structure Queries*.

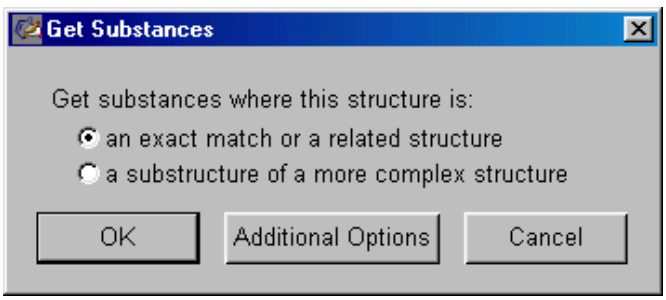
Searching for Multiple Fragments or Components

If you wish to retrieve substance answers that contain particular structure fragments or multiple components, draw a query that contains one or more structures that are not connected to each other. When you click **Get Substances** (see the following section for details), SciFinder Scholar will alert you that there are multiple fragments in your query and ask if you would like to continue. Click **OK**.

Performing an Exact Structure Search

When you have completed a chemical structure drawing, you are ready to perform a structure search. Structure searches may be performed on structures drawn in SciFinder Scholar or structures opened from files in other formats. For information on importing a structure from another application, see Appendix B, *Importing and Exporting Structure Queries*.

Click **Get Substances** to initiate a search. If you have the SciFinder Substructure Module (SSM), the **Get Substances** dialog box is displayed.



SSM users may choose either:

- an exact match or a related structure
- a substructure of a more complex structure (see Chapter 5)

For this example, select **an exact match or a related structure**. Exact structure searching allows you to retrieve one or more substance candidates. These may include:

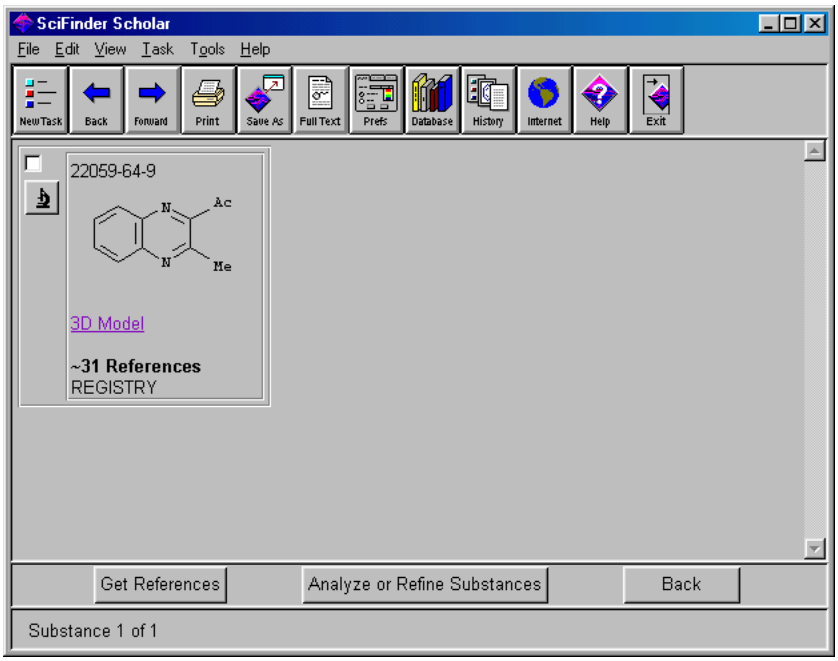
- The structure exactly as you have drawn it
- Stereoisomers
- Tautomers (including keto-enol)
- Coordination compounds
- Charged compounds
- Radicals or radical ions
- Isotopes
- Polymers in which the structure is a monomer

To exclude particular types of substance answers, click **Additional Options** and modify the settings. Or, modify the settings in the **Explore** tab of the **Preference Editor**. See Appendix A, *Preferences*, for details.

Click **OK** to submit your structure query.

SciFinder Scholar uses a CAS intelligent searching process, called Smartsearch, to provide maximum recall for your "exact match" structure query. For more information on Smartsearch, see Appendix C, *Smartsearch: Inside Explore by Chemical Structure*.

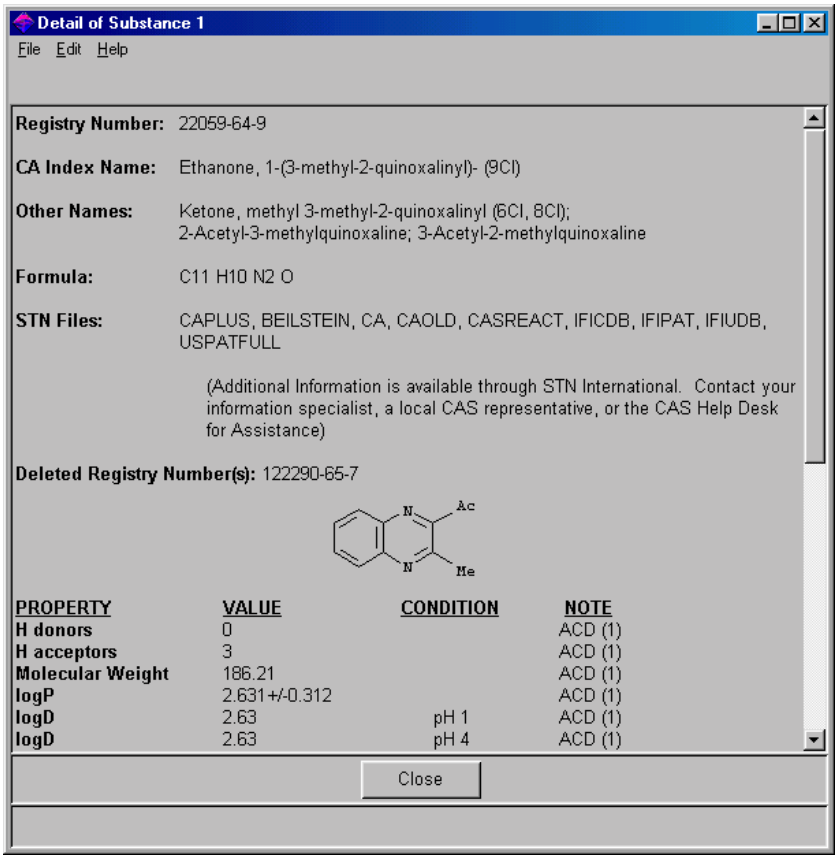
While SciFinder Scholar is searching, a Stop sign appears in the bottom right corner. It allows you to cancel the search, if needed. If you allow the search to go to completion and substances are found, they are displayed in the **SciFinder Scholar** window.



Your query structure is highlighted in each structure in the answer set. Results are displayed in the default format and order. To change the display, select from options in the **View** menu. Or, change the defaults in the **Display** tab of the **Preference Editor**. See Appendix A, *Preferences*, for details.

Viewing Substance Details

To view substance details, click the **microscope** icon next to the substance. A **Detail of Substance #** dialog box is displayed. A substance record may include the CAS Registry Number, chemical names, molecular formula, the chemical structure, and other related information.



Details are displayed in the default format for this window, specified in the **Display** tab of the **Preference Editor**. See Appendix A, *Preferences*, for details..

The STN Files list identifies databases and inventories that contain additional information for this CAS Registry Number. Contact your Site Administrator to find out how you can access and use these STN files and inventories to locate more information on a CAS Registry Number.

You may print or save the record by selecting **Print** or **Save As** from the **File** menu. See Chapter 2 for details.

To return to the **SciFinder Scholar** window, click **Close**.

Keeping Substances of Interest

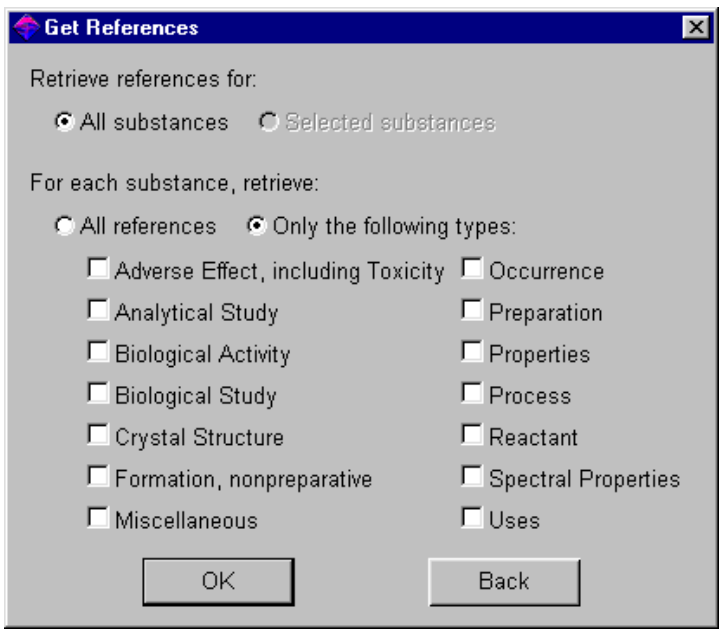
Use the **Keep Substances** option to retain only the substances that interest you. Click the boxes next to the substances you would like to keep. Then select **Keep Substances** from the **Tools** menu. SciFinder Scholar displays only the substances that you selected.

Refining and Analyzing Substances

Substance answer sets may be refined by chemical structure and/or commercial availability. They may also be analyzed by precision and by ring skeletons, atoms, and bonds. Additional analysis options are available for substructure answer sets. Descriptions of the Refine Substances and Analyze Substances features are provided in Chapter 5.

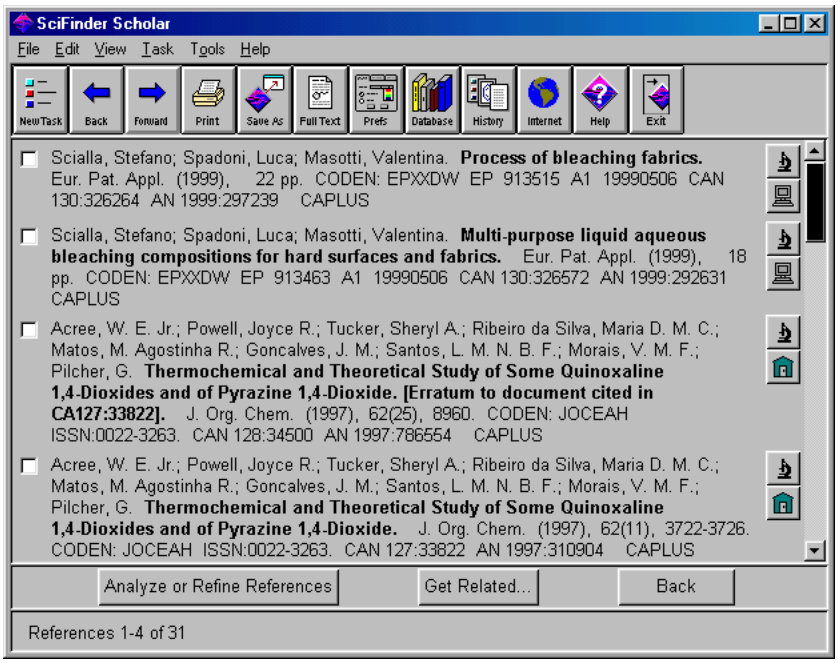
Retrieving References for Substances

To retrieve references that cite a substance or group of substances, click **Get References**. You may optionally select substances of interested before clicking **Get References**. The **Get References** dialog box is displayed.



Choose to retrieve references for all substances or only those you selected in the previous screen. You may then opt to minimize the number of references retrieved by selecting specific substance types under **For each substance, retrieve**. Click the radio button next to **Only the following types**. Then select the substance types of interest, e.g., Preparation. Click **OK**.

The references for the substances you selected are displayed in the **SciFinder Scholar** window.



References are displayed in the default format and order. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Ending Your Explore Session

To begin a new task, click the **New Task** button on the **Main Menu Toolbar** or select **New Task** from the **File** menu.

To exit SciFinder Scholar, select **Exit** from the **Main Menu Toolbar** or select **Exit SciFinder Scholar** from the **File** menu.

5

Exploring by Substructure

SciFinder Scholar's substructure searching feature allows you to draw a chemical structure (see Chapter 4) and retrieve answers that may include:

- Exact structure search results, plus
- Matches in which the query structure is a part of a more complex structure, which may have substitution at positions left "open" in the query
- Matches where your query structure is embedded in a larger ring system

Chapter 5 expands on Chapter 4 and includes the following topics:

- Applying substructure-specific tools
- Previewing your results
- Performing a substructure search
- Refining and analyzing your results

Introduction to Substructure Searching

Substructure searches often retrieve large substance answer sets because the search requirements are quite general. Details on the types of substance answers you can expect from your substructure search are given in Appendix C, *Smartsearch: Inside Explore by Chemical Structure*.

These answers may also provide information concerning:

- Preparation methods
- Commercial sources and regulatory information
- Bibliographic references and abstracts

Substructure searching capabilities include:

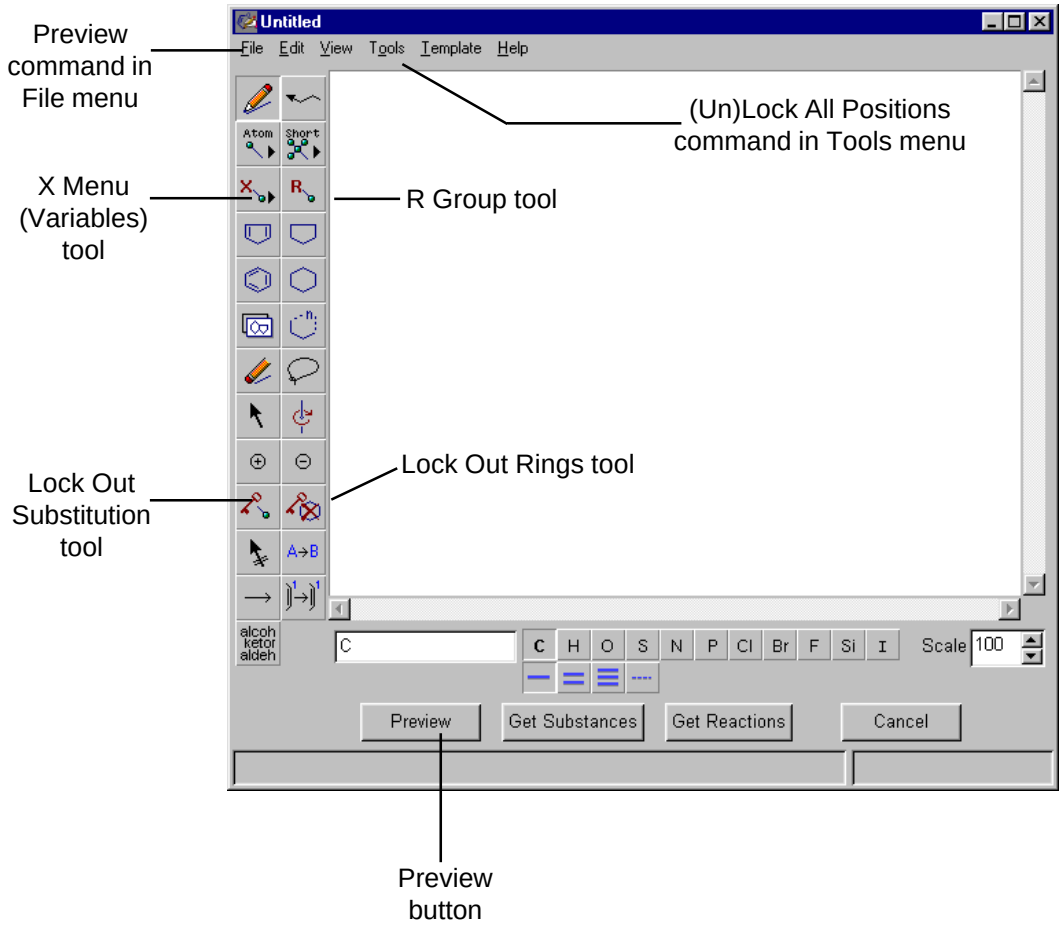
- Executing substructure searching capabilities for structures drawn in SciFinder Scholar's Explore by Chemical Structure
- Isolating rings from further ring fusion or allowing rings to be embedded in other ring systems.
- Allowing a chain to be in a ring or chain in answers or to be chain only
- Opening and closing sites for substitution in rings and chains
- Defining R groups, multiple allowable substituents at a position, to include atoms, shortcuts, and variables with up to 10 R groups per structure
- Using predefined variables, i.e., generic nodes
- Importing and exporting queries with substructure attributes
- Accessing all SciFinder Scholar tools, features, and tasks

A Preview feature is provided that allows you to view or analyze sample answers prior to actually performing the search. This will assist you in drawing a query that will be searched successfully and in a reasonable time frame, while allowing you to retrieve a manageable number of relevant answers. Preview also can provide insight into the potential structure answers you may retrieve.

Once you have completed a substructure search, the Analyze feature allows you to categorize and evaluate your answer set in several ways. These features are discussed later in this chapter.

Accessing Explore by Substructure

To Explore by substructure, open a Structure Drawing window by clicking **Explore** in the **New Task** window. Then click **Chemical Substance or Reaction**. Finally, click **Chemical Structure**. An **Untitled** Structure Drawing window is displayed.



Substructure Drawing Features

The Structure Drawing window includes tools for drawing structure queries as well as tools, menu items, and buttons that are used specifically for substructure searching. These items, which are indicated on the previous page, include:

- **Lock Out Substitution** tool – prohibits additional substitution at designated nodes
- **Lock Out Rings** tool – prohibits additional ring fusion and sets chain bonds to chain only
- **Unlock All Positions** in the **Tools** menu – allows substitution at all nodes
- **Lock All Positions** in the **Tools** menu – inhibits substitution at all nodes
- **X Menu** tool – allows variable groups to be placed in your structure
- **R Group** tool – opens the **R Group Definition** dialog box where you may create up to 10 R groups, i.e., define multiple substituents allowed at a position
- **Preview** in the **File** menu and **Preview** button near the bottom of the window – allows you to analyze your query and retrieve a set of sample answers

Substructure Drawing Defaults

The following table identifies the defaults that SciFinder Scholar assumes.

If your substructure contains:	**SciFinder Scholar finds structure matches where:**
Rings	The skeleton ring system you drew is: - Exactly as you drew it - Further substituted - Embedded within a larger ring system
Chains	The *nodes* in the chain are: - Further substituted - Part of a Ring - Part of a Chain The *bonds* in the chain are part of a: - Chain - Ring
Terminal Shortcuts from the Short Menu, with the exception of Ak	The terminal shortcut is locked from substitution

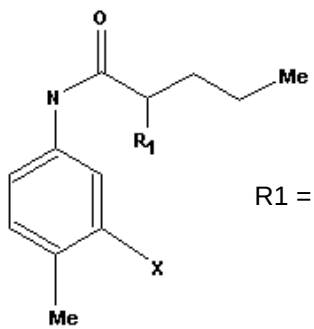
Changing Substructure Drawing Defaults

You may change the substructure drawing defaults by using the SciFinder Scholar drawing tools described in the following table.

If the substructure contains:	Use this SciFinder Scholar tool:
Ring System	**Lock Out Rings** tool to *isolate* the ring system. No further fusion, including spiro, is allowed on the drawn ring system.
Chain Bonds	**Lock Out Rings** tool to set bonds to *chain only.* Node default cannot be reset.
Ring or Chain Nodes	**Lock Out Substitution** or **Lock All Positions** in the **Tools** menu command to prevent further substitution.

Drawing a Substructure

To perform a substructure search, first draw a structure you would like to search. For this example, draw the following structure in your Structure Drawing window:



R1 = C, O, N, S, H

Details about drawing structures are provided in the *Drawing a Structure* section of Chapter 4. Drawing tools are also described individually in Chapter 4.

1. Use the **Benzene** tool to place a benzene ring in the center of the Structure Drawing window.

2. Click the **Short Menu** tool, and hold down the mouse button to display the menu. Select **Me**. Use the **Pencil** tool to attach Me to the ring by a single bond.

3. Click the **X Menu** tool and hold down the mouse button to display the menu. Select **X Any halogen**. Use the **Pencil** tool to attach X to the ring by a single bond.

4. Click the N in the **Common Atoms Palette**. Click the **Pencil** tool to attach N to the ring by a single bond.

5. Use the **Chain** tool to draw a 5-membered chain attached to the N.

6. Click the **Short Menu** tool and hold the mouse button to display the menu. Select **Me**. Place your cursor over the node at the end of the chain. Click to replace the carbon atom with Me.

7. Click the **R Group** tool. In the **R1 =** box, type *C, O, N, S, H*. Use the **Pencil** tool to attach R1 to the chain by a single bond.

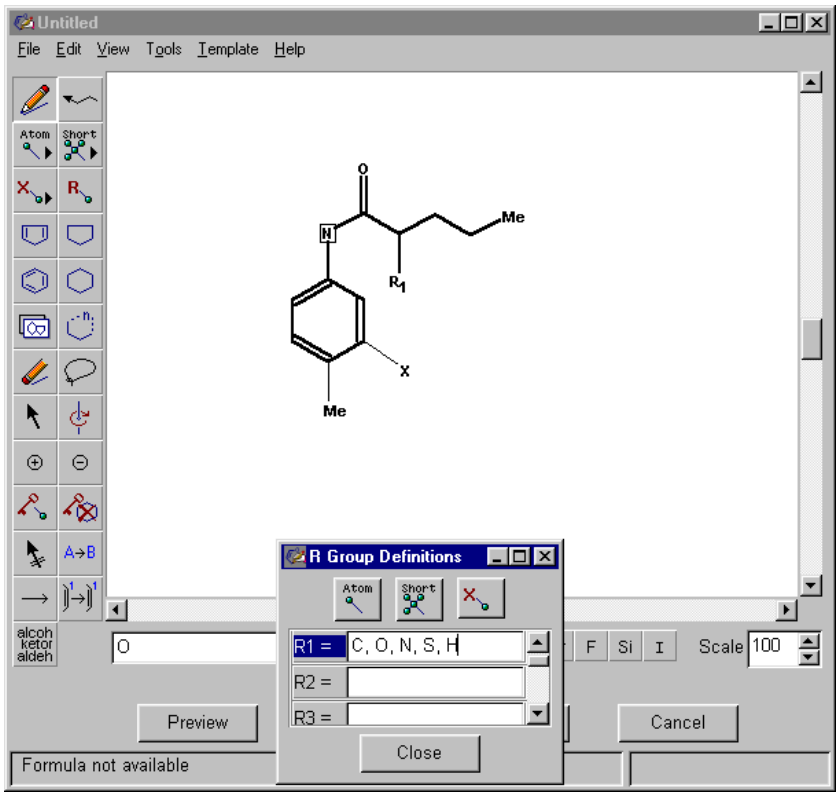
8. Click O on the **Common Atoms Palette**. Click the double bond on the **Common Bonds Palette**. Use the **Pencil** tool to attach O to the chain by a double bond.

9. Click the **Lock Out Substitution** tool. Place your cursor over the N to highlight it and click. This isolates the N from further substitution.

10. Click the **Lock Out Rings** tool. Place your cursor over a bond in the ring to highlight the ring and click. This isolates the ring from further ring fusion.

    Place your cursor over any bond in the chain to highlight the chain and click. This sets the chain bonds to chain only.

When you have completed the drawing, your Structure Drawing window should look similar to this:

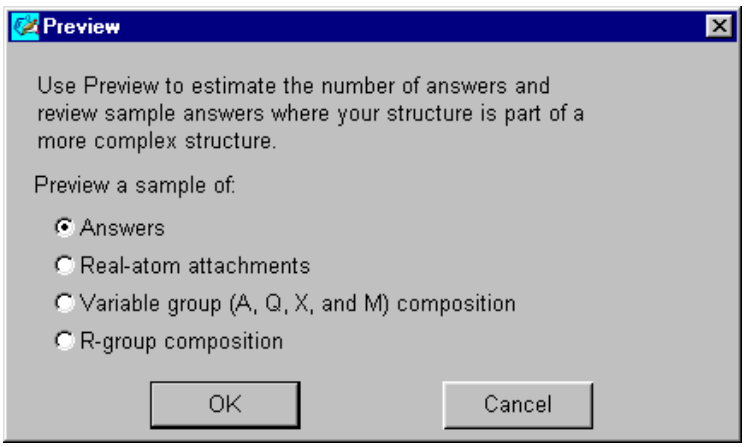


Alternatively, you may open a previously saved structure file by selecting **Open** from the **File** menu or by pasting a structure into the Structure Drawing window from the clipboard. See Appendix B, *Importing and Exporting Structure Queries*, for more information.

Previewing Substructures

The Preview feature gives an estimate of the number of answers you can expect and shows some sample answers. With Preview, you can analyze sample answers to predict whether your substance query will retrieve answers and what kind of answers you will retrieve.

After your structure is complete, click the **Preview** button. The **Preview** dialog box is displayed.



You can Preview by:

- **Answers** – allows you to view representative answers
- **Real-atom attachments** – allows you to get estimates of the types of attachments you can expect at real atoms on the structure
- **Variable group composition** – allows you to get frequency of occurrence estimates of the atoms at each variable site
  - **A** – any atom except H
  - **Q** – any atom except C or H
  - **X** – any halogen
  - **M** – any metal
- **R-group composition** – allows you to get frequency of occurrence estimates of the atoms at each R group site

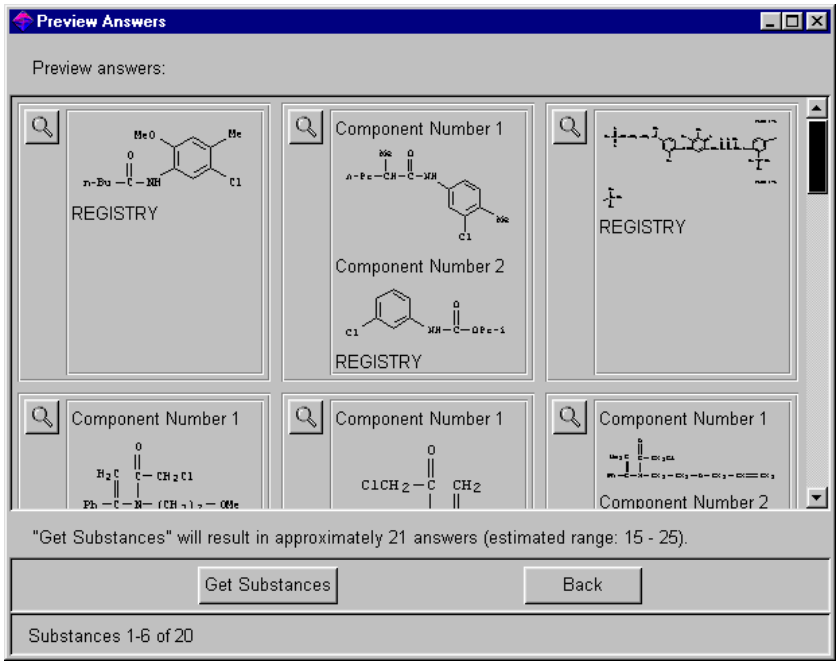
Each Preview option also gives you an estimate of the total number of answers this structure will retrieve via **Get Substances**.

Preview Not Completed

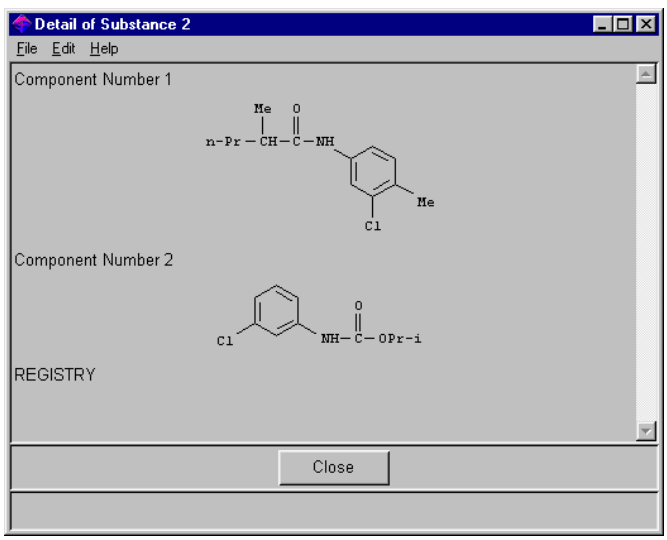
If a large number of potential answers are identified, an alert message is displayed. The **AutoFix** feature may help narrow your query. Clicking the **Autofix** button locks out all rings and chains, as if you had applied the **Lock Out Rings** tool. This prohibits fusion to the ring and sets all chain bonds to chain only. You are returned to the Structure Drawing window, and all of the rings and chains in your structure appear in bold. Click **Preview** to try again.

Previewing Answers

To preview a sample of answers, click the radio button next to **Answers** in the **Preview** dialog box. Then click **OK**. The **Preview Answers** window is displayed. It contains a set of sample answers and an estimate of the total number of answers **Get Substances** will find.



To view a structure at a larger size, click the **magnifying glass** icon next to the structure. A **Detail of Substance #** window is displayed.

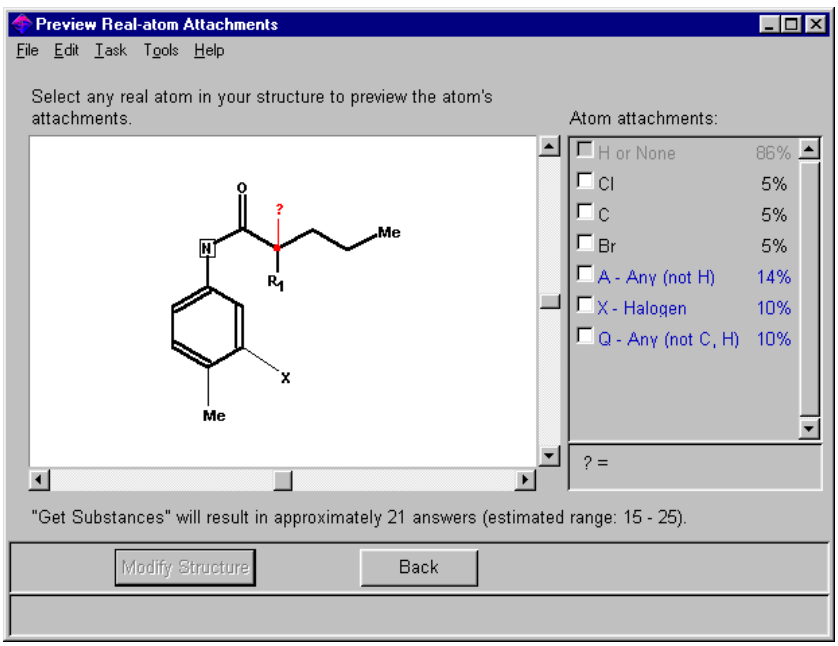


Click **Close** to return to the **Preview Answers** window. Then click **Back** to return to the **Preview** dialog box to choose another Preview option.

Previewing Real-Atom Attachments

To preview real-atom attachments, click the radio button next to **Real-atom attachments** in the **Preview** dialog box. Then click **OK**. The **Preview Real-atom Attachments** window is displayed.

Click an atom in the structure to get an estimate of the attachments you can expect at that node in your **Get Substances** answer set. The node you click is labeled with a bond to a question mark. The preview information for that node is displayed in the **Atom attachments** box to the right. Definite substitutions appear in black, and variable substitutions, e.g., A, appear in blue. The total number of answers is the sum of the definite substitutions. The variable substitution answers are also represented by definite substitution answers.



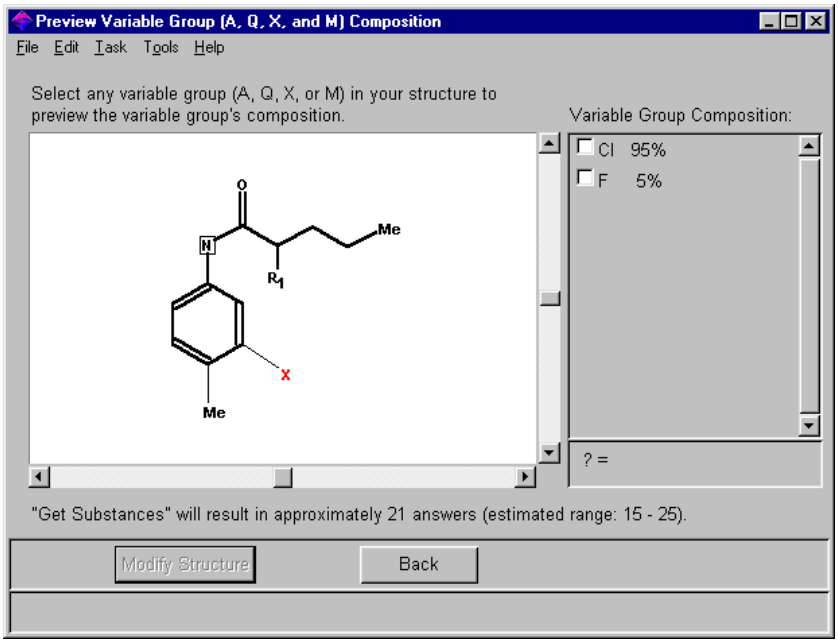
You may click a check mark in one or more boxes under **Atom attachments** to include those nodes in your query. Then click **Modify Structure**. The structure in your Structure Drawing window will be modified to reflect this change.

Or, click **Back** to return to the **Preview** dialog box to choose another Preview option.

Previewing Variable Group Composition

To preview variable group composition, click the radio button next to **Variable group (A, Q, X, and M) composition** in the **Preview** dialog box. Then click **OK**. The **Preview Variable Group (A, Q, X, and M) Composition** window is displayed.

Click a variable, e.g., X, to highlight it. The Preview information for that variable is displayed in the **Variable Group Composition** box to the right.

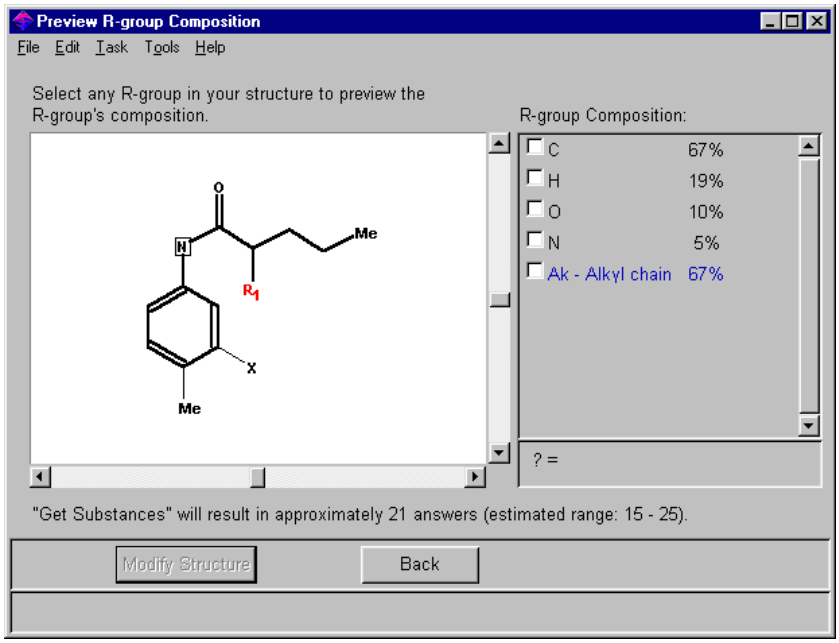


You may click a check mark in one or more boxes under **Variable Group Composition** replace the variable with the selected nodes. Then click **Modify Structure**. The structure in your Structure Drawing window will be modified to reflect this change.

Or, click **Back** to return to the Preview dialog box to choose another **Preview** option.

Previewing R-group Composition

To preview by R-group composition, click the radio button next to **R-group composition** in the **Preview** dialog box. Then click **OK**. The **Preview R-group Composition** window is displayed. Click an R group, e.g., R1, to highlight it. The Preview information for that R group is displayed in the **R-group Composition** box to the right.



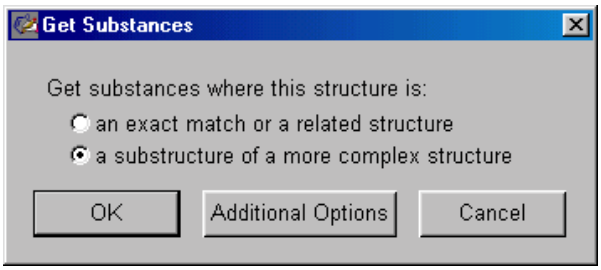
You may click a check mark in one or more boxes under **R-group Composition** to narrow your query to only those structures. Then click **Modify Structure**. The structure in your Structure Drawing window will be modified to reflect this change.

Or, click **Back** to return to the **Preview** dialog box.

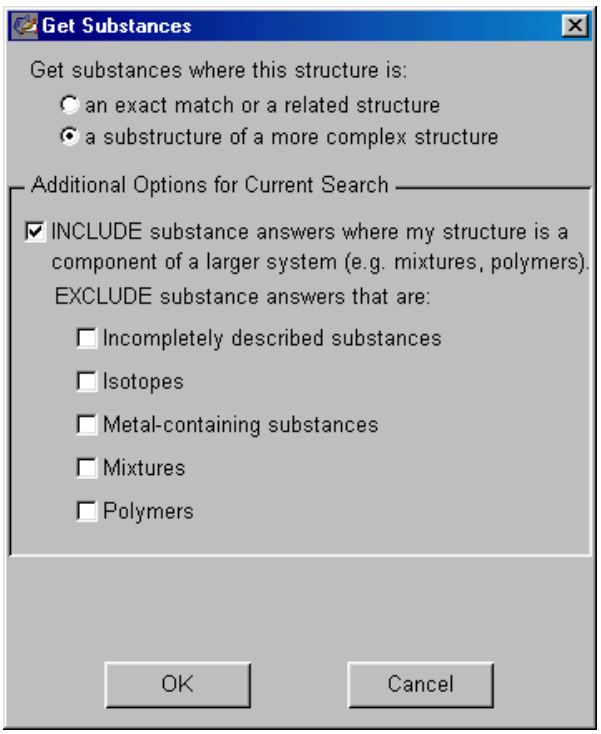
When you are satisfied with your query, click **Cancel** in the **Preview** dialog box to return to the Structure Drawing window.

Performing a Substructure Search

When you are satisfied with your search structure, click **Get Substances** in the Structure Drawing window to perform the search. The **Get Substances** dialog box is displayed.



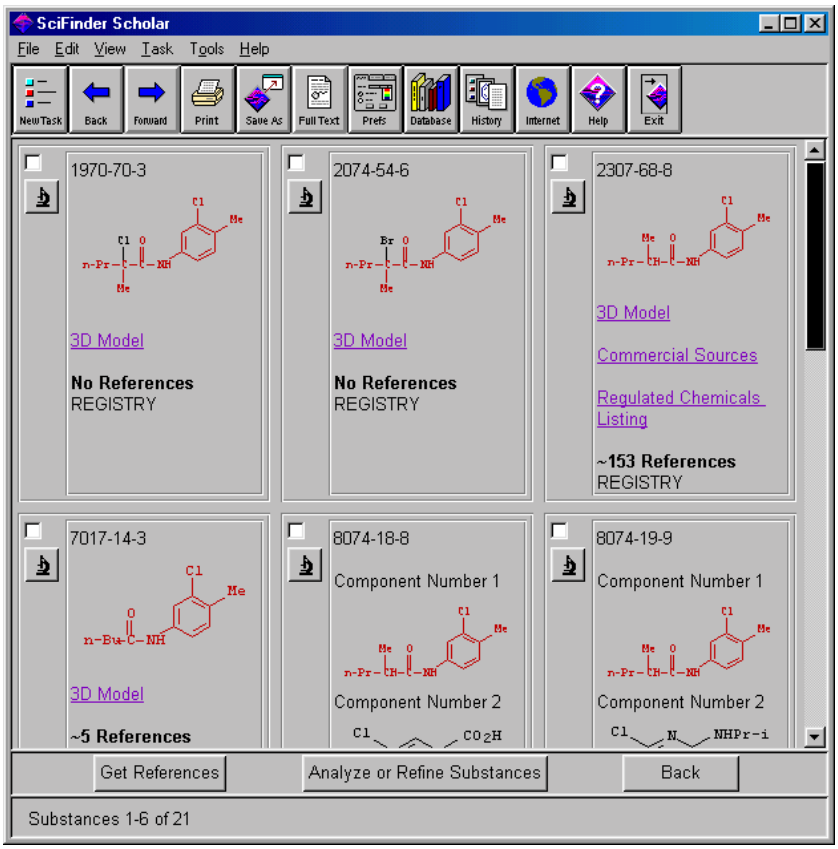
To modify your Explore options for the current search only, click the **Additional Options** button.



The options are the same as those found in the **Explore** tab of the **Preference Editor**. Select the substance types to include or exclude from your search. For details about Explore options or changing your Explore Preferences, see Appendix A, *Preferences*.

To submit a substructure search, click the radio button next to **a substructure of a more complex structure.** Then click **OK**.

SciFinder Scholar conducts the search and displays the answers in the **SciFinder Scholar** window.



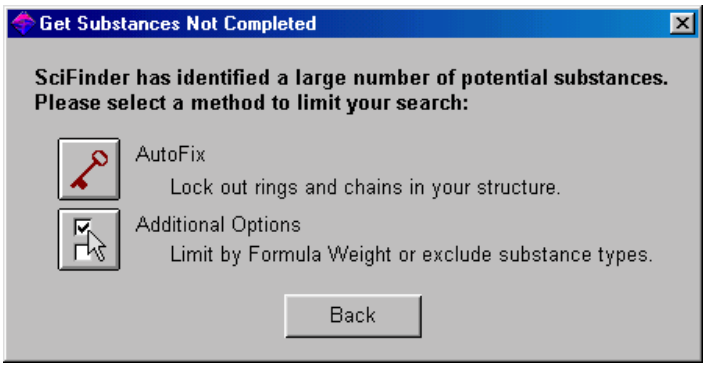
Your query structure is highlighted within the structures in the answer set. This helps you more readily identify where your structure is contained in the answer structures and perhaps why particular answers were retrieved.

Results are displayed in the default format and order. To change the display, select from options in the **View** menu. Or, change the defaults in the **Display** tab of the **Preference Editor**. See Appendix A, *Preferences*, for details.

You may view the structures with the **microscope** icon, select and keep specific answers, **Get References**, and **Refine Substances**, just as you would for an exact structure search. See the corresponding sections on these topics in Chapter 4. For saving and printing instructions, see Chapter 2.

Get Substances Not Completed

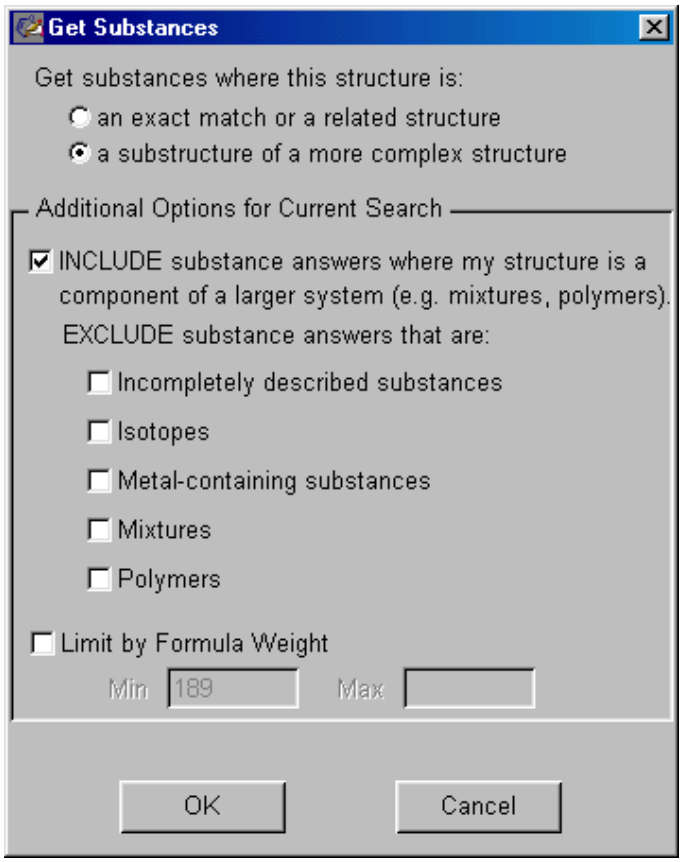
If a large number of potential answers are identified, an alert is displayed.



The AutoFix feature and Additional Options may help narrow your query.

Click the **AutoFix** button to lock out all rings and chains, as if you had applied the **Lock Out Rings** tool. This prohibits fusion to the ring and sets all chain bonds to chain only. You are returned to the Structure Drawing window, and all of the rings and chains in your structure appear in bold. Click **Get Substances** to try the search again.

Alternatively, click **Additional Options** to modify your Explore options for current search only.



The options are similar to those found in the **Explore** tab of the **Preference Editor**. Select the substance types to include or exclude from your search. For details about Explore options or changing your Explore Preferences, see Appendix A, *Preferences*.

The **Limit by Formula Weight** option allows you to narrow your query to substances in a particular formula weight range. This option is only available for single-component structure queries. The **Min** box is prefilled by SciFinder Scholar with the formula weight of your query, provided at the bottom right of the Structure Drawing window. Edit the **Min** and **Max** to reflect the formula weight range of interest.

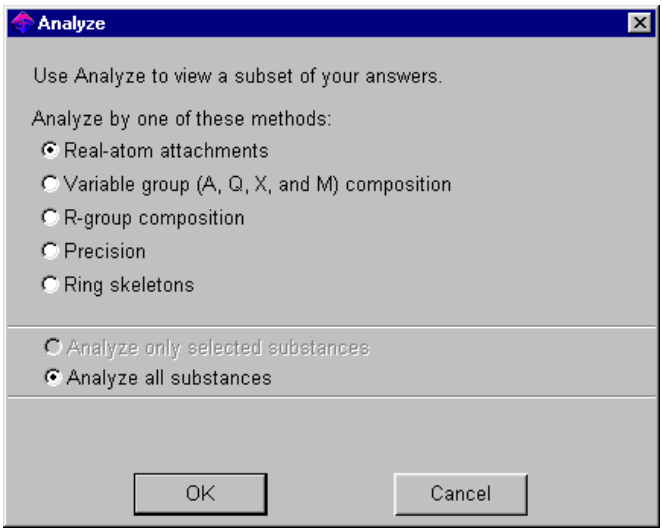
Multiple-component answers will be retrieved if at least one component matches the structure query *and* falls in the formula weight range.

Click **OK** to try the search again.

Analyzing Substances

The Analyze Substances feature is useful for working with large answer sets obtained by substructure searching. This feature works similarly to the Preview feature described earlier in this chapter.

To begin analyzing your answer set, click the **Analyze Substances** button in the **SciFinder Scholar** window. The **Analyze** dialog box appears, displaying the analysis options.



Select an analyze method by clicking the appropriate radio button:

- **Real-atom attachments** – allows you to determine the types of attachments present at a particular site
- **Variable group (A, Q, X, and M) composition** – allows you to determine the atoms at particular variable sites
- **R-group composition** – allows you to determine the atoms that make up particular R groups
- **Precision** – identifies the types of answers that make up your answer set, i.e., conventional substructure, closely or loosely associated tautomers and zwitterions, or other
- **Ring Skeletons** – divides the answer set on the basis of substances' skeletons, atoms, and bonds

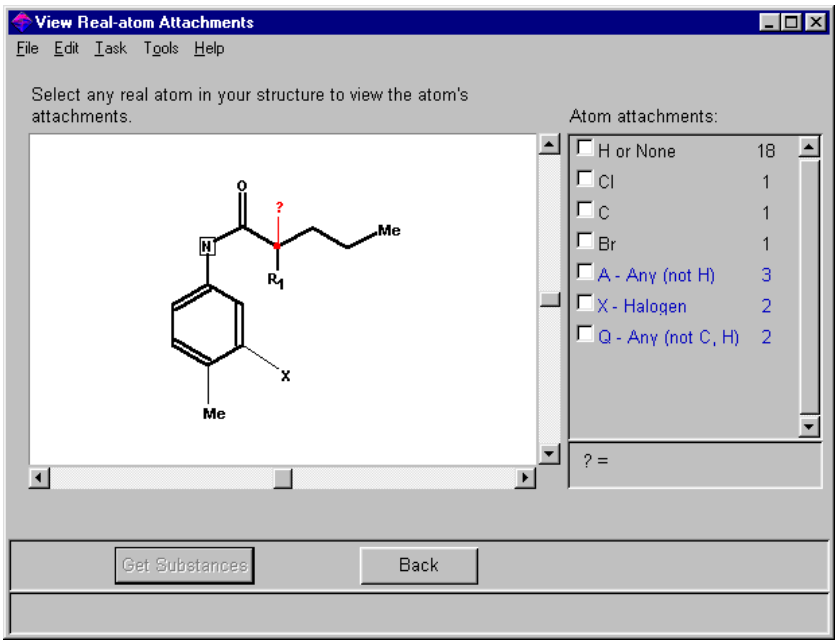
You may choose to analyze the full answer set or a subset of the answers. To select a subset of answers to analyze, click **Cancel** to return to the **SciFinder Scholar** window. Then select a subset of answers by clicking in boxes next to the substances you would like to analyze. Click **Analyze Substances** to redisplay the **Analyze** dialog box. The radio button next to **Analyze only selected substances** is selected.

Click **OK** to begin analyzing.

Analyzing by Real-Atom Attachments

To analyze by real-atom attachments, click the radio button next to **Real-atom attachments** in the **Analyze** dialog box. Then click **OK**. The **View Real-atom Attachments** window is displayed, which shows your query structure.

Click an atom in the structure to display the types of attachments at that atom in the answer set structures. The node you click is labeled with a bond to a question mark, and the results are displayed in the **Atom attachments** box to the right. Definite substitutions appear in black, and variable substitutions, e.g., A, appear in blue. The total number of answers is the sum of the definite substitutions. The variable substitution answers are also represented by definite substitution answers.



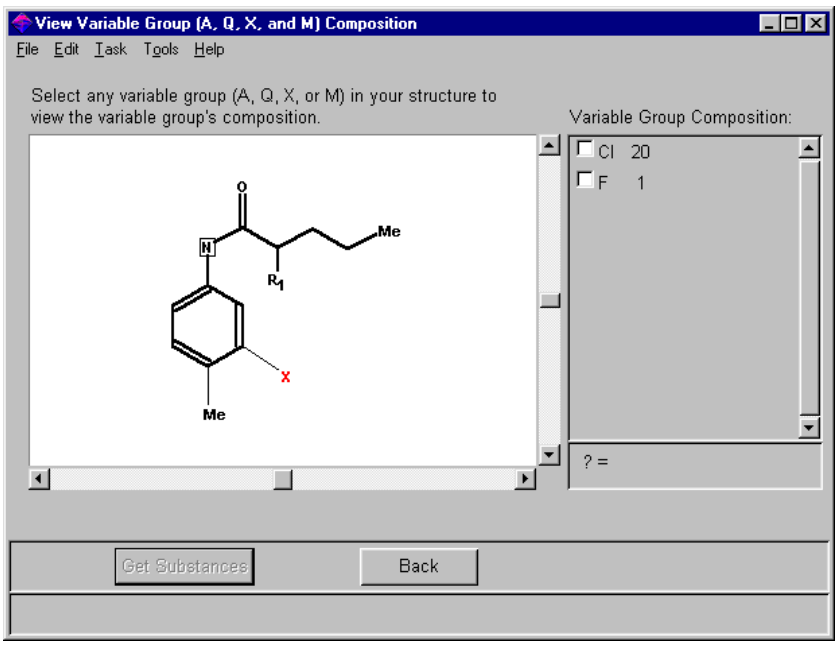
You may click a check mark in one or more of the boxes under **Atom attachments** to narrow your answer set to only those structures that have the specified attachments. Click **Get Substances** to create the smaller answer set.

Or, click **Back** to return to the **Analyze** dialog box to choose another Analyze option.

Analyzing by Variable Group Composition

To analyze by variable group, click the radio button next to **Variable group (A, Q, X, and M) composition** in the **Analyze** dialog box. Then click **OK**. The **View Variable Group (A, Q, X, and M) Composition** window is displayed.

Click a variable, e.g., X, to highlight it. The composition at that variable in the answer set is displayed in the **Variable Group Composition** box to the right.



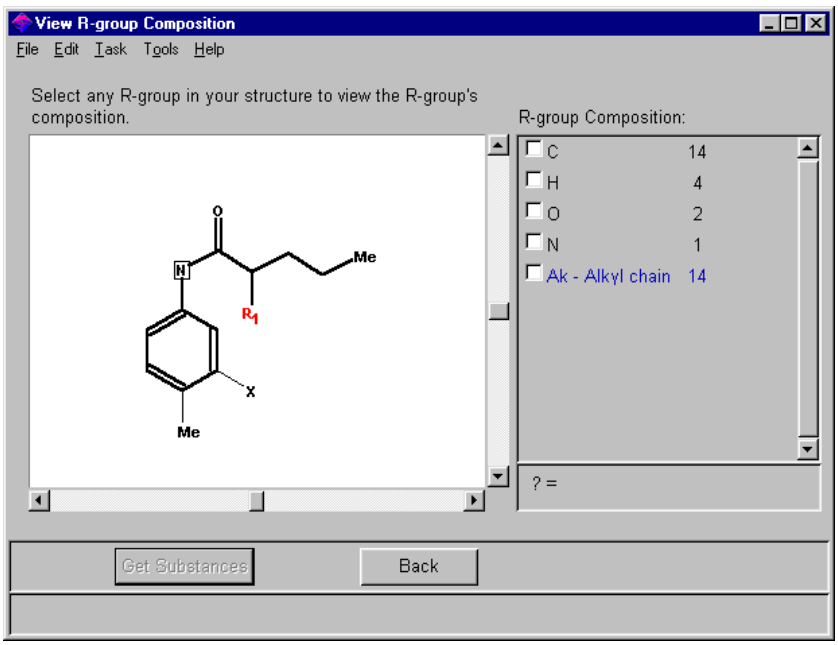
You may click a check mark in one or more of the boxes under **Variable Group Composition** to narrow your answer set to only those structures that have the specified composition attached at this position. Click **Get Substances** to create the smaller answer set.

Or, click **Back** to return to the **Analyze** dialog box to choose another Analyze option.

Analyzing by R-group Composition

To analyze by R group, click the radio button next to **R-group composition** in the **Analyze** dialog box. Then click **OK**. The **View R-group Composition** window is displayed.

Click an R group, e.g., R1, to highlight it. The composition of that R group in your answer set is displayed in the **R-group Composition** box to the right.



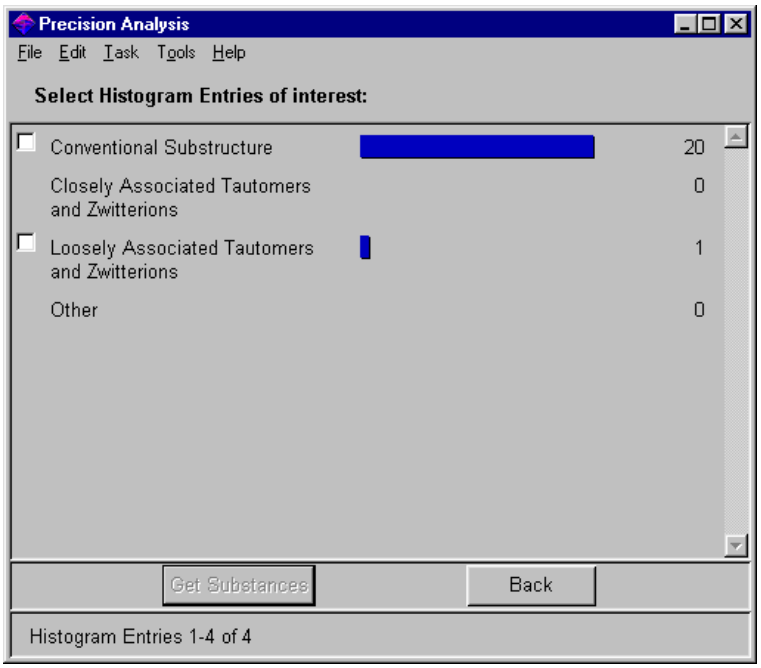
You may click a check mark in one or more boxes under **R-group Composition** to narrow your answer set to only those structures that have the specified atom at this position. Click **Get Substances** to create the smaller answer set.

Or, click **Back** to return to the **Analyze** dialog box to choose another Analyze option.

Analyzing by Precision

Analyze by Precision allows you to see the types of answers that make up your answer set.

To analyze by precision, select the radio button next to **Precision** in the **Analyze** window and click **OK**. The **Precision Analysis** window is displayed, showing the makeup of the answer set.



The answers are divided into four categories:

- Conventional Substructure
- Closely Associated Tautomers and Zwitterions
- Loosely Associated Tautomers and Zwitterions
- Other

You may click a check mark in one or more boxes in the **Precision Analysis** window to narrow your answer set to only those answers in a particular category. Click **Get Substances** to create the smaller answer set.

Or, click **Back** to return to the **Analyze** dialog box to choose another Analyze option.

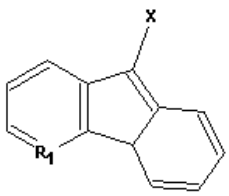
Analyzing by Ring Skeletons

Analyze by Rings divides a substance answer set into subsets, or buckets, of substances that contain rings with similar skeletons, atoms, or bonds. Each bucket shows a ring for which there is at least one atom from the query structure. These rings are referred to as "matched rings." The number of substances in the answer set that contain the matched ring is indicated.

Answer sets may be analyzed on the basis of:

- Ring skeleton only
- Ring skeleton and atoms contained in the rings
- Ring skeleton, atoms contained in the rings, and bonds involved

For this example, build the following structure in a Structure Drawing window:



R = C, N

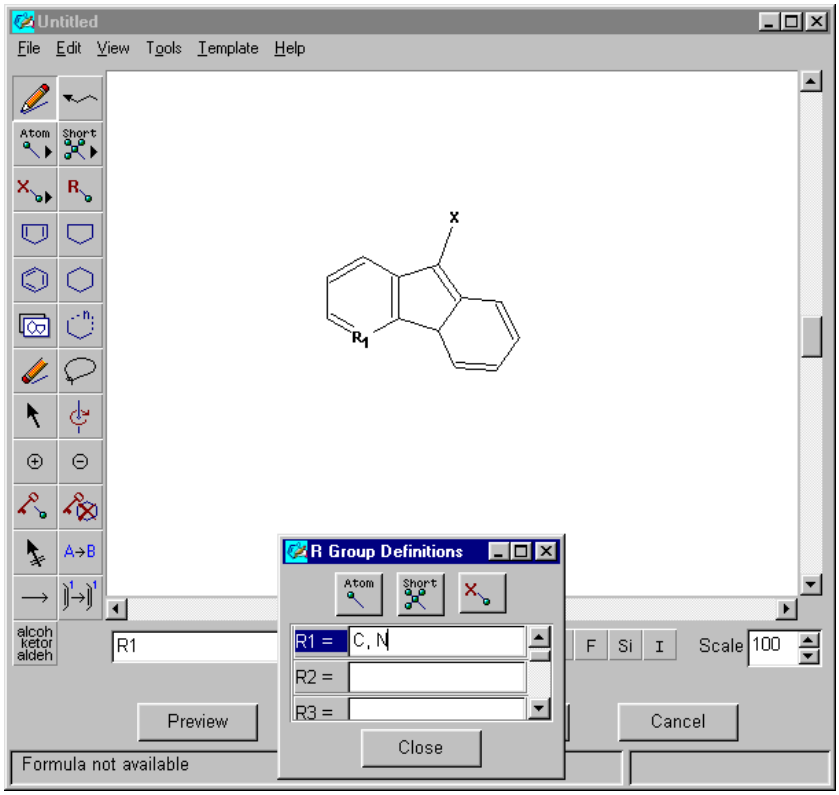
1. Begin by drawing the ring skeleton. Click the **Benzene** tool icon on the **Vertical Tool Palette**. Place the cursor in the Structure Drawing window, and click to draw a benzene ring.

   Click the **Cyclopentadiene** tool icon. Position your cursor over the rightmost bond of the benzene ring. Click to draw a cyclopentadiene ring fused to the benzene.

   Click the **Benzene** tool icon again. Position your cursor over the bottom right bond of the ring system already drawn in the Structure Drawing window. Click to fuse a benzene ring to the ring system.

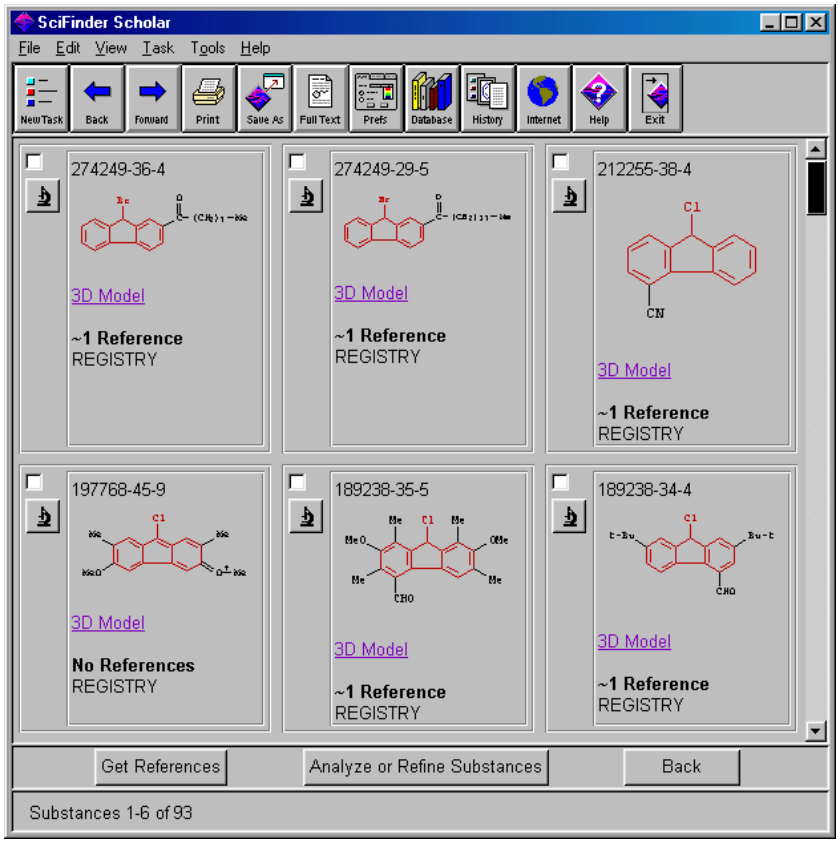
2. Click and hold the **X Menu (Variables)** tool icon to display the variables menu. Select **X Any halogen**. Add an X substituent to the ring skeleton as shown above.

3. Click the **R Group** tool icon to display the **R Group Definitions** box. Replace a carbon in the ring system with R1 as shown above. In the **R Group Definitions** box, define R1 as C or N.



Searching the substructure as shown above will retrieve structures where additional rings may be fused to the ring skeleton. In addition, substituents may appear at any open site. Ring fusion and additional substitution may optionally be blocked with use of the **Lock Out Rings Tool** and **Lock Out Substitution Tool**.

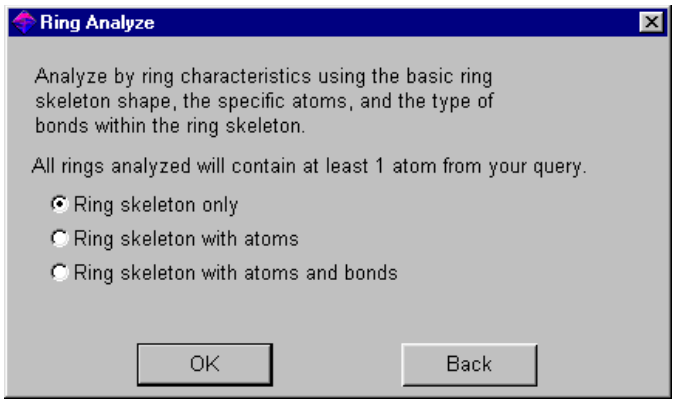
To retrieve substances that contain your substructure query, click **Get Substances**. Select **a substructure of a more complex structure**. Then click **OK**. SciFinder Scholar conducts the search and displays the answers in the **SciFinder Scholar** window.



Your query structure is highlighted within the structures in your answer set. Analyzing by Rings will divide the answer set into groups of substances that contain rings with similar skeletons, atoms, or bonds.

Click **Analyze or Refine Substances**. Then click **Analyze**. To analyze only a portion of the answer set, select boxes next to substances of interest before clicking **Analyze Substances**. The **Analyze** dialog box is displayed. Select **Ring Skeletons**, and choose whether to analyze all answers or only those selected. Click **OK**.

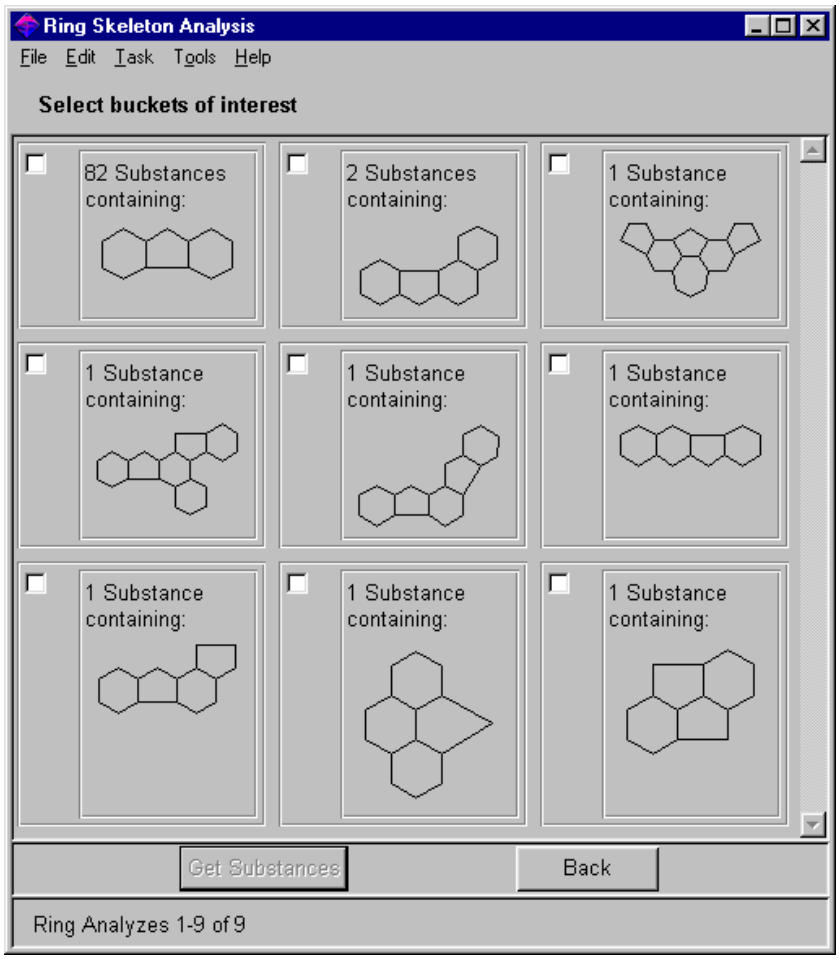
The **Ring Analyze** dialog box is displayed.



Select an option in the **Ring Analyze** dialog box. Then click **OK**.

Analyzing by Ring Skeleton Only

Analyzing by Ring Skeleton Only divides the answer set on the basis of ring framework without regard to the atoms or bonds involved. In the **Ring Analyze** dialog box, select **Ring skeleton only**. Then click **OK**. Buckets are displayed for all ring skeletons in the substance answer set that contain at least one atom from the query structure.



Buckets containing the most substances from the answer set are displayed first. The number of substances and a ring image are given. In some rare instances, an image for a matched ring cannot be generated. In this event, a “no ring image available” message is displayed instead of the ring image.

One or more additional buckets may appear after the matched ring buckets:

- Rings Not Matched – substances in the answer set that contain rings, but none of the rings contain at least one atom from the query structure
- No Rings – substances that do not contain any rings
- Other – substances for which ring analysis could not be completed

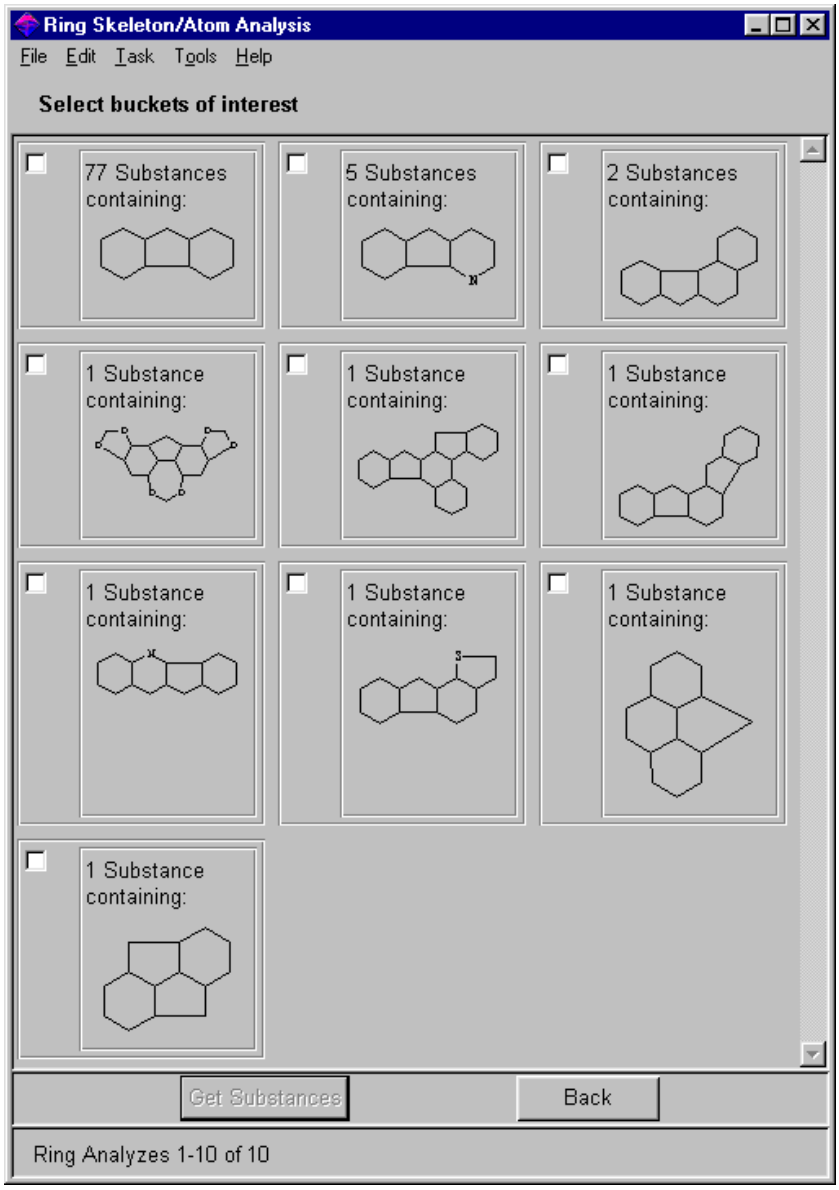
Because a substance answer may contain more than one matched ring, individual answers may appear in more than one ring bucket. Thus, the buckets are not mutually exclusive.

If you are interested in only answers in particular buckets, click the appropriate check boxes. Then click **Get Substances** to view only the substances of interest.

When you have finished viewing the answer set, click **Back** to return to the Ring Analyze options.

Analyzing by Ring Skeleton with Atoms

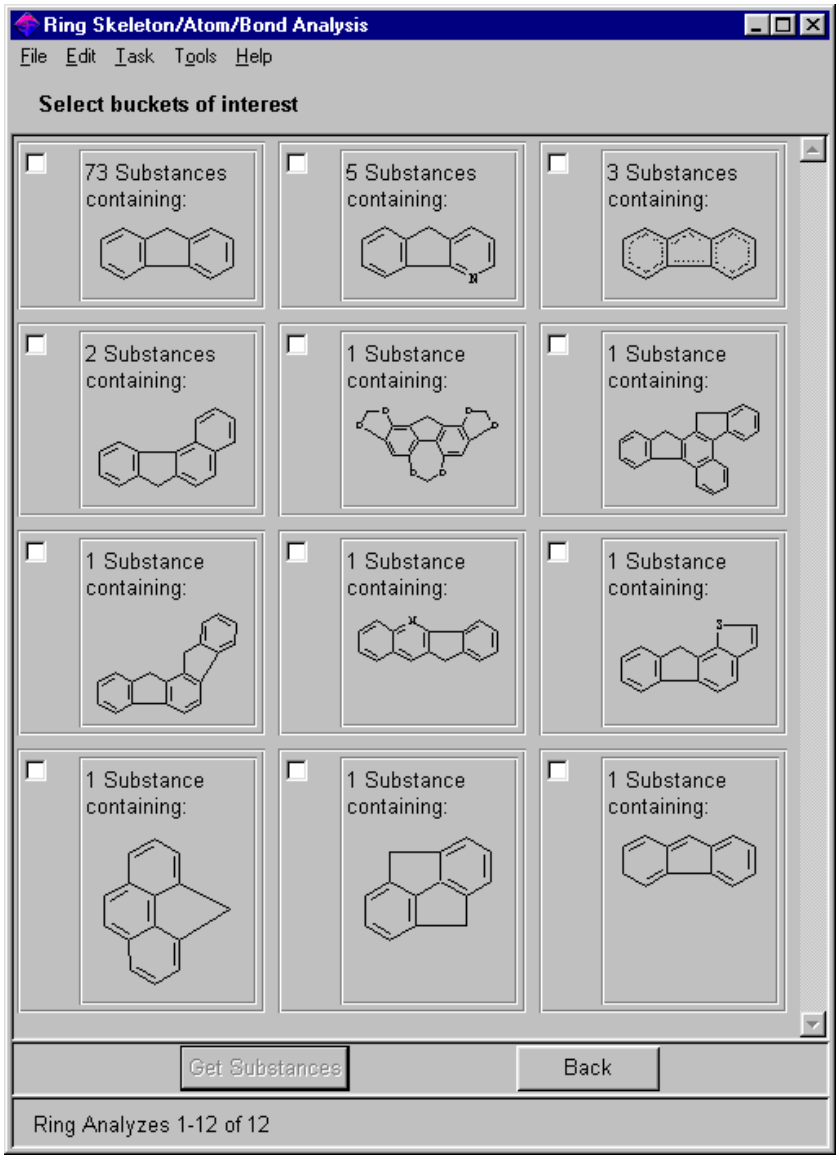
Analyzing by Ring Skeleton with Atoms divides the answers set into groups of substances that contain the same ring skeleton and specific atoms within that skeleton. In the **Ring Analyze** dialog box, choose **Ring skeleton with atoms**. Then click **OK**. Buckets are displayed for ring skeletons that have atoms in the same positions as a ring system in the query structure.



You may select buckets of interest and click **Get Substances**. Or, click **Back** to return to the Ring Analyze options.

Analyzing by Ring Skeleton with Atoms and Bonds

Analyzing by Ring Skeleton with Atoms and Bonds divides the answers set into groups of substances that contain the same ring skeleton and specific atoms and bonds within that skeleton. In the **Ring Analyze** dialog box, choose **Ring skeleton with atoms and bonds**. Click **OK**. Buckets are displayed for ring skeletons that have atoms and bonds in the same positions as a ring system in the query structure.



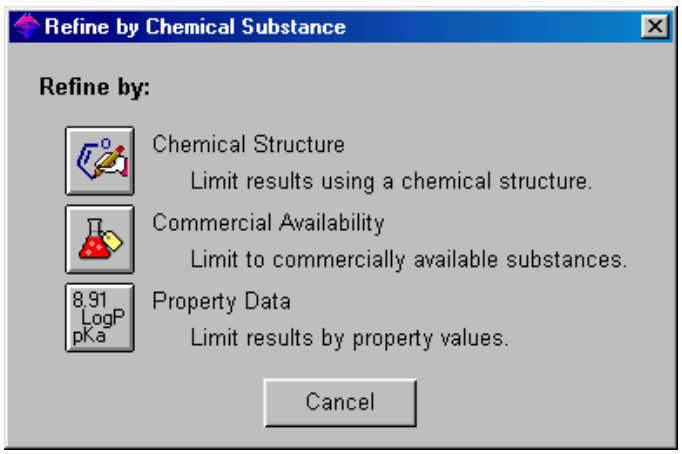
You may select buckets of interest and click **Get Substances**. Or, click **Back** to return to the Ring Analyze options. Click **Back** again to return to the original answer set.

To leave your substructure session, select **New Task** from the **File**

Refining Substances

If you get a large number of substances with your search, the Refine Substances feature may help reduce the size of your answer set. This feature allows you to add additional search criteria to your original search strategy.

Click **Refine or Analyze Substances**. Then click **Refine** to display the **Refine by Chemical Substance** options.



Refine Substances allows you to narrow your answer set by **Chemical Structure**, **Commercial Availability**, or **Property Data** (for SSM users only).

Refine by Chemical Structure

Click **Chemical Structure** to return to the Structure Drawing window. You may make your query more precise by modifying your original structure or by adding a fragment that must be present. After editing the structure, click **Get Substances**. SciFinder Scholar creates a new substance list with your new structure requirements.

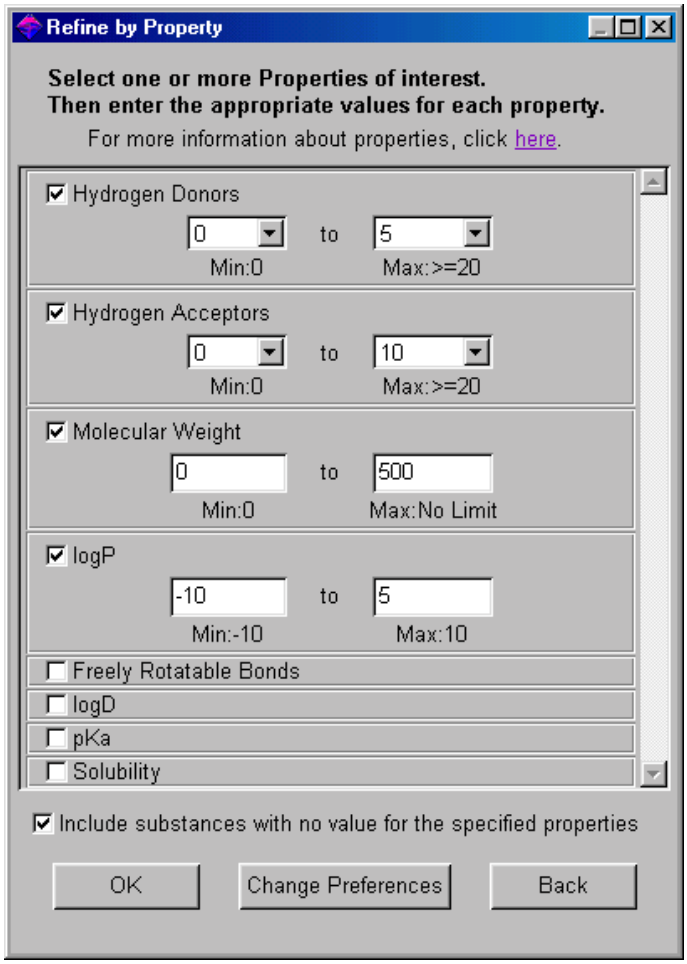
If there is a chemical moiety that you want to require in your answers, e.g., a carboxyl group, but you do not have any particular site where you want it to be attached, delete the original structure and draw that moiety alone. **Get Substances** will then do a subset search on your original answer set.

Refine by Commercial Availability

Click **Commercial Availability** if you are only interested in substances that are commercially available. SciFinder Scholar returns only the substances from your answer set that have Commercial Availability information.

Refine by Property Data

SSM users may click **Properties** to refine the answer set by physical properties. The **Refine by Property** dialog is displayed.



Select the properties you wish to include in your refinement, and indicate the appropriate values for those properties. When multiple properties are selected, results must meet all of the selected property conditions.

Include substances with no value for the specified properties ensures that substances without values available for selected properties are retained in your answer set. Deselect this option if you do not wish to retain those substances.

The first four properties are preselected and prefilled with parameters developed by Christopher A. Lipinski and colleagues at Pfizer Central Research, Groton, CT. Refining by these parameters is helpful in identifying potential drug candidates. These parameters are the initial default values for Refine by Property, found on the **Analyze** tab of the **Preference Editor**.

To change your defaults, click the **Change Preferences** button. If you do not change your defaults, the property selections are kept only for the current search.

The **Preference Editor** opens to the **Analyze** tab (see Appendix A for details). The **Refine by Property** section displays the selections you chose in the **Refine by Property** dialog box. You may make additional changes to the Preferences. Click **OK** to save the new defaults and return to your search.

Once you have made your selections, click **OK** to refine your answer set.

Ending Your Explore Session

To leave your substructure session, select **New Task** from the **File** menu or click the **New Task** icon on the **Main Menu Toolbar**.

To exit SciFinder, select **Exit SciFinder** from the **File** menu or click **Exit** on the **Main Menu Toolbar**.

6

Exploring by Reaction

The reaction searching capability of SciFinder Scholar allows you to search for chemical structures and/or functional groups in reactants/reagents or products. You can search only one side of a reaction or a full reaction. Reaction tools also allow you to map atoms within a reaction and specify reaction sites.

Chapter 6 describes reaction searching via SciFinder Scholar. Examples demonstrate how to draw and perform the following types of reaction searches:

- Chemical structure
  - One side of the reaction
  - Both sides of the reaction
- Functional group
  - Functional group only
  - Combinations of functional group and structure

Introduction to Reaction Searching

The Get Reactions feature initiates a search where you may find:

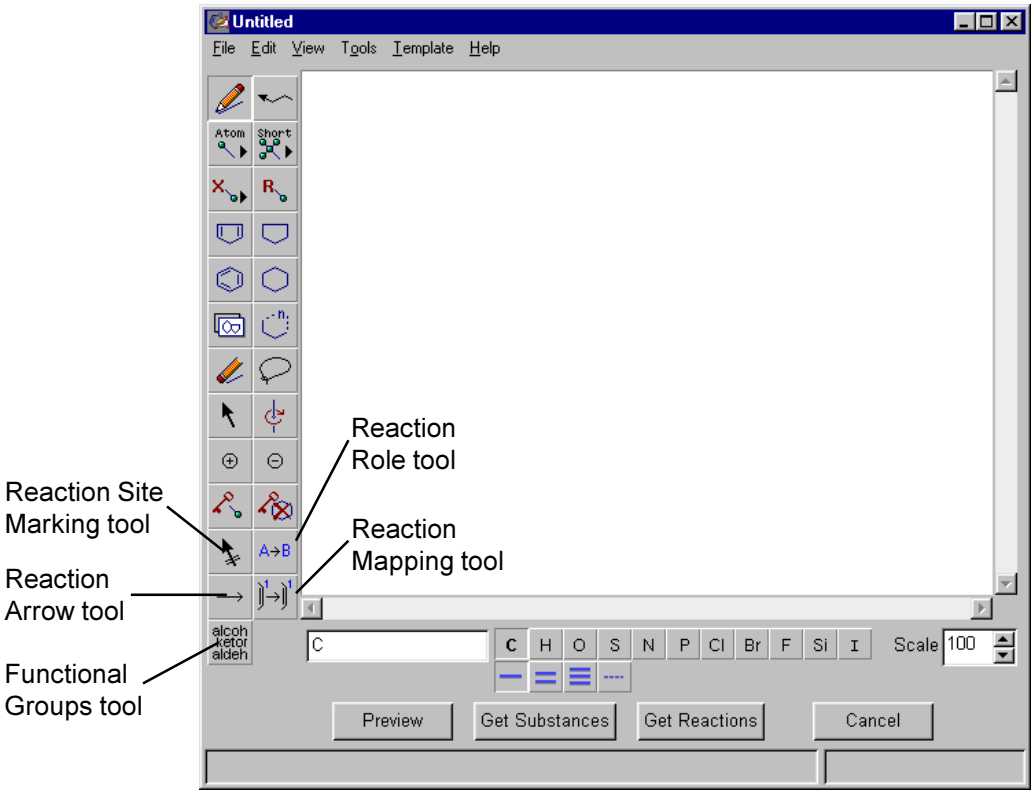
- Reactions that match or contain your query substructures and/or functional groups
- Preparation methods for a specific substance
- Commercial sources for the reaction materials
- Regulated chemicals listings for substances
- Abstracts and references describing the reactions in more detail

SciFinder Scholar searches for reactions in a document-based database. Thus, retrievals are actually documents containing reactions. For example, if a search retrieves 10 answers, SciFinder Scholar displays the first hit reaction from each document, i.e., the first single step or multiple step reaction in the document that matches your query substructure, for each of the 10 documents. Additional hit reactions can be displayed by clicking the **microscope** icon for that answer.

Reaction searching does not use the convention-free Smartsearch capabilities described in Appendix C.

Accessing Explore by Reaction

Reaction queries are drawn in a Structure Drawing window. To access a Structure Drawing window, click the **Chemical Substance or Reaction** icon in the **Explore** window. Then click **Chemical Structure**. An **Untitled** Structure Drawing window is displayed.

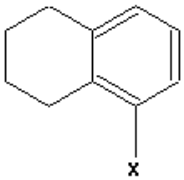


The tools labeled above are used exclusively for reaction queries. More information on these drawing tools, located in the **Vertical Tool Palette**, can be found in Chapter 4.

Rather than draw a reaction in the Structure Drawing window, you may use previously saved structure or reaction queries by selecting the **Open** command from the **File** menu. See Appendix B, *Importing and Exporting Structure Queries*, for details.

Searching One Side of a Reaction

To find reactions that contain a structure, first build the structure. Follow these steps to build the structure shown here.

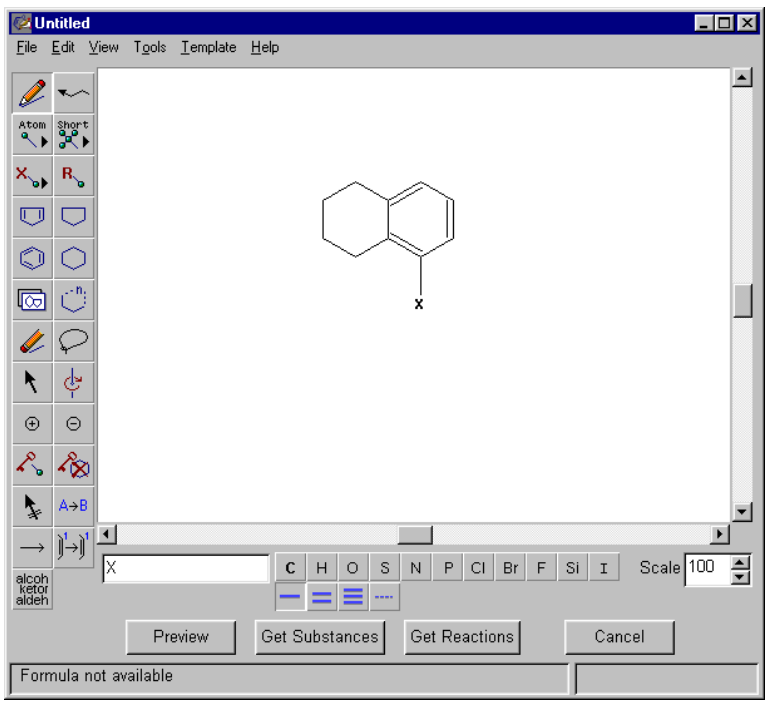


1. Select the **Benzene Ring** tool from the **Vertical Tool Palette**. Place the ring cursor arrowhead in the center of your Structure Drawing window and click to place the benzene ring.

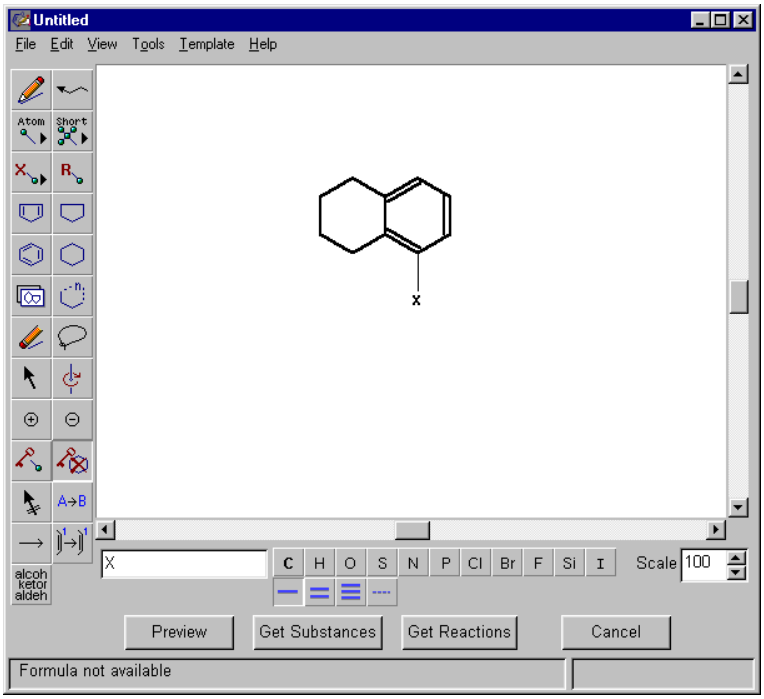
2. Click the **Cyclohexane Ring** tool icon from the **Vertical Tool Palette**. Place the ring cursor arrowhead on the left bond of the benzene ring to highlight that bond. Click to fuse the cyclohexane ring to the benzene ring.

3. Click the **X Menu** tool icon from the **Vertical Tool Palette**. Continue to hold your mouse button to display the X menu. Select **X Any Halogen**.

   Place the pencil tip on the bottom node of the benzene ring. Press your mouse button and drag the pencil away from the node to create a 1-atom chain. Release your mouse button to display X single bonded to the ring.

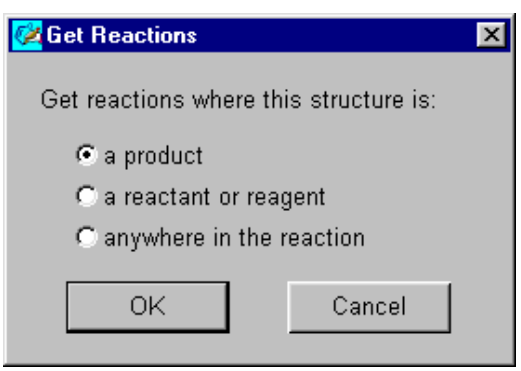


4. Click the **Lock Out Rings** tool icon from the **Vertical Tool Palette**. Place the cursor tip on any ring bond to highlight the entire ring system and click. The entire ring system displays in bold. This means that no other rings will be fused to this ring system in the search results.



Retrieving Reactions That Contain Your Structure

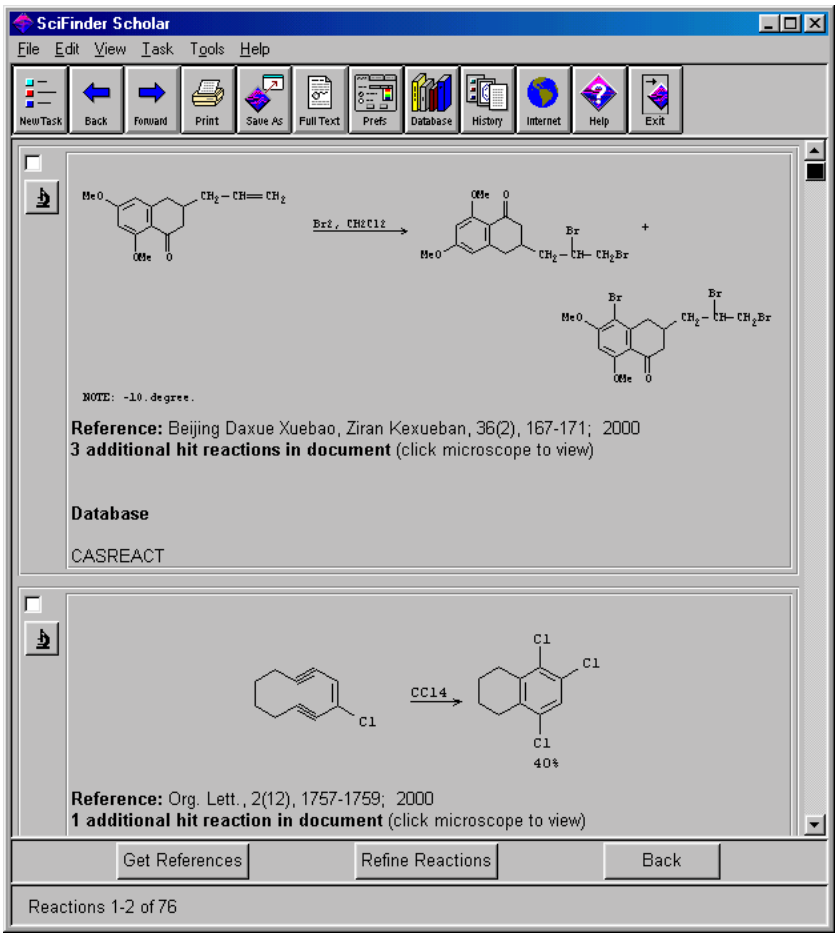
When you have completed the structure drawing, click **Get Reactions**. The **Get Reactions** dialog box is displayed and provides options to define the role of your structure: product, reactant/reagent, or any role, i.e., the structure may occur anywhere in the reaction.



For this example, click **a product**. Then click **OK**. SciFinder Scholar finds any reaction that contains your substructure as a product. Substitution may take place anywhere on the structure, unless prohibited by use of the **Lock Out Substitution** tool.

Viewing Reaction Candidates

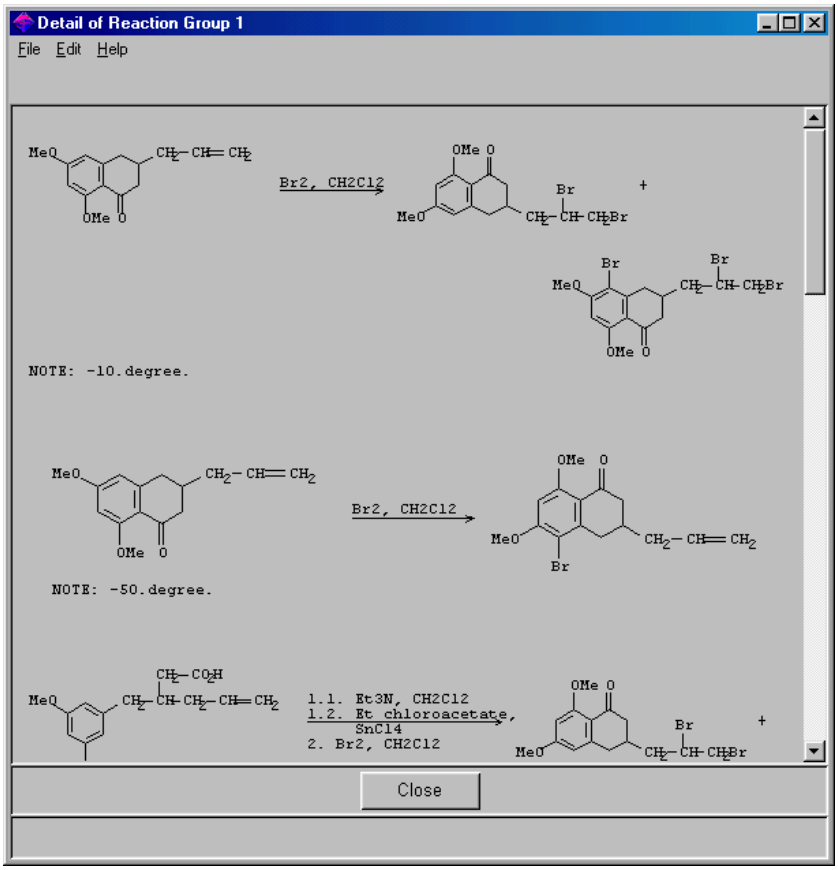
If matches are found, the reaction candidates are displayed in the **SciFinder Scholar** window.



For reactions, only the Full display format is available. It includes the first hit reaction, i.e., the first reaction in the document that matches your query substructure, bibliographic information, and, if applicable, notes about the reaction and the number of hit reactions in the document. Hit reactions may be multiple step reactions in which your query is only a part of the full reaction.

Viewing Additional Hit Reactions

When additional hit reactions exist in a document, they can be viewed by clicking the **microscope** icon next to the answer. A **Detail of Reaction Group #** window is displayed that contains all hit reactions for that reference.



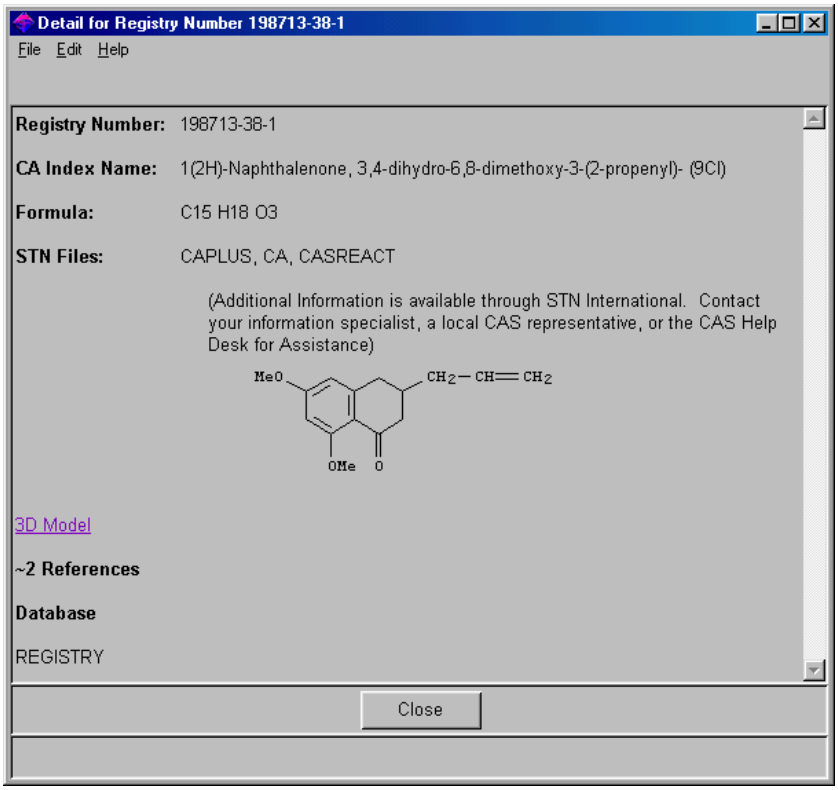
Other reactions may also exist for a given document besides the hit reactions. However, these reactions cannot be displayed.

You may print or save the details by selecting **Print** or **Save As** from the **File** menu. See Chapter 2 for details.

To return to the **SciFinder Scholar** window, click **Close**.

Viewing Substance Records for Reaction Components

To see the CAS Registry Number, Chemical Name, Molecular Formula, and more for any substance participating in a reaction, place your cursor over that substance and click. A **Detail for Registry Number #** window is displayed.



The substance record is displayed in the default format. The default may be changed in the **Display** tab of the **Preference Editor**. See Appendix A, *Preferences*, for details.

You may print or save the substance record by selecting **Print** or **Save As** from the **File** menu. See Chapter 2 for details.

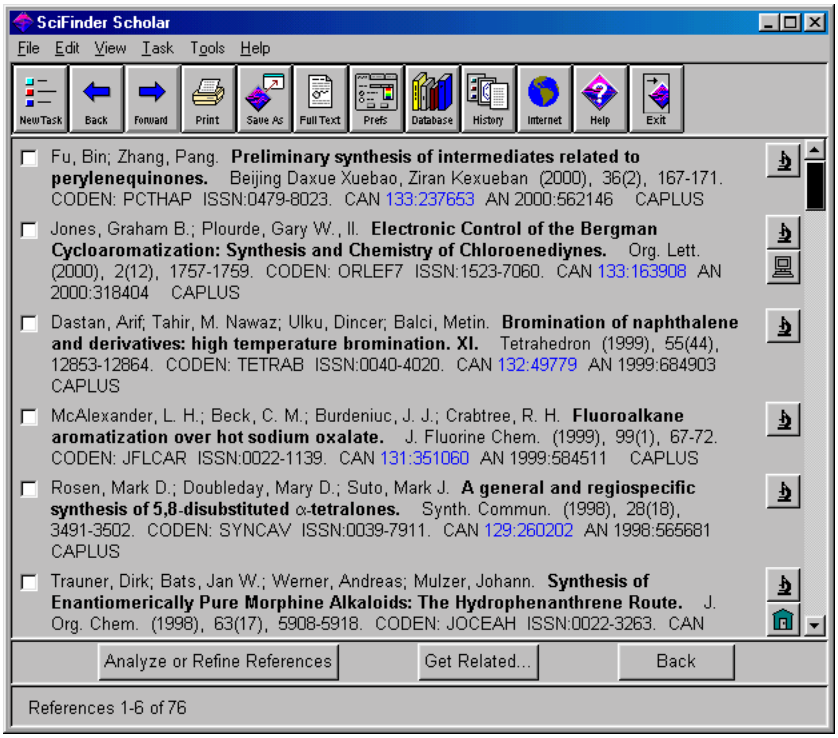
To return to the **SciFinder Scholar** window, click **Close**.

Retrieving References for Reaction Results

To retrieve references discussing hit reactions in more detail, click the boxes to the left of reactions of interest. You may click as many boxes as you like. Then click **Get References**. The **Get References** dialog box is displayed.

Choose to retrieve references for all reactions or only those you selected. Then click **OK**.

The references are displayed in the **SciFinder Scholar** window.



References are displayed in the default format and order. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

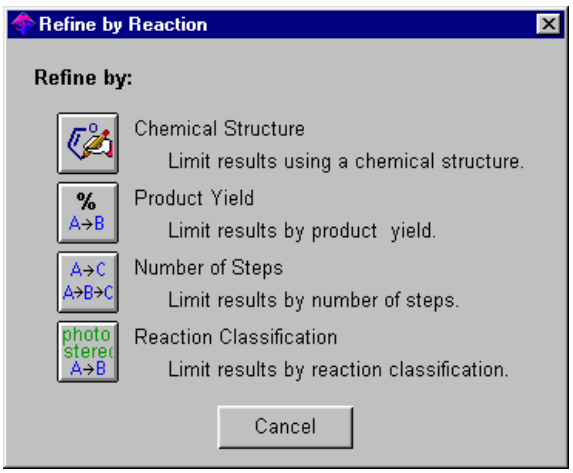
Click **Back** to return to the reaction results.

Keeping Reactions

If a large number of reaction hits are returned, you may choose to keep only a subset of those hits. To do so, click the check boxes next to the reactions you would like to keep. Then select **Keep Reactions** from the **Tools** menu. SciFinder Scholar displays only those candidates you selected.

Refining Reactions

Refine Reactions allows you to change or narrow an existing reaction query. Click the **Refine Reactions** button at the bottom of the **SciFinder Scholar** window to view reaction refinement options. The **Refine by Reaction** dialog box is displayed.



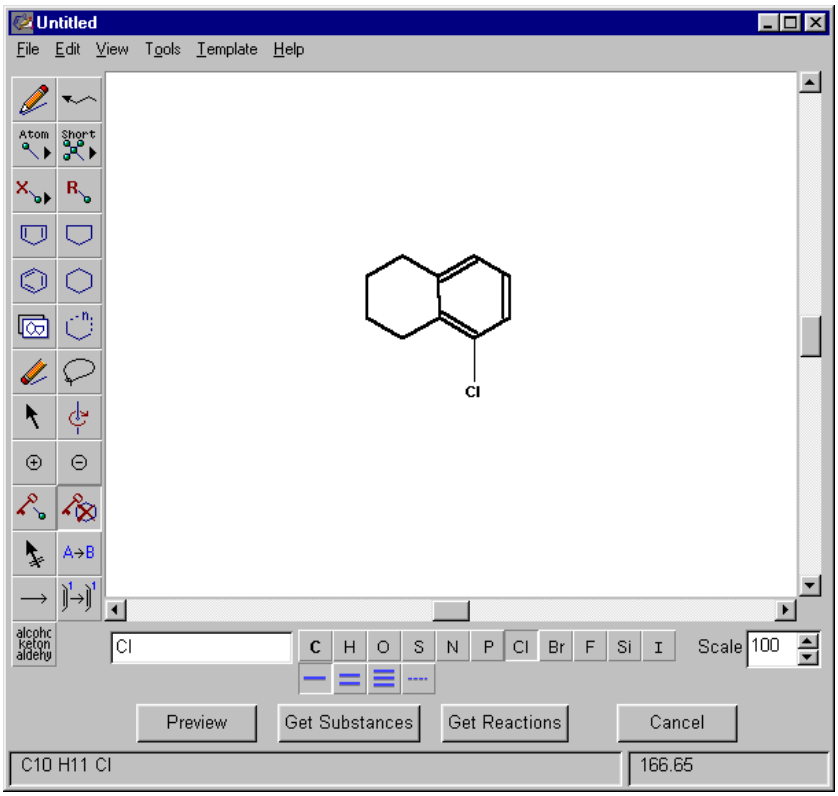
You may refine by:

- Chemical Structure
- Product Yield
- Number of Steps
- Reaction Classification

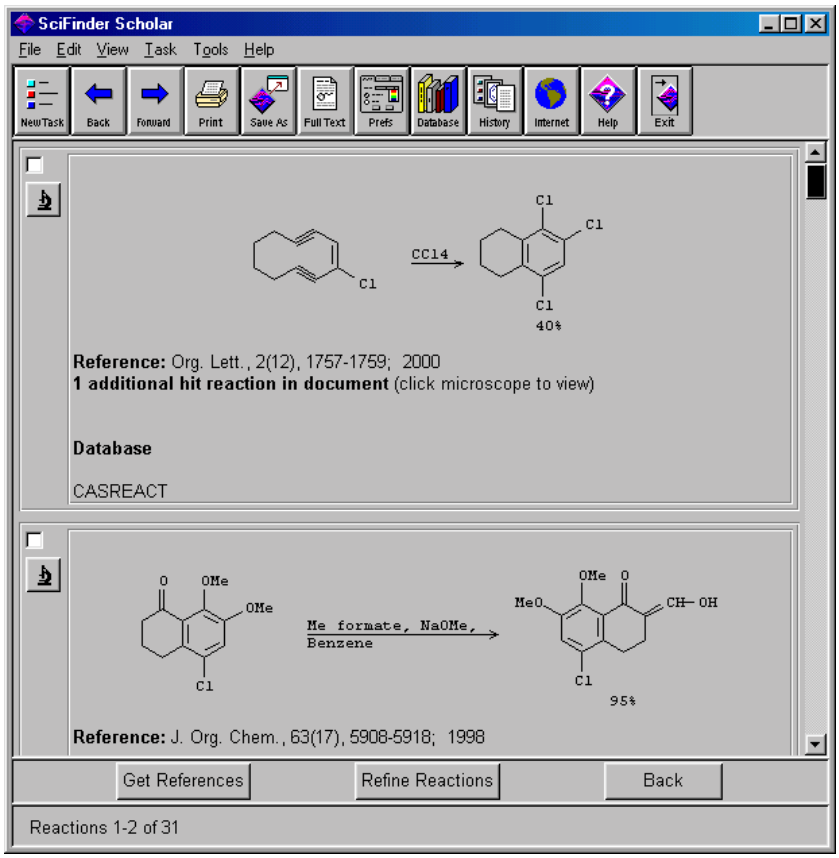
Refining by Chemical Structure

Refine by Chemical Structure allows you to add structural requirements to your original reaction query. Click **Chemical Structure** in the **Refine by Reaction** dialog box. A Structure Drawing window containing your current reaction query is displayed.

For this example, refine your answer set to include only answers that have Cl at the X position. Click **Cl** on the **Common Atoms** palette. Then place the cursor over the **X** in the structure and click. The X is replaced by Cl.



Click **Get Reactions** to retrieve the subset of reactions that contain the new structure. The first hit reaction for each answer is displayed in the **SciFinder Scholar** window.

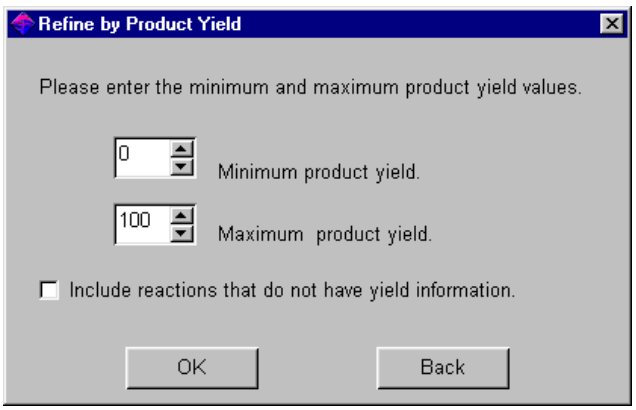


When you are finished viewing the answer set, click **Back**. Then click **Cancel** in the Structure Drawing window to return to your original answer set. Click **Refine Reactions** to return to the refine options.

Refining by Product Yield

Refine by Product Yield allows you to limit your answer set to reactions with a specific percent yield or a range of percent yields.

Click **Product Yield** in the **Refine by Reaction** dialog box. The **Refine by Product Yield** dialog box is displayed.



Set the minimum and maximum product yields you would like to include. Click the up or down arrows to increase or decrease the displayed number by 5. Or, type any number directly into the box.

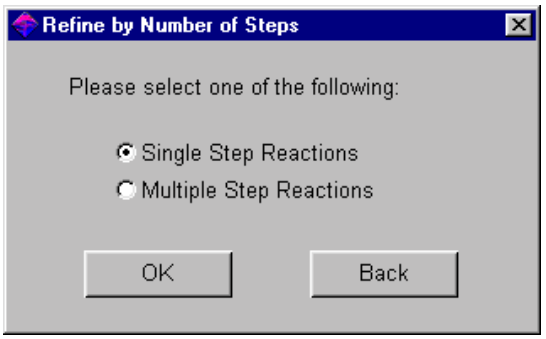
Some products do not have yield information available. To retain these reactions in the answer set, check the box next to **Include reactions that do not have yield information**. Click **OK**. Your revised answer set is displayed in the **SciFinder Scholar** window.

When you are finished viewing the answers, click **Back**. Then click **Back** again to return to your original answer set. Click **Refine Reactions** to select another refine option.

Refining by Number of Steps

Refine by Number of Steps allows you to distinguish single step reactions from multiple step reactions.

Click **Number of Steps** in the **Refine by Reaction** dialog box. The **Refine by Number of Steps** dialog box is displayed.



Choose **Single Step Reactions** or **Multiple Step Reactions**, and click **OK**. The appropriate reactions are displayed in the **SciFinder Scholar** window.

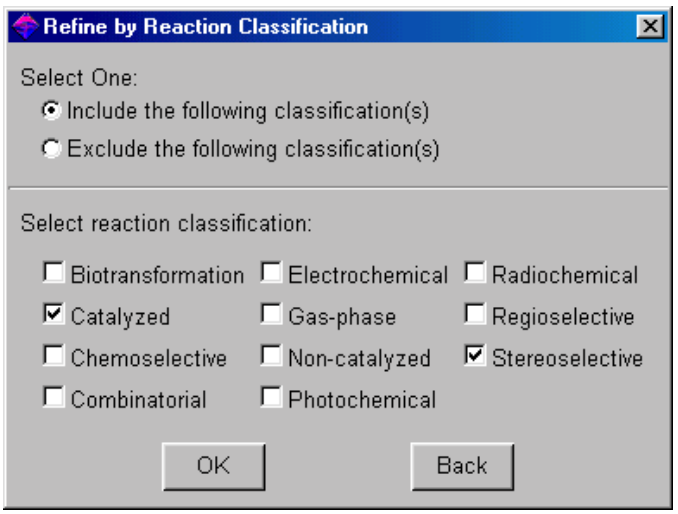
You may click **Get References** or refine your search even more. Or, click **Back** to return to the Structure Drawing window. Click **Refine Reactions** to select another refine option.

Refining by Reaction Classification

Refine by Reaction Classification allows you to limit your answer set to particular types of reaction documents. Likewise you may exclude particular types of reaction documents. Because answers may fit more than one classification, the categories are not mutually exclusive.

SciFinder Scholar determines which documents contain reactions with particular attributes, e.g., stereoselective, gas phase, or electrochemical. You may choose one or more attributes to include in, or exclude from, your answers.

Click **Reaction Classification** in the **Refine by Reaction** dialog box. The **Refine by Reaction Classification** dialog box is displayed.



Select whether to include or exclude specific reaction classifications. Then select one or more classifications. Click **OK**. The reaction documents with the attributes you selected are displayed in the **SciFinder Scholar** window.

When you are finished viewing the answer set, click **Back**. Then click **Back** again to return to your original answer set.

Searching Both Sides of a Reaction

To perform a full-reaction search, build the reaction you would like to search. Follow these steps to build the reaction shown here.

1. Select the **Pencil** tool from the **Vertical Tool Palette**. Draw a two-atom chain, for the reactant, at the left of the Structure Drawing window.

2. Click the **Cyclohexane** tool from the **Vertical Tool Palette**. Draw a cyclohexane ring, for the product, to the right of the reactant, leaving room to add the arrow.

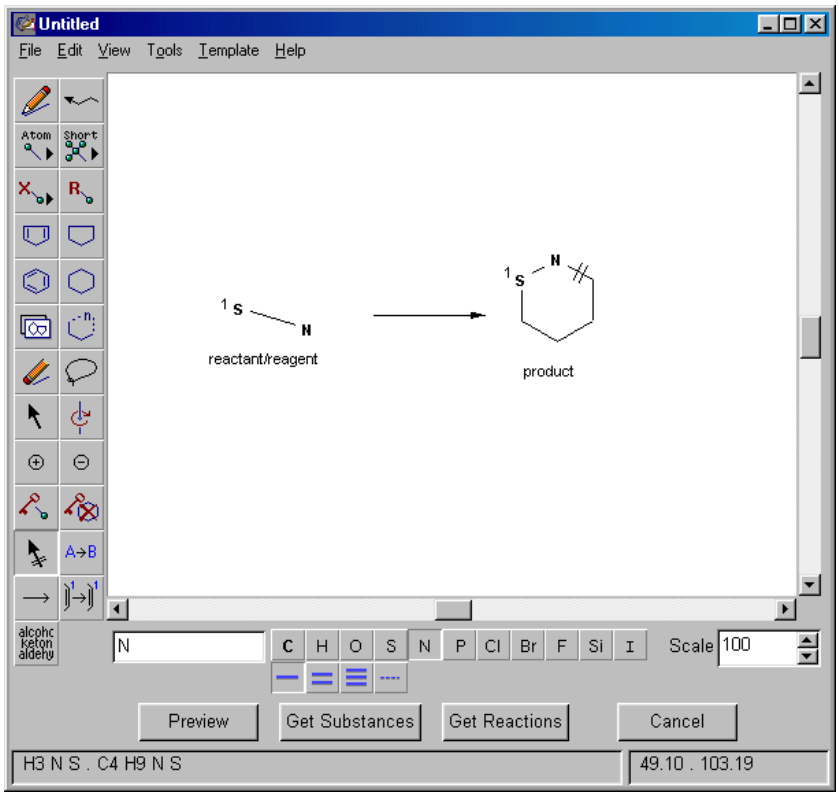
3. Click the **S** on the **Common Atoms Palette**. Place an S at the left end of the single bond and at the top left of the 6-membered ring. Click the **N** on the Common Atoms Palette. Place an N at the right of the single bond and at the top of the 6-membered ring.

4. Click the **Reaction Arrow** tool. Position the cursor near the reactant and click and drag it toward the product. When you let go of the mouse button, the arrow appears as you drew it and the structures are labeled as **reactant/reagent** and **product**.

5. Click the **Reaction Mapping** tool. Position the cursor over the S in the reactant to highlight it. Click and a 1 is placed beside that node. Then position the cursor over the S in the product to highlight it and click. A 1 is placed beside that node also.

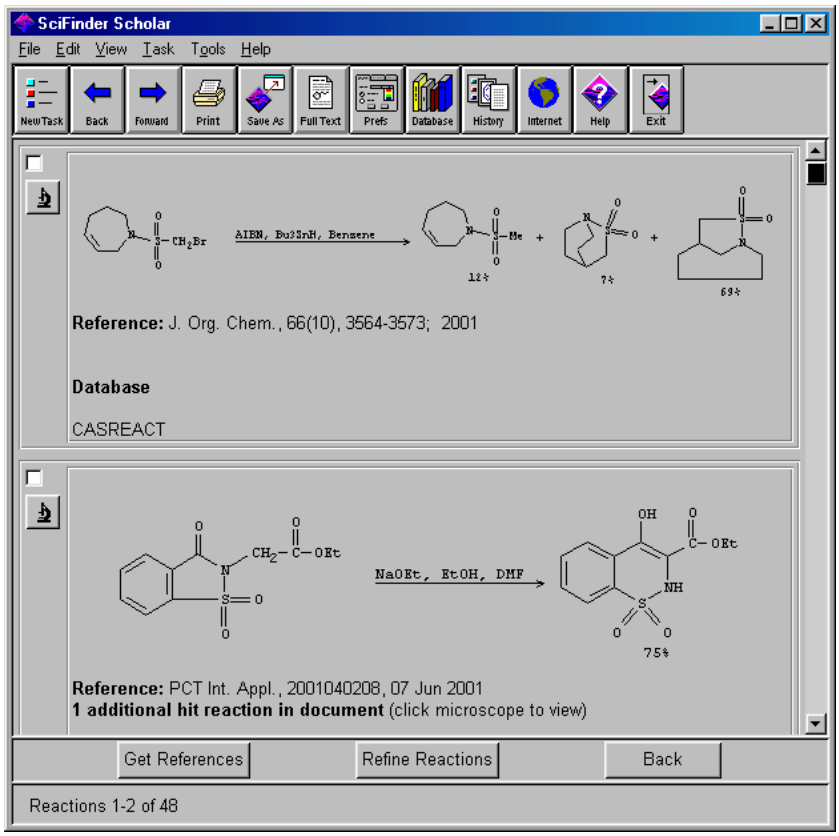
6. Click the **Reaction Site Marking** tool. Position it over the bond in the product between the N and the carbon next to it to highlight the bond. Click and the reaction site is marked.

When you are finished drawing the reaction, your Structure Drawing window should look like the one below.



Retrieving Matches to Your Full-Reaction Query

After you have completed the reaction drawing, click **Get Reactions**. The results are displayed in the **SciFinder Scholar** window.



You may proceed by viewing the reaction candidates, additional hit reactions, and substance records as described in earlier sections of this chapter. You may also keep or refine your answer set and retrieve references. For saving and printing instructions, see Chapter 2.

Exploring Reactions by Functional Groups

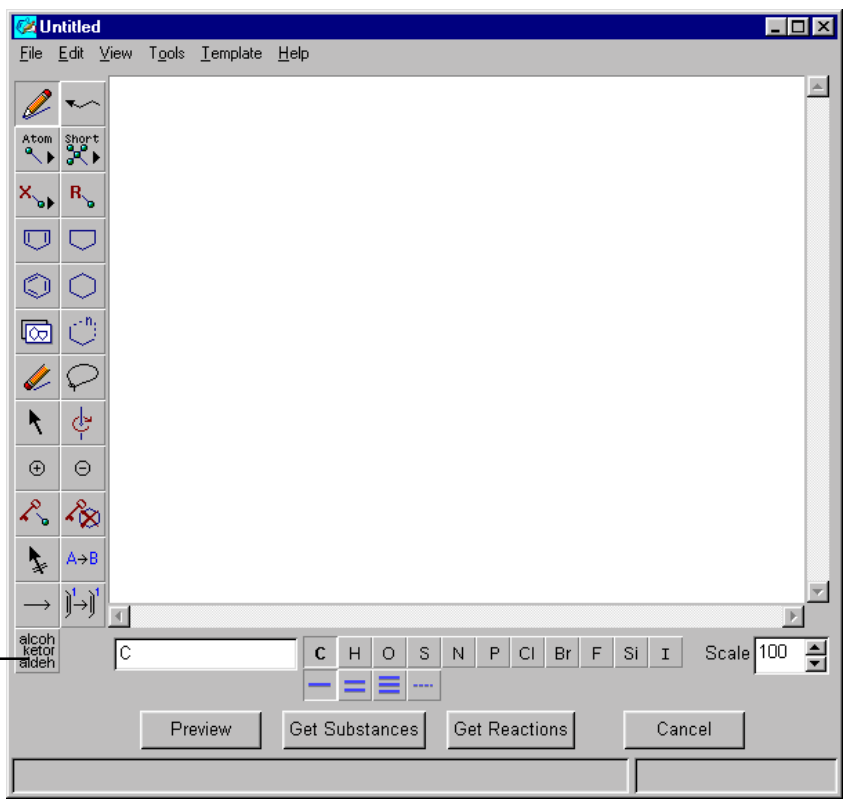
The Explore by Functional Groups feature allows you to examine functional group transformations between reactants/reagents and products. Use functional group searching to specify the functional groups present in a reaction and the role each functional group performs, either:

- Product – is formed by the reaction
- Reactant/Reagent – is transformed by the reaction
- Any role – is a product, reactant/reagent, or non-reacting substance
- Non-reacting – is a participant but is unaffected by the reaction

Functional group searching is an ideal way to obtain a broad set of reactions with common structural features. You can then use the refinement tools to limit the answer set. See the *Refining Reactions* section for more details.

Accessing Explore by Functional Groups

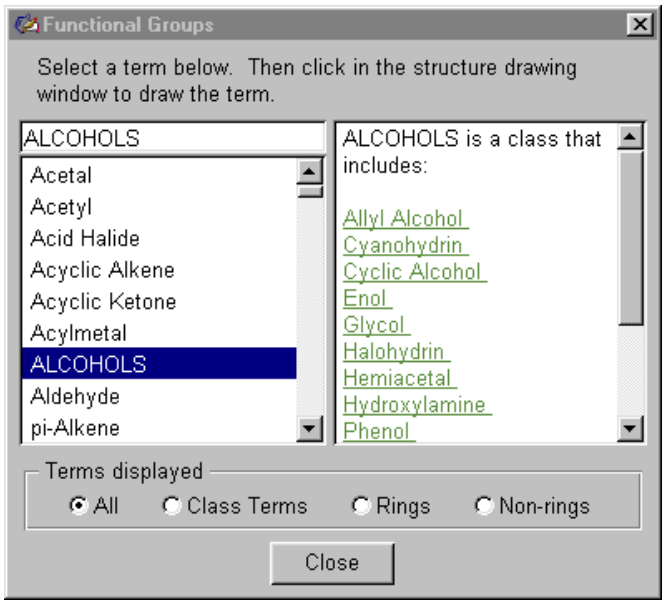
Functional group queries are drawn in a Structure Drawing window. To access a Structure Drawing window, click **Chemical Substance or Reaction** in the **Explore** window. Then click **Chemical Structure**. A Structure Drawing window is displayed. The **Functional Group** tool allows you to select functional groups.



Functional Group tool

Selecting Functional Groups

To access functional groups, click the **Functional Group** tool icon. The **Functional Groups** dialog box is displayed.



Four display options are available for functional group terms listed in the left-hand scrolling frame:

- All (default)
- Class Terms
- Rings
- Non-rings

The default display is **All**, which shows all of the functional group terms available in SciFinder Scholar. The class terms and functional groups are displayed alphabetically, followed by the ring terms.

Click the **Class Terms** radio button to display only the class terms. These terms are broad classes of substances. Click a class term name to see a list of the functional groups within that class. For example, click **ALCOHOLS**. The functional groups within the alcohols class are displayed in the right-hand frame. All of these functional groups are searched if **ALCOHOLS** is placed in the Structure Drawing window.

Click the **Rings** radio button to display only the ring terms. Click a term to display its structure diagram in the right-hand frame. For example, click **1,2-C4NS**. The right-hand frame displays a structural representation of the functional group searched if **1,2-C4NS** is placed in the Structure Drawing window.

Click the **Non-rings** radio button to display only the non-ring terms. Click a term in the list to select it. For example, click **Aldehyde**. Its structure diagram is shown in the right-hand frame.

The class term, ring term, or non-ring term that is selected displays in the box at the top left of the **Functional Groups** dialog box. It also displays in the **Current Atom** box near the bottom of the Structure Drawing window. Rather than selecting a term from the list, you may type a term into the **Current Atom** box and press **<Return>**. If what you enter does not exactly match an item in the list, SciFinder Scholar will choose its closest match from the list.

Once you have selected a term to use in your reaction, move your cursor to the Structure Drawing window and click. The selected term displays as the term name. This “name” indicates that the item is a functional group term and differentiates it from a structure drawing. If you place your mouse over a functional group term, a tooltip displays the structural representation or a list of functional groups that will be searched.

Drawing a Functional Group Reaction Query

To find reactions that contain particular functional groups, build the reaction in the Structure Drawing window. You may draw just one functional group or multiple functional groups within a reaction query. Each functional group must be given a role, e.g., product. Use the **Reaction Role** tool or the **Reaction Arrow** tool to assign the roles.

Functional group terms must stand on their own. The following rules apply:

- Structures cannot be bonded to functional group terms
- Charges may not be placed on functional group terms
- **Reaction Mapping** and **Reaction Site Marking** tools may not be applied to functional group terms
- Functional group terms cannot be rotated

Functional group terms may, however, be searched in the same reaction query as chemical structures. See *Combinations of Functional Groups and Chemical Structures*, later in this chapter, for details.

For this example, build a reaction in which a secondary alcohol is converted to a ketone and a primary alcohol is present but non-reacting.

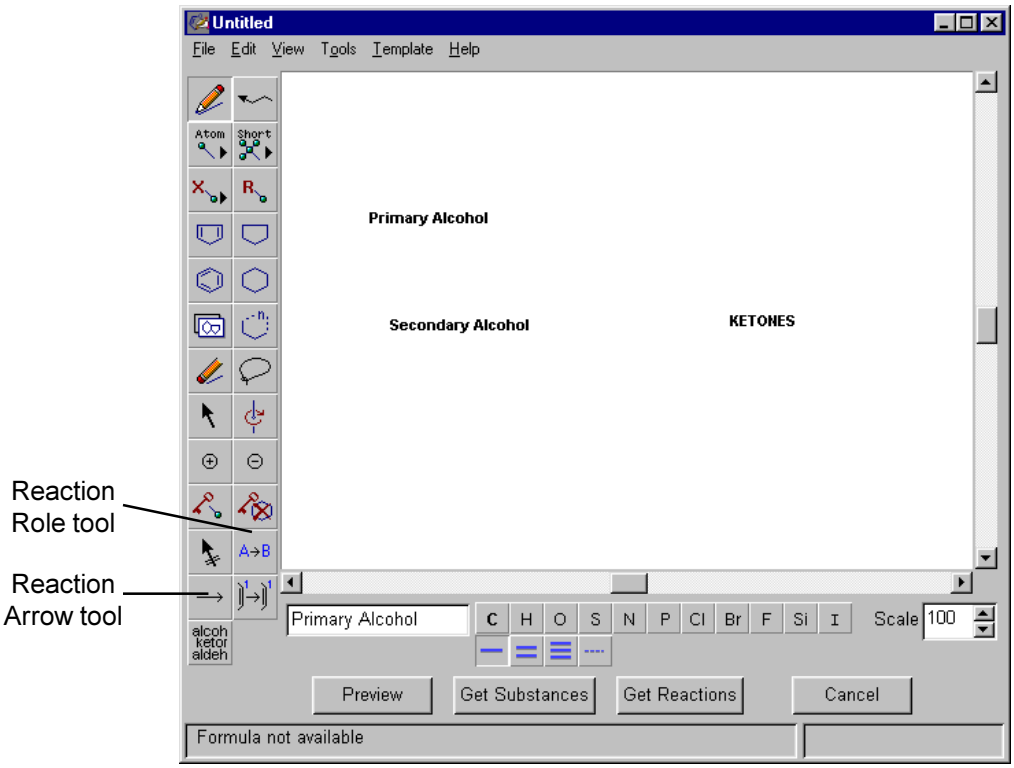
1. Select the **Functional Group** tool from the **Vertical Tool Palette**. The **Functional Groups** dialog box is displayed.

2. Scroll down the left-hand frame to find Secondary Alcohol in the list. Click **Secondary Alcohol** to highlight it. Then place the cursor on the left side of the Structure Drawing window and click. The term **Secondary Alcohol** is drawn.

3. Scroll to find KETONES in the left-hand frame. Click **KETONES**. Then place the cursor on the right side of the Structure Drawing window and click. The term **KETONES** is drawn.

4. Scroll to find Primary Alcohol in the left-hand frame. Click **Primary Alcohol**. Then place the cursor above the **Secondary Alcohol** term in the Structure Drawing window and click. The term **Primary Alcohol** is drawn.

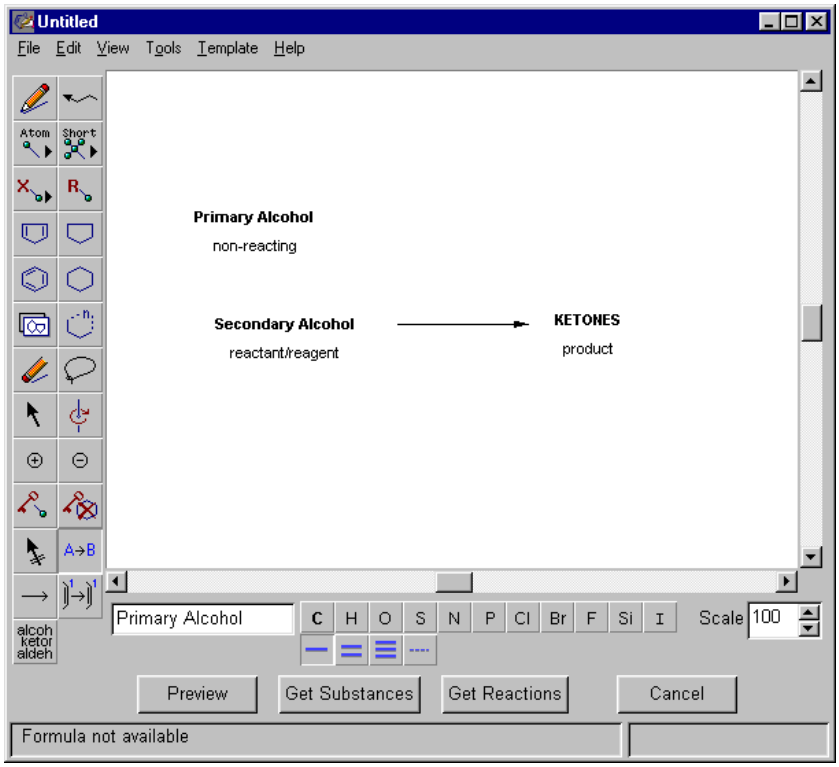
   Click **Close** in the **Functional Group** dialog box.



5. Select the **Reaction Arrow** tool from the **Vertical Tool Palette**. Click just to the right of **Secondary Alcohol** and drag the cursor toward **KETONES**. An arrow is drawn from left to right. Roles are assigned to the terms, depending on their location with respect to the arrow.

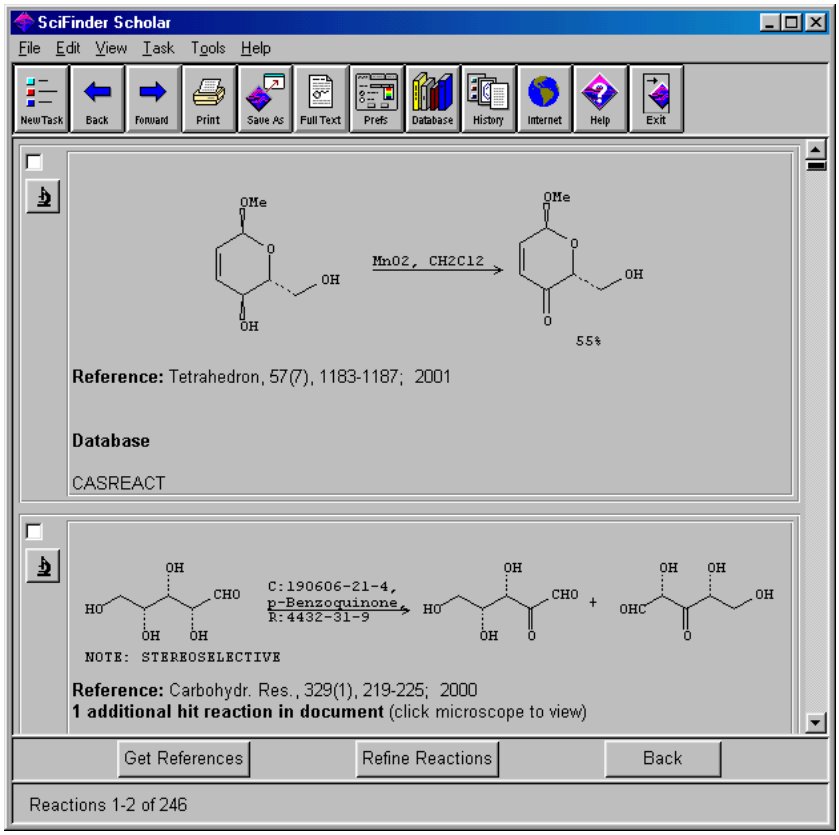
6. The **Reaction Arrow** tool labeled the **Primary Alcohol** as a Reactant/Reagent because of its location. To relabel it as non-reacting, select the **Reaction Role** tool from the **Vertical Tool Palette**. Click **Primary Alcohol**. The **Reaction Roles** dialog box is displayed. Select **non-reacting**, and click **OK**. The role is changed appropriately.

Your functional group query should look like the one below.



Retrieving Reactions That Match Your Functional Group Query

When you have completed the reaction drawing, click **Get Reactions**. If reactions that match your functional group query are found, they are displayed in the **SciFinder Scholar** window.



The first hit reaction for each document, i.e., the first reaction in the document that matches your functional group query, is displayed. To view additional hit reactions, if present, click the **microscope** icon next to the reaction.

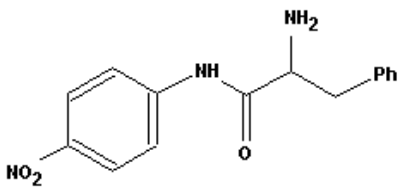
Functional group searches are broad and, in general, retrieve large answer sets. You may wish to refine the reaction, e.g., by adding a chemical structure to the reaction query, to reduce the size of the answer set. Click **Refine Reactions** to view the refine options, or see *Refining Reactions*, earlier in this chapter, for details.

You may also retrieve references for one or more of the reactions. Select reactions of interest. Then click **Get References**. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Combinations of Functional Groups and Chemical Structures

Mixtures of functional group terms and chemical structures can be searched within the same reaction query. Draw the reaction you would like to search. Then assign a role to each fragment.

Find reactions in which a carboxylic acid is converted to an amide and the following structure is also a reactant/reagent:



1. Draw the structure shown above in the top left portion of the Structure Drawing window. For details about structure drawing, see Chapter 4.

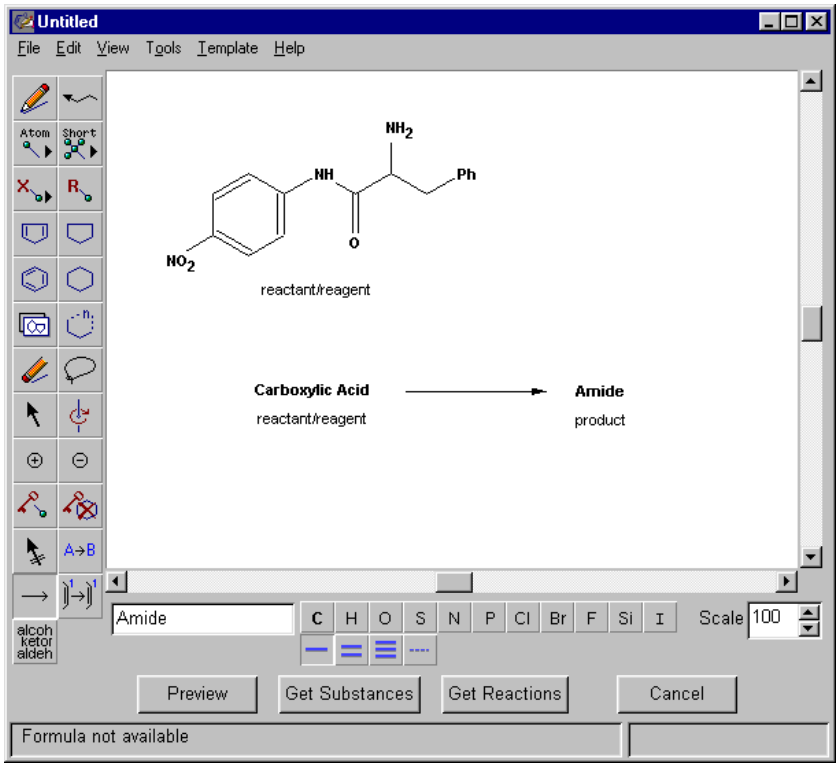
2. Select the **Functional Group** tool from the **Vertical Tool Palette**. The **Functional Groups** dialog box is displayed. Scroll the left-hand frame to find Carboxylic Acid. Click the term to highlight it. Place the cursor below the structure in the lower left portion of the Structure Drawing window and click. The term **Carboxylic Acid** is drawn.

3. In the **Functional Groups** dialog box, scroll to find Amide. Click the term to highlight it. Place the cursor on the right side of the Structure Drawing window and click. The term **Amide** is drawn.

4. Select the **Reaction Arrow** tool from the **Vertical Tool Palette**. Click to the right of the **Carboxylic Acid** term and drag toward the **Amide** term. A reaction arrow is drawn, and roles are assigned to the fragments, depending on their location with respect to the arrow.

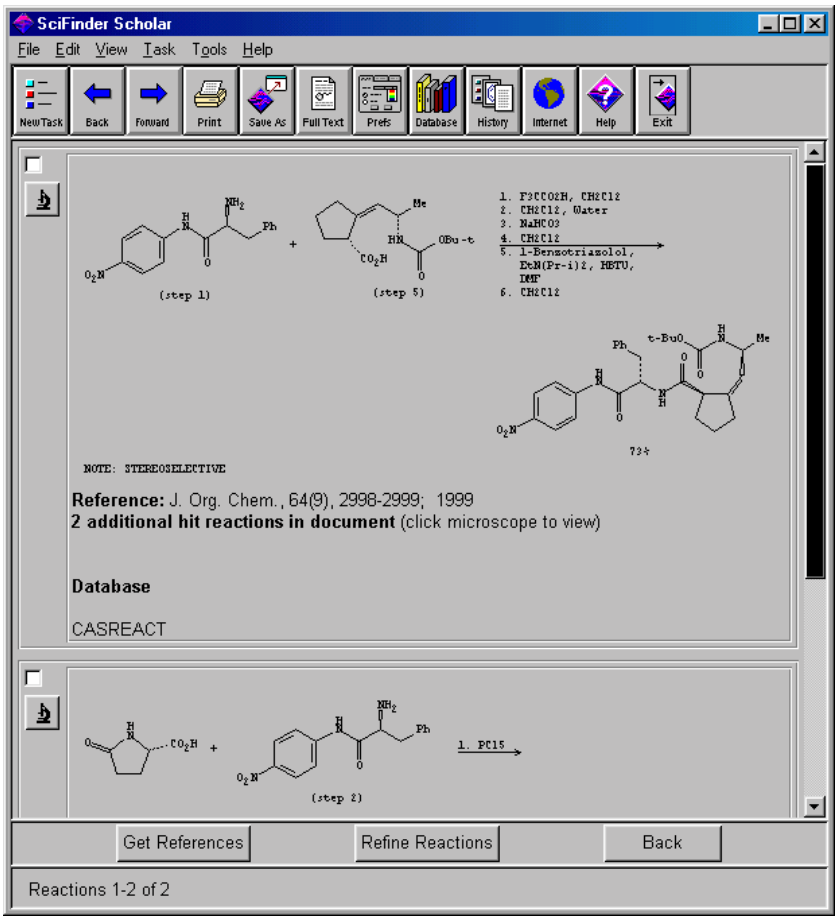
   Click **Close** in the **Functional Group** dialog box.

Your functional group query should look like the one below.



Retrieving Reactions That Match Your Combination Query

When you have completed the reaction drawing, click **Get Reactions**. If reactions that match your query are found, they are displayed in the **SciFinder Scholar** window.



For large answer sets, you may wish to refine your reaction query. Click **Refine Reactions** to see the refinement options. See *Refining Reactions*, earlier in this chapter, for details.

Click **Get References** to retrieve references that contain the hit reactions. See Chapter 7 for details on working with references. For saving and printing instructions, see Chapter 2.

Ending Your Explore Session

To begin a new task, select **New Task** from the **File** menu or click the **New Task** button on the **Main Menu Toolbar**.

To exit SciFinder Scholar, select **Exit SciFinder Scholar** from the **File** menu or click the **Exit** button on the **Main Menu Toolbar**.

7 Working with References

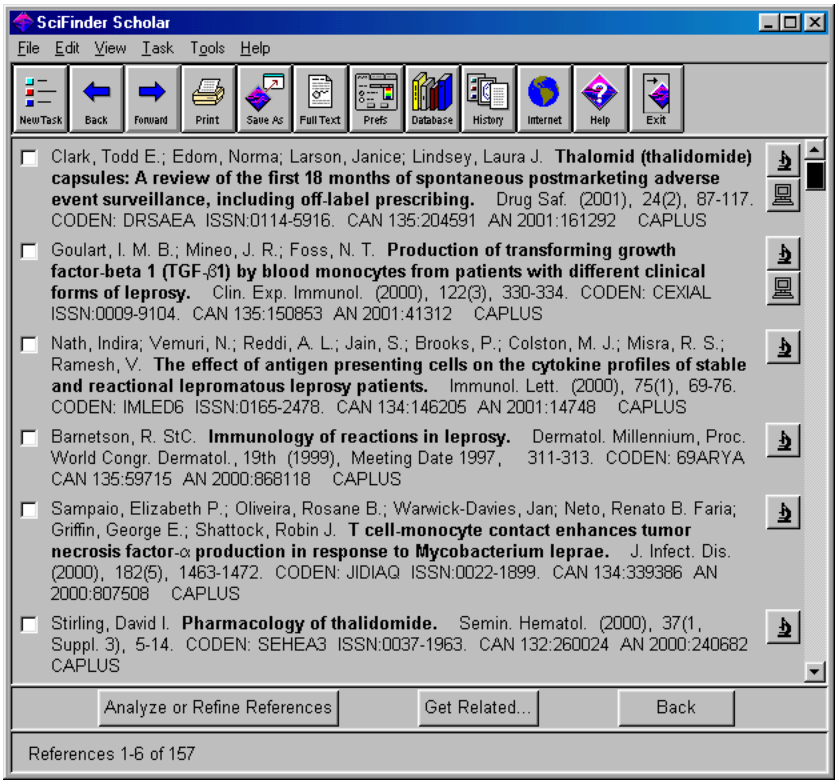
SciFinder Scholar provides many tools for manipulating reference answer sets, such as analyzing, refining, and retrieving citations and substances.

Chapter 7 explains the many ways you can work with reference answer sets:

- Change the sort order and display format
- Keep references of interest
- View individual references in detail
- Access full text of references
- Analyze answer sets
- Refine answer sets
- Get references cited in the document(s)
- Get references that site the document(s)
- Get substances from the document(s)

After you have completed a task and retrieved references, SciFinder Scholar tools allow you to work with your reference answer set.

Your reference answer set is displayed in the **SciFinder Scholar** window.



Display Format and Sort Order

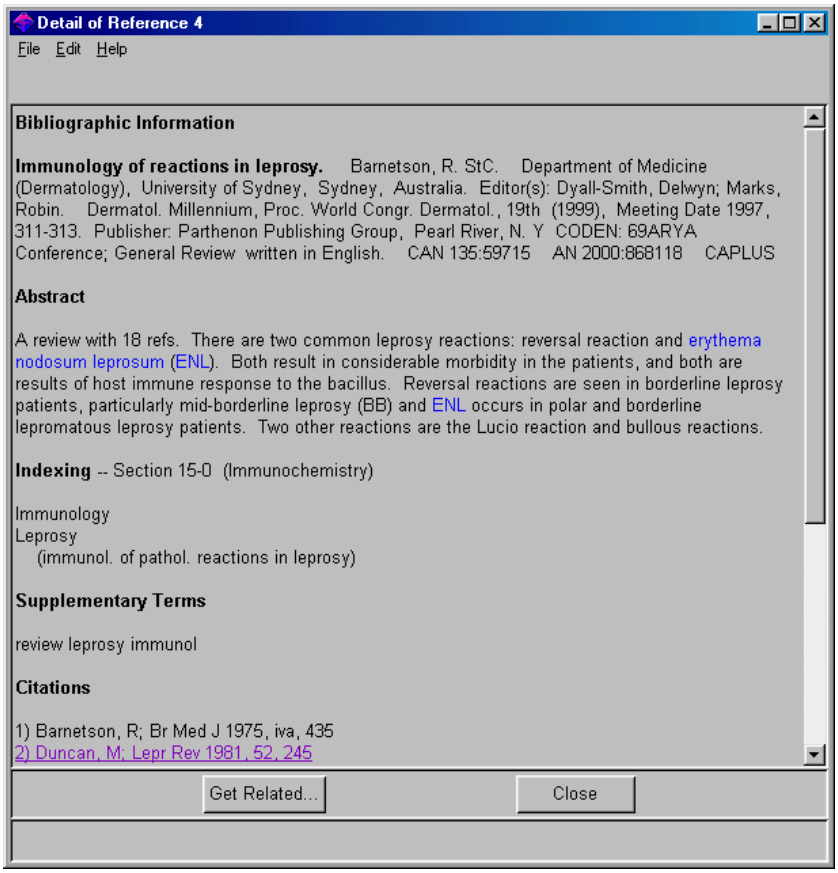
References are displayed in the default format and order. To change the display of your current answer set, choose an alternative option from the **View** menu. The format and order options are defined in the *View Menu* section of Chapter 2. For information on changing the defaults, refer to *Display Preferences* in Appendix A.

Keeping References of Interest

If an answer set contains a large number of references, you may choose to keep only the references that are of interest to you. Click the box next to each reference that you would like to keep. Then select **Keep References** from the **Tools** menu. SciFinder Scholar displays only the references you selected.

Viewing Details of References

In a reference answer set, a **microscope** icon is displayed to the right of each reference. Click the **microscope** icon to display details for a particular reference. A **Detail of Reference #** window is displayed that contains full bibliographic information, the abstract, and other details about the reference.



Information is displayed in the default format for the window. The default may be changed in the **Display** tab of the **Preference Editor**. See *Display Preferences* in Appendix A for details.

In the detail window, links to additional information, such as CAS Registry Numbers or citations, may be present.

If full text is available via ChemPort, an **e-document** icon is displayed at the top right of the window. See Chapter 8 for more details.

To retrieve citations or substances, or to link to eScience, click the **Get Related** button. See the end of this chapter and Chapter 8 for details.

To return to the **SciFinder Scholar** window, click **Close**.

Accessing Full-Text Documents

For journal articles and patents that are available electronically from the publisher or patent office via ChemPort, an **e-document** icon is located to the right of the reference (below the **microscope** icon). For details about accessing full text, see *Accessing Full-Text Documents* in Chapter 8.

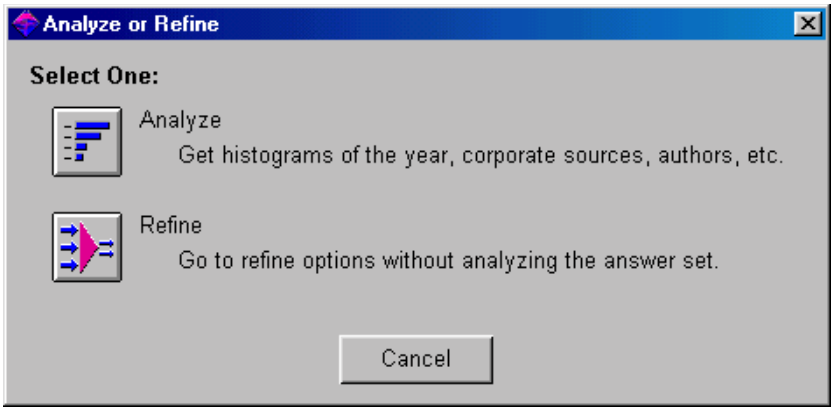
Some users may see **house** icons in place of **e-document** icons. The Site Administrator for your organization has provided CAS with a list of journals available to you in-house. **House** icons work similarly to **e-document** icons. Please see your Site Administrator for details about the in-house journals list.

Analyzing References

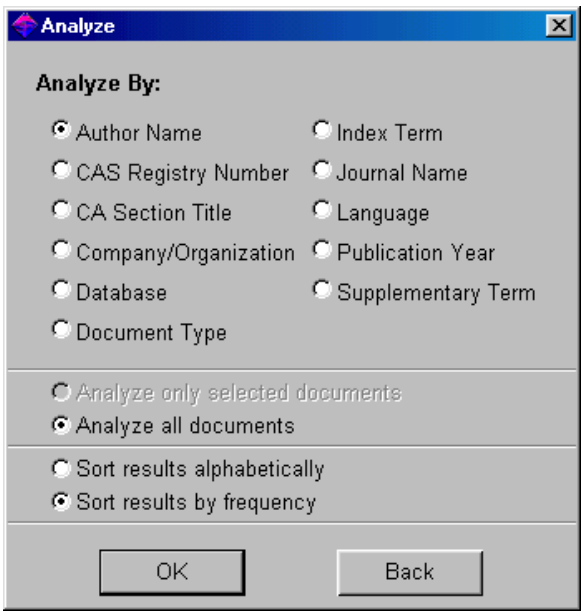
The Analyze References feature is used to create subsets of reference answer sets that fit specific criteria. Histograms allow you to see a visual representation of the answer set based on frequency. You may analyze references according to these attributes:

- Author Name
- CAS Registry Number
- CA Section Title
- Company/Organization
- Database
- Document Type
- Index Term
- Journal Name
- Language
- Publication Year
- Supplementary Term

To analyze references, click the **Analyze or Refine References** button. The **Analyze or Refine** dialog box is displayed.

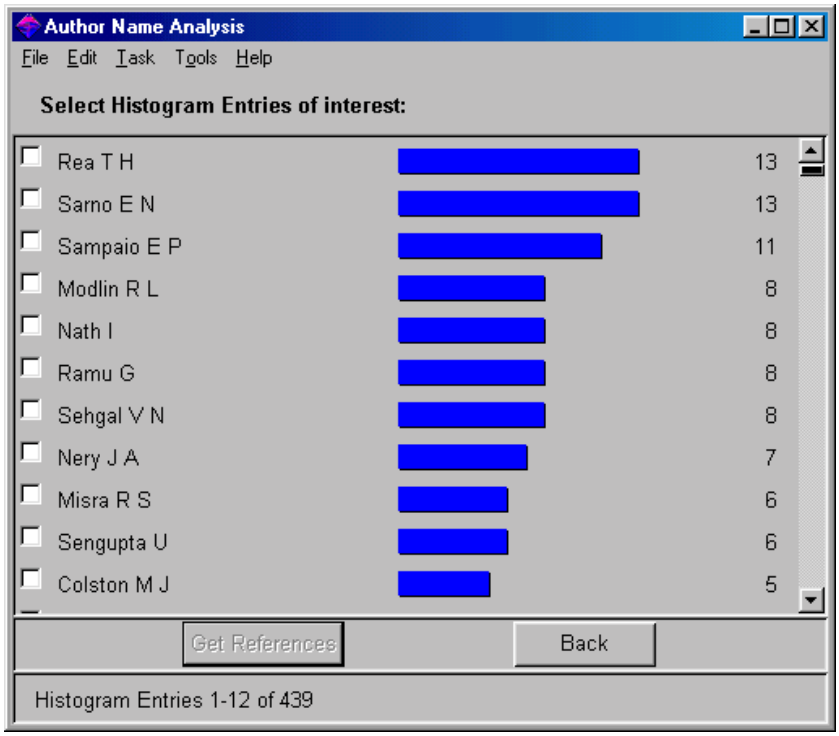


Click the **Analyze** button to display the **Analyze** dialog box.



Choose an attribute on which to analyze and whether to analyze all of the documents or only those you have selected. You may display alphabetically or by frequency. Click **OK**.

SciFinder Scholar displays an **Analysis** window that contains your analyzed results.



The number of references corresponding to each entry is displayed at the right. You may select one or more histograms and click **Get References** to retrieve those references. Or, click **Back** to analyze by a different attribute.

In some cases, you will retrieve more than the number of references listed at the right. SciFinder Scholar retrieves not only references for the histograms you select but also references for some related histogram entries. For example, if you analyze by company/ organization and select *Kyoto Univ, Japan*, SciFinder Scholar also retrieves references for *Kyoto Prefect Univ, Japan* to provide retrieval of additional relevant answers.

Some records may not include information for a particular analysis. When this occurs, the references are placed in a histogram titled “References not containing information for this analysis.”

If you click the **Stop** button during an Analyze operation, you get the results of analyzing part of your answer set. However, if you then select items and choose **Get References**, the selection will be applied to the entire answer set.

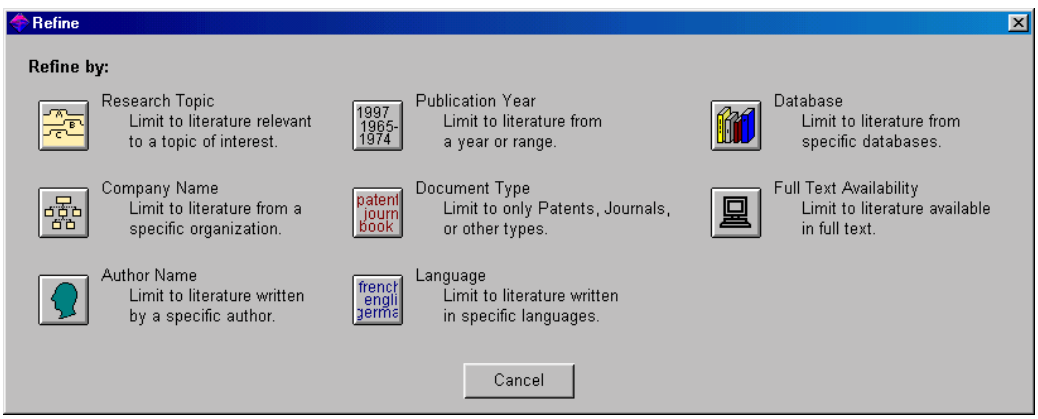
The histograms from the analyze results may be printed or saved by using the **Print** or **Save As** options under the **File** menu. See Chapter 2 for more details.

Refining References

The Refine References function allows you to narrow your search by adding to your original search criteria.

To use Refine References, click the **Analyze or Refine References** button. Click the **Refine** button to display the **Refine** dialog box. You may choose to refine by:

- Research Topic
- Company Name
- Author Name
- Publication Year
- Document Type
- Language
- Database
- Full Text Availability

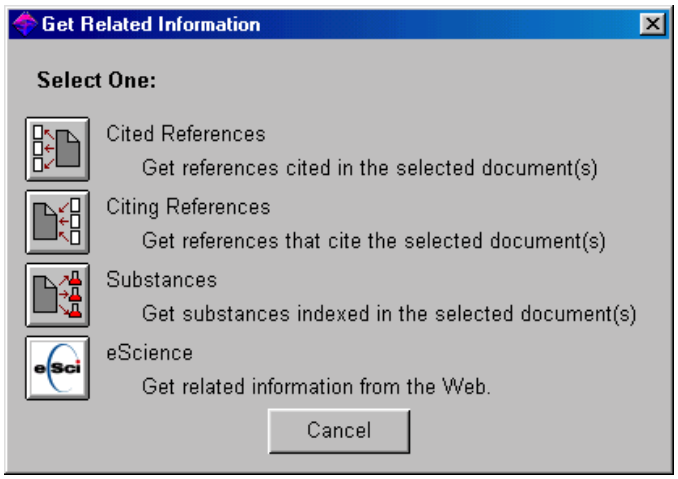


When you choose one of these options, a dialog box displays that allows you to add additional information to your search criteria. You may refine your reference list as many times as you like.

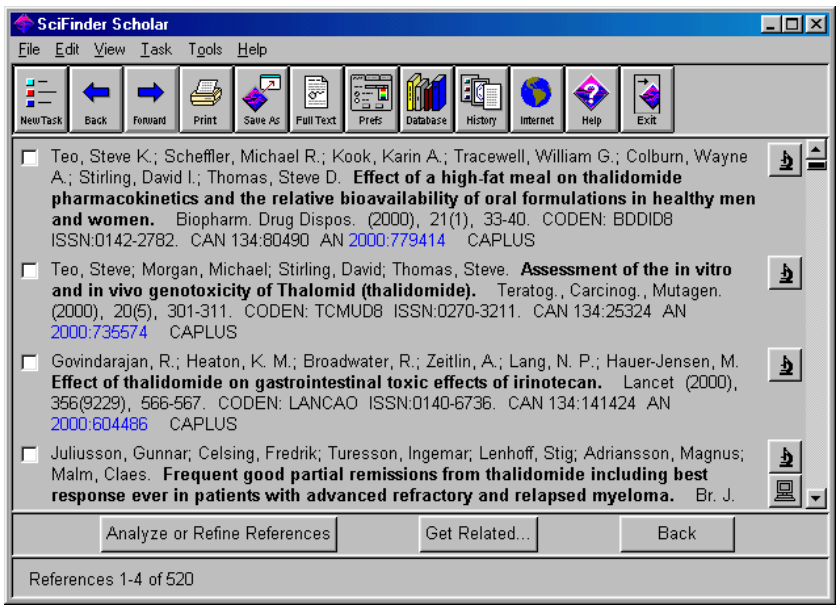
Get Cited References

References that are cited within a document or set of documents can be retrieved with the Get Cited References feature.

To retrieve cited references, click the **Get Related** button. The **Get Related Information** dialog is displayed.



Then click **Cited References**. SciFinder Scholar displays the references cited by the document(s).

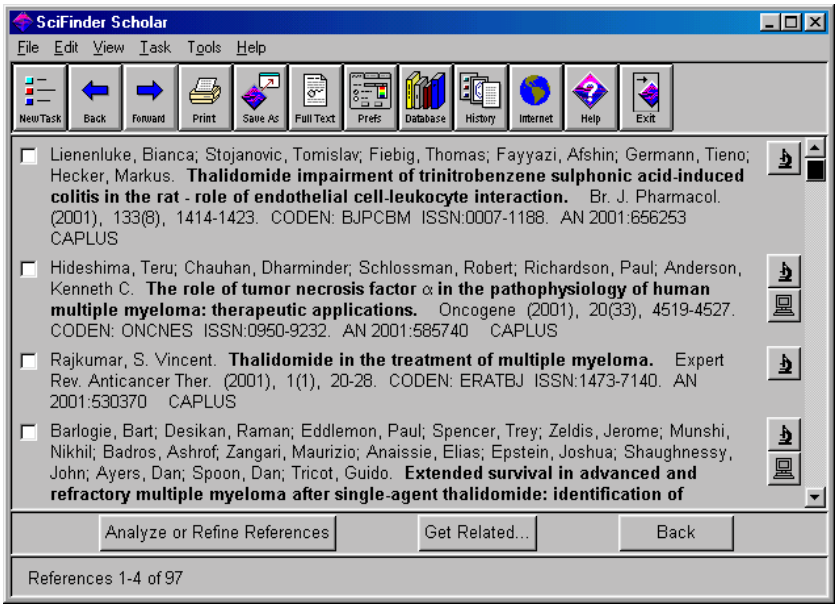


If no cited references are available for the selected documents, a message indicates that the search results in no hits.

Get Citing References

The Get Citing References feature allows you to retrieve references that cite a document or set of documents.

To retrieve Citing References, click the **Get Related** button. Then click **Citing References**. SciFinder Scholar displays references that cite the document(s).

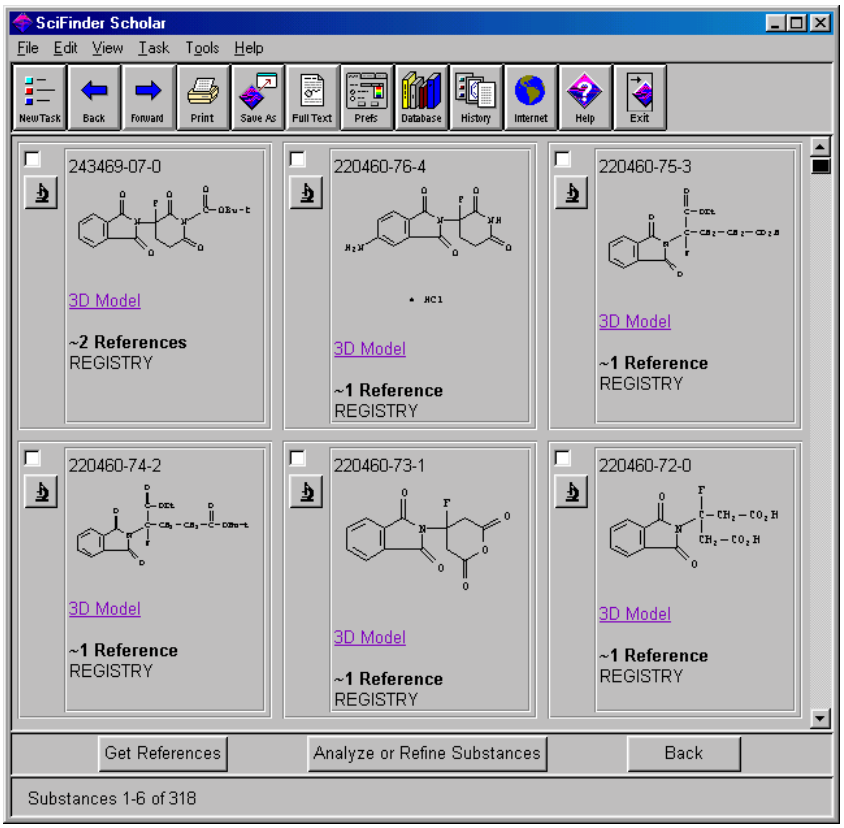


If no citing references are available for the selected documents, a message indicates that the search results in no hits. This is frequently the case for recently published documents.

Get Substances from Reference Answer Set

With the Get Substances feature, subscription users can retrieve all substances associated with a reference or set of references.

To Get Substances, click the **Get Related** button. Then click **Substances**. SciFinder Scholar displays the substances associated with the reference(s).



If no substances are available for the selected documents, a message indicates that the search results in no hits.

Ending Your Session

To end your session, select **New Task** from the **File** menu or click the **New Task** button on the **Main Menu Toolbar**.

To exit SciFinder Scholar, select **Exit SciFinder Scholar** from the **File** menu or click **Exit** on the **Main Menu Toolbar**.

8

Linking to Additional Information

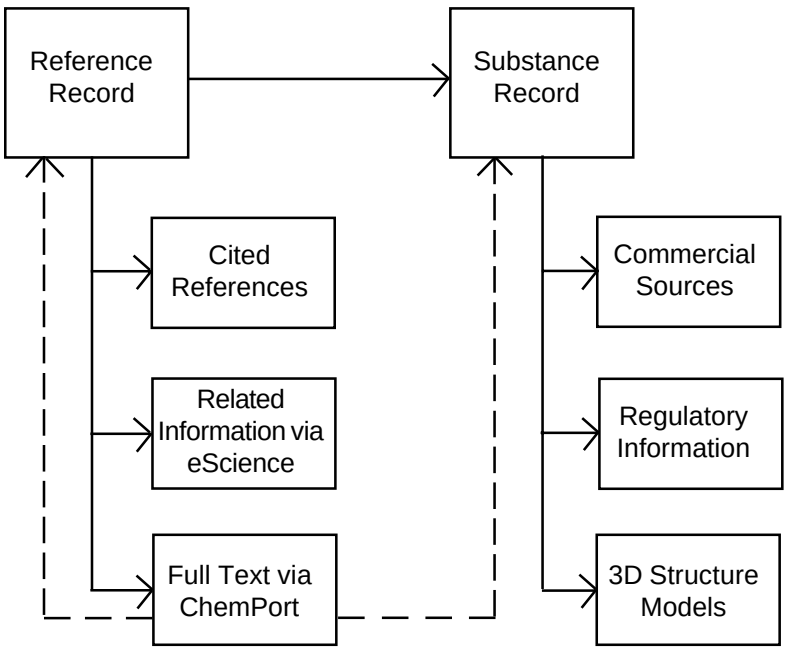
SciFinder Scholar provides many opportunities to link among sources to obtain additional information about substances or references. For example, you may link from reference records to substance records, and from substance records to regulated chemicals information.

Chapter 8 acquaints you with linking options available in SciFinder Scholar. Convenient links are provided to:

- Substance records in the CAS REGISTRY database
- Commercial sources
- Regulatory information
- Individual cited references
- 3D structure models (with WebLab® Viewer™)
- Related information on the Web via eScience®
- Full-text documents (via ChemPort℠)

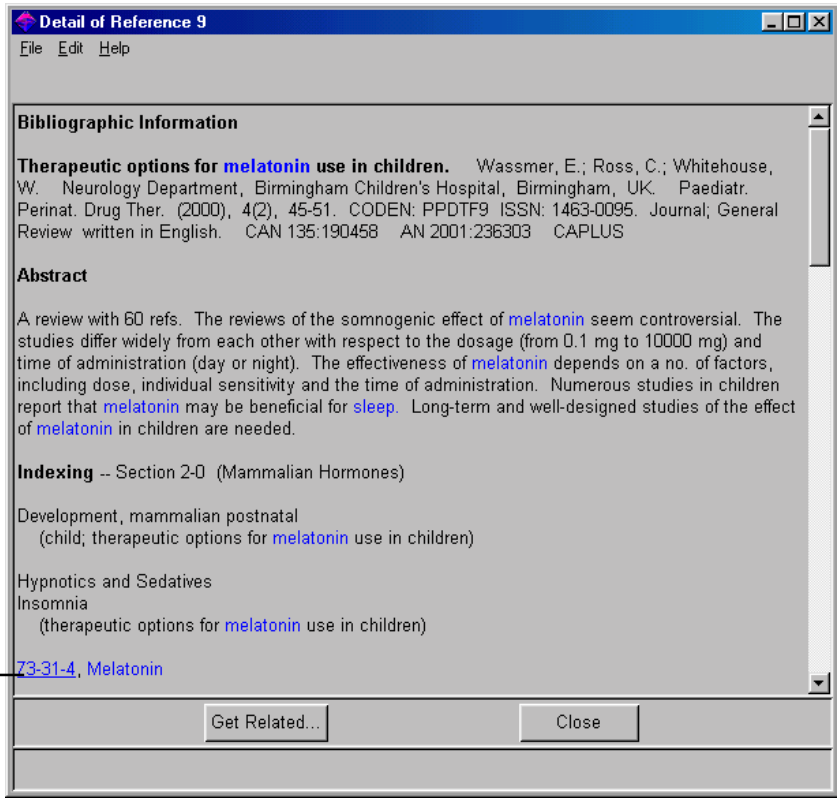
Additionally, you can link to SciFinder Scholar from an e-article (at several publisher web sites) and explore for information related to that article. Links discussed in this chapter are outlined in the chart below.

Links to Additional Information



Linking to Substance Records

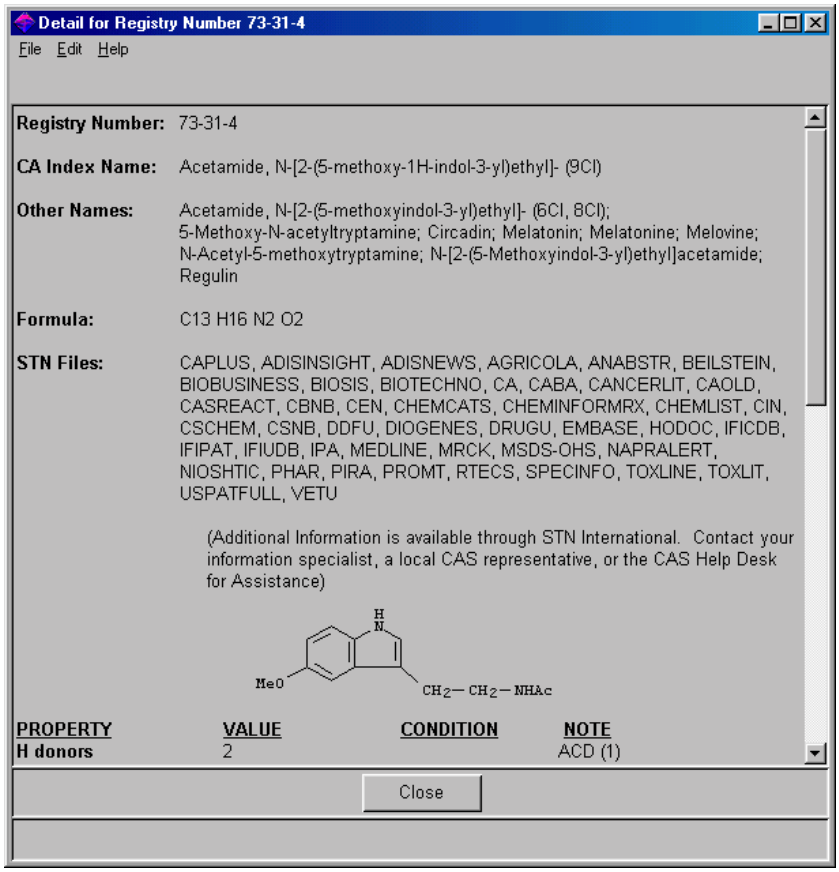
CAS Registry Numbers are included in many detailed references.



hypertext link

Click the CAS Registry Number hypertext link to view details about the corresponding substance.

A **Detail for Registry Number #** dialog box is displayed.



The full substance record may include the CAS Registry Number, chemicals names, molecular formula, chemical structure, and other related information.

The STN Files list identifies databases and inventories that contain additional information for this CAS Registry Number. Contact your site administrator or the CAS Help Desk to find out how you can access and use these STN files and inventories to locate more information on a CAS Registry Number.

You may print or save the record by selecting **Print** or **Save As** from the **File** menu.

To return to the previous window, click **Close**.

Linking to Substance Records from Reactions

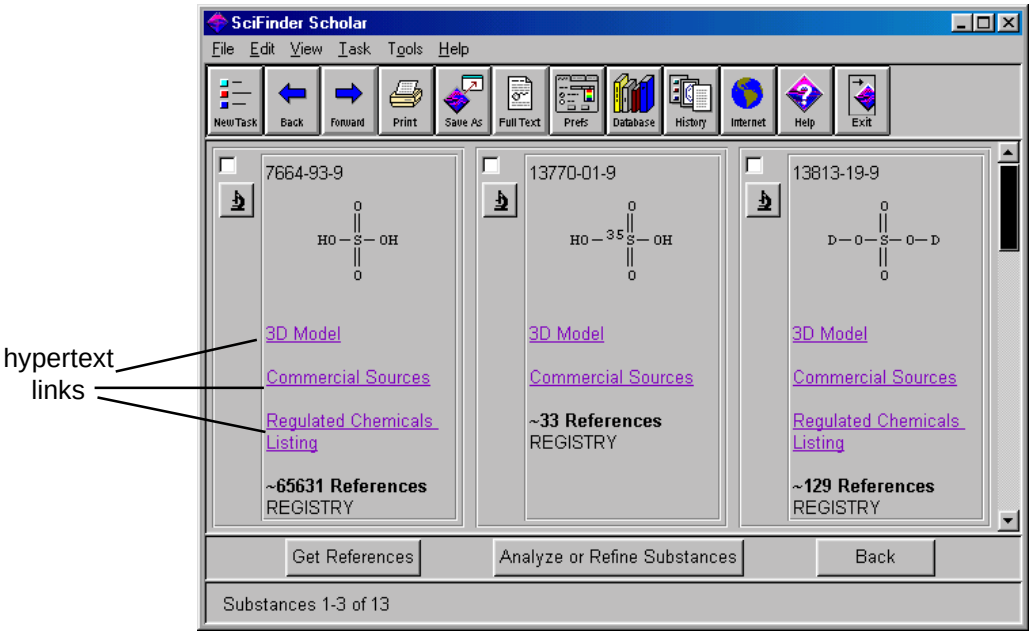
While displaying a reaction obtained via a reaction search, you may view the substance record for any substance participating in the reaction.

To view a substance record, click a reactant, reagent, product, or catalyst. A **Detail for Registry Number #** dialog box is displayed and may include the CAS Registry Number, CA Index Name, formula, and more. For details and to view examples, refer to the *Viewing Substance Records within a Reaction* section in Chapter 5.

Linking to Commercial Sources

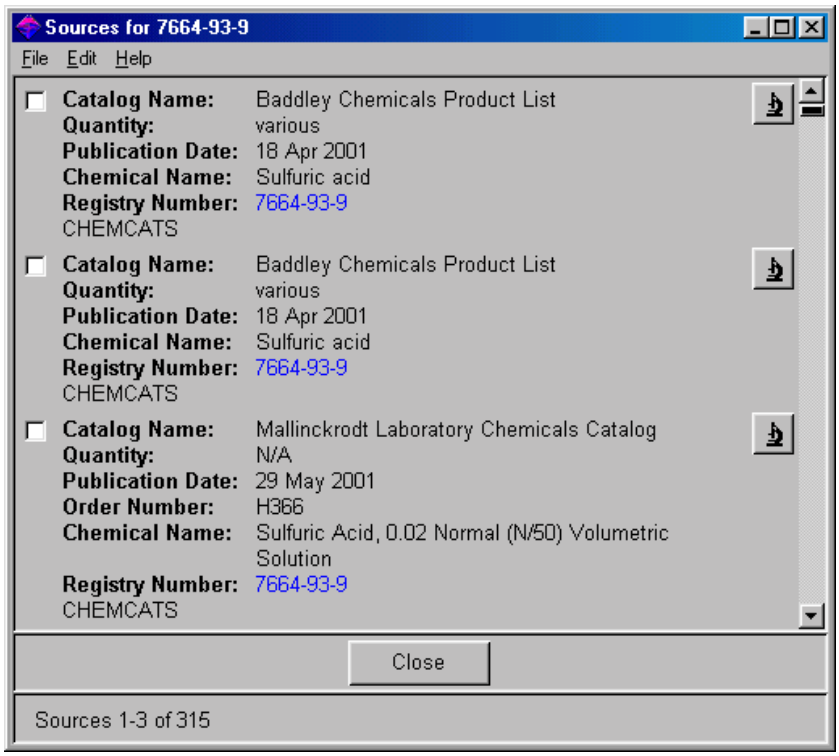
Over 3,300,000 products accessed via SciFinder Scholar are linked to information concerning their commercial availability. This information is from more than 700 chemical catalogs and libraries.

Commercial Sources links, when available, are found in substance records.



To retrieve chemical supplier information for substances, click the **Commercial Sources** link.

The **Sources for #** dialog box is displayed.

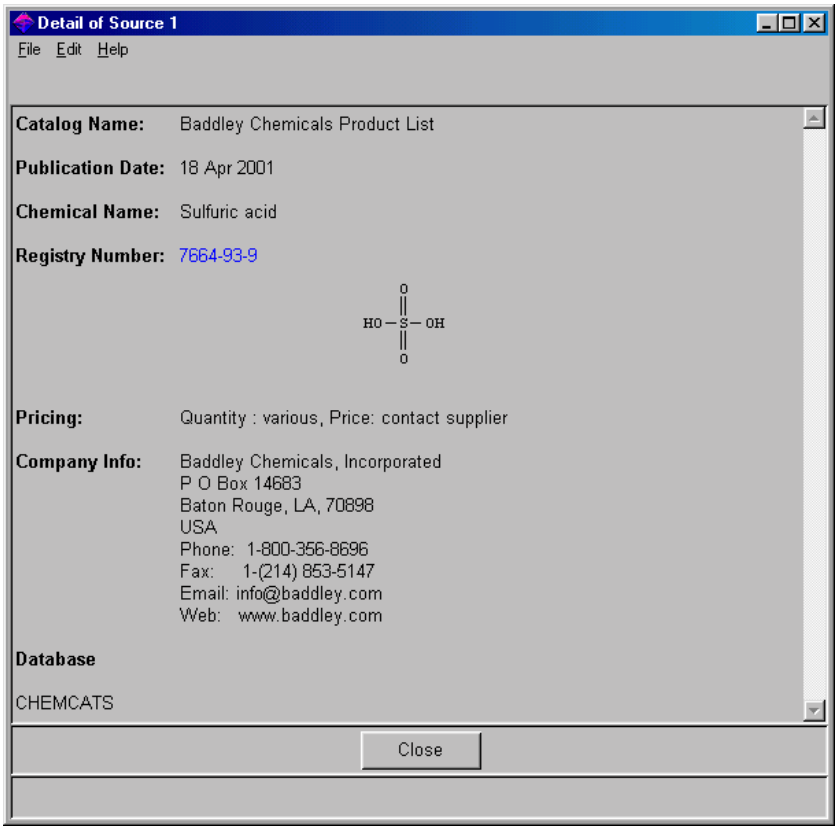


Chemical supplier information may include the catalog name, quantities available, publication date of the catalog, order number, chemical names, synonyms, and CAS Registry Number.

To ensure that this data is current, contact the supplier.

The check boxes at the left allow you to save or print a subset of the sources. To do so, click one or more boxes. Select **Save As** or **Print** from the **File** menu.

You may obtain further information for the source by clicking the **microscope** icon that follows each commercial source. This displays the **Detail of Source #** dialog box.



This information includes more in-depth data including company information, quantity, pricing, and structure diagrams. Company information includes the names, addresses, and phone numbers of distributors. The CAS Registry Number for the substance is highlighted.

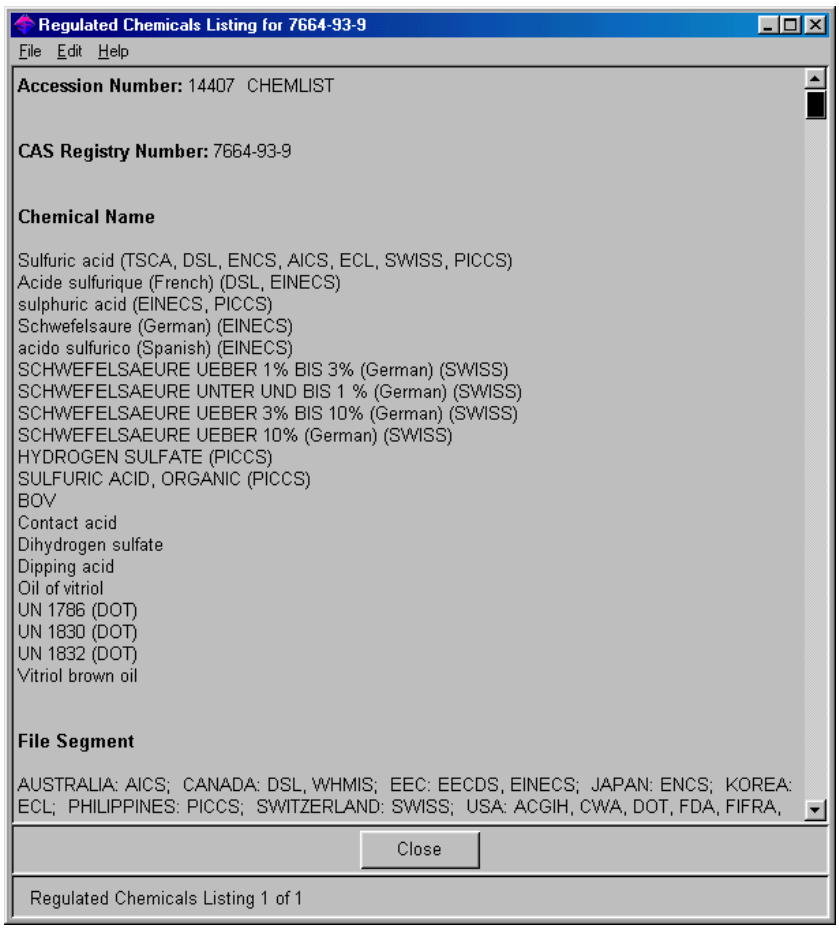
To print or save detailed source information, select **Print** or **Save As** from the **File** menu. To exit the detailed source information, click **Close**. You are returned to the **Sources for #** dialog box.

Linking to Regulated Chemicals Listing

Regulatory information can be accessed via **Regulated Chemicals Listing** links. This information may contain a list of worldwide inventories, including the U.S., Australia, Japan, Korea, Canada (DSL & NDSL), and European (ELINCS & EINECS) inventories, in which the substance appears.

Regulated Chemicals Listing links, when available, are found in substance records. See the previous section, *Linking to Commercial Sources*, for an example.

To retrieve the list of inventories for a substance, click the **Regulated Chemicals Listing** link. The **Regulated Chemicals Listing for #** dialog box is displayed.

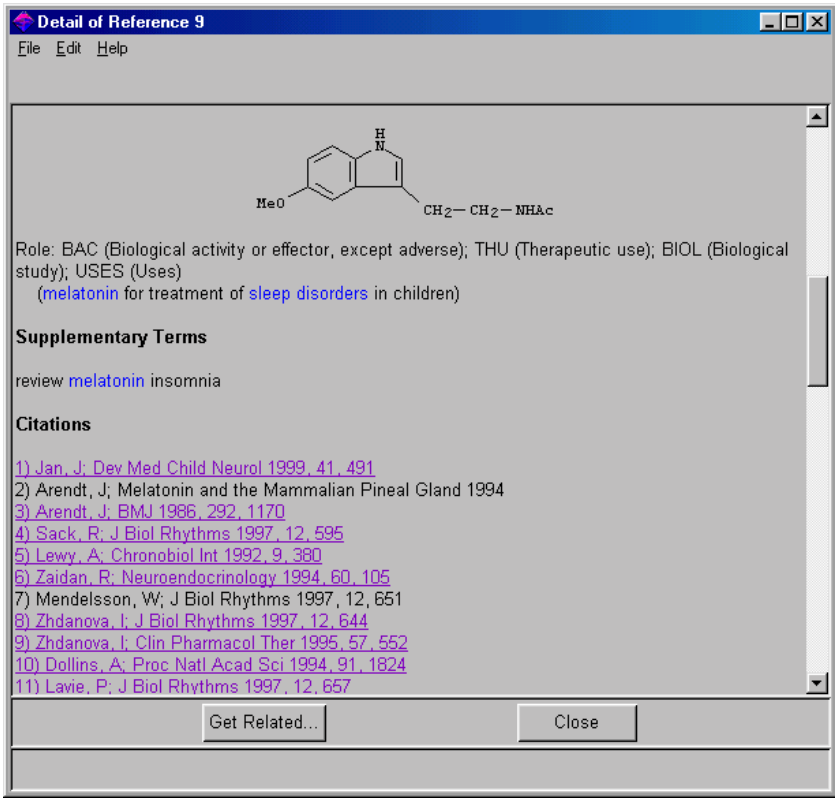


Regulatory chemicals listings may include the CAS Registry Number; chemical names; the inventory (File Segment), using the name, countries, and inventories citing the substance; confidentiality status; Regulatory List Numbers; inventory status; and more.

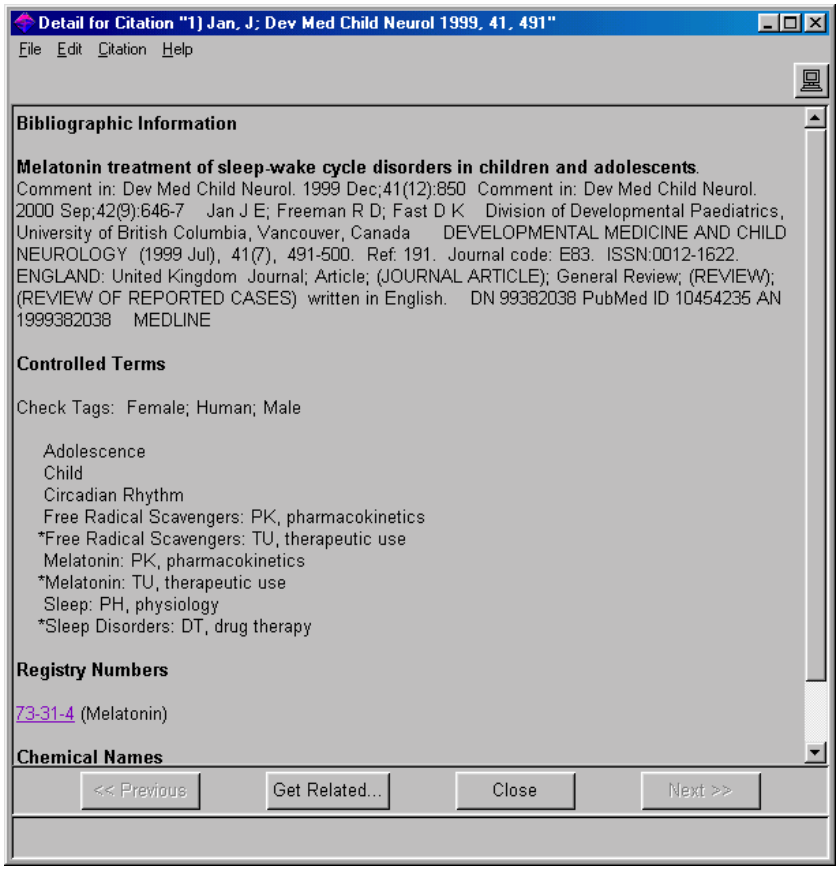
To print or save a regulated chemical listing, select **Print** or **Save As** from the **File** menu. To exit this window, click **Close**. You are returned to the previous window.

Linking to Cited References

For over 965,000 records added to the CAS databases from 1999 to the present, a list of cited references, or citations, appears in the Full display. If Full is the display format selected for the References Viewer in the **Display** tab of your **Preference Editor**, simply click the **microscope** icon for the document. Or, select **Full** from the **View** menu for documents displayed in the main **SciFinder Scholar** window. You may need to scroll down to view the citations.



From the **Citations** portion of the record, you may link to the CAplus or MEDLINE record being cited. Click a linked citation to view the detailed record. The record displays in the **Detail for Citation #** window. If both a CAplus and MEDLINE record are associated with the link, the CAplus record is displayed.



The **e-document** icon is displayed in the top right corner of the **Detail for Citation #** window for documents that are available electronically via ChemPort. Click the icon to view options for electronic access. See *Accessing Full-Text Documents* later in this chapter for details.

The **Detail for Citation #** window can be left open for viewing several citations consecutively. Use the **Previous** and **Next** buttons to move among citations you have already displayed. Citations are redisplayed based on the order the links were clicked. For example, if you click citations in the order 1, 9, 4, 7, they are redisplayed with the **Previous** button in the order 7, 4, 9, 1.

To retrieve related information, click the **Get Related** button. For details, see Chapter 7 and *Linking to eScience* later in this chapter.

To print or save a cited reference, select **Print** or **Save As** from the **File** menu. To exit this window, click **Close**.

Linking to 3D Structure Models (Windows only)

Windows users may use WebLab ViewerLite or ViewerPro software along with SciFinder Scholar to view 3D structure models. The WebLab Viewer products are high-end molecular visualization applications that use Open GL graphics for visualizing models of molecules. Models can be rotated, scaled, edited, labeled, and analyzed to provide better understanding of 3D structure.

WebLab ViewerPro is available for purchase from Accelrys (visit http://www.accelrys.com/about/msi.html for details). WebLab ViewerLite is available via free download from the Accelrys web site. SciFinder Scholar accesses the version of WebLab Viewer that was most recently installed on your PC.

Installing WebLab ViewerLite

Close all Windows applications and anti-virus software, except your Internet browser. *Installation may not proceed properly if other programs are running.*

1. Open your Internet browser to:

   http://www.accelrys.com/viewer/register/lite/viewerlite_reg.php

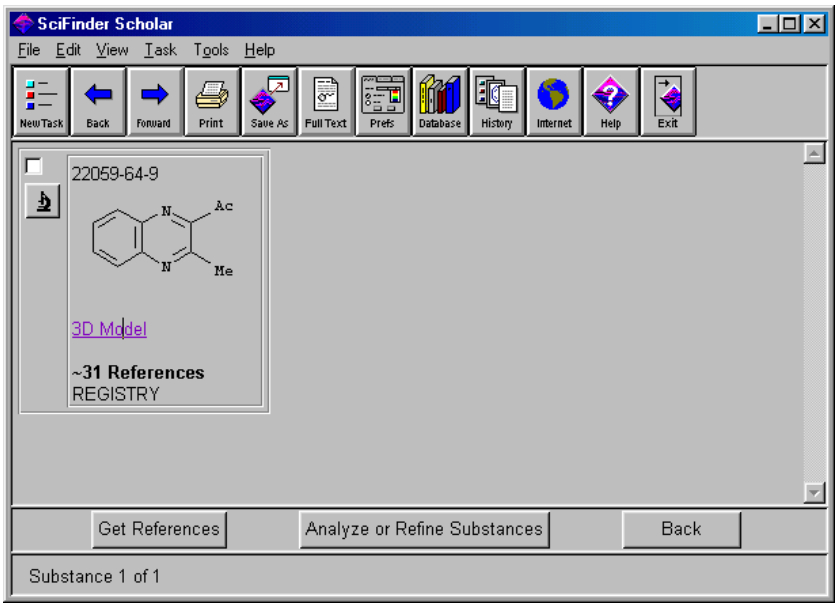
2. After reading the license agreement, enter the appropriate information. Then click the **Submit Form** button at the bottom of the page.

3. Click the **WLViewerLite40.exe** link to download the software. The **Save As** window displays. Choose a folder. Click **Save** to download the file to your computer.

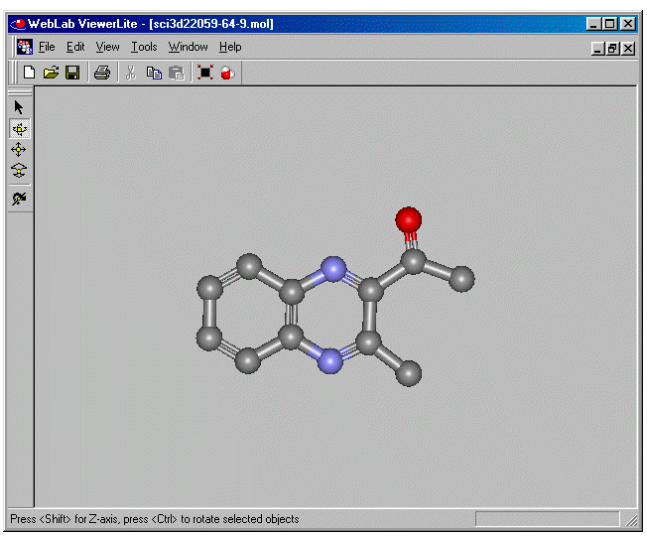
4. Open the folder you chose in step 3. Double-click the *WLViewerLite40.exe* icon. A **WinZip Self-Extractor** window displays. Click **Setup** to begin the installation, and follow the prompts.

Viewing 3D Models

Once you have properly installed the WebLab Viewer, **3D Model** links are displayed for many of the substances in SciFinder Scholar.



Click the **3D Model** link to display the 3D model for that structure.

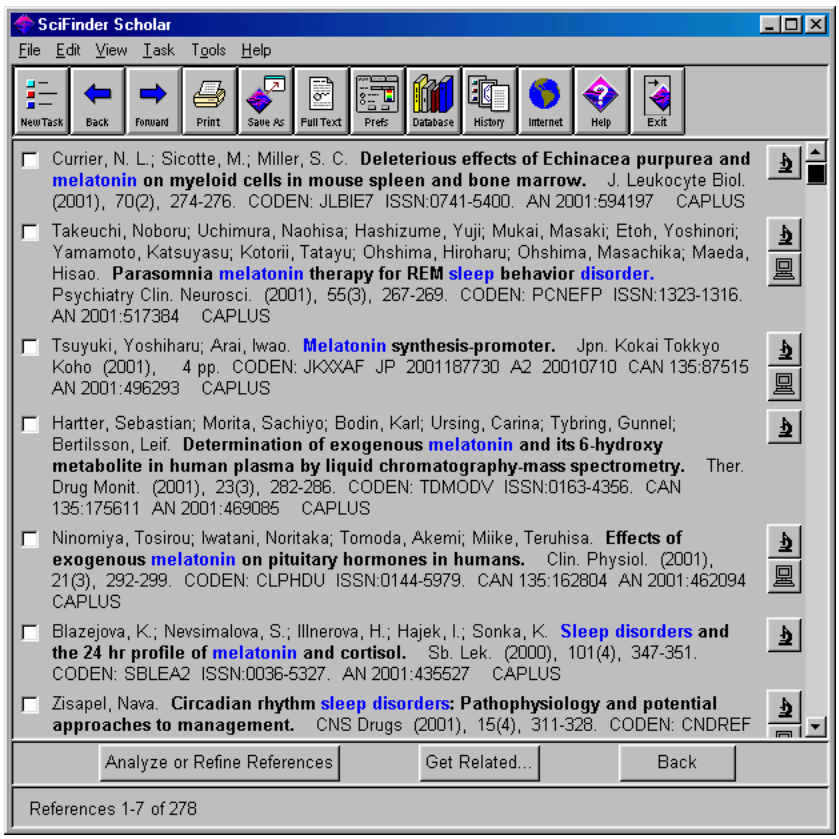


Use the menu items to manipulate the display and to save or print the file. The **Help** menu provides explanations of the functions available. For more information on the features of WebLab Viewer, visit the Accelrys web site at http://www.accelrys.com/weblab/index.html.

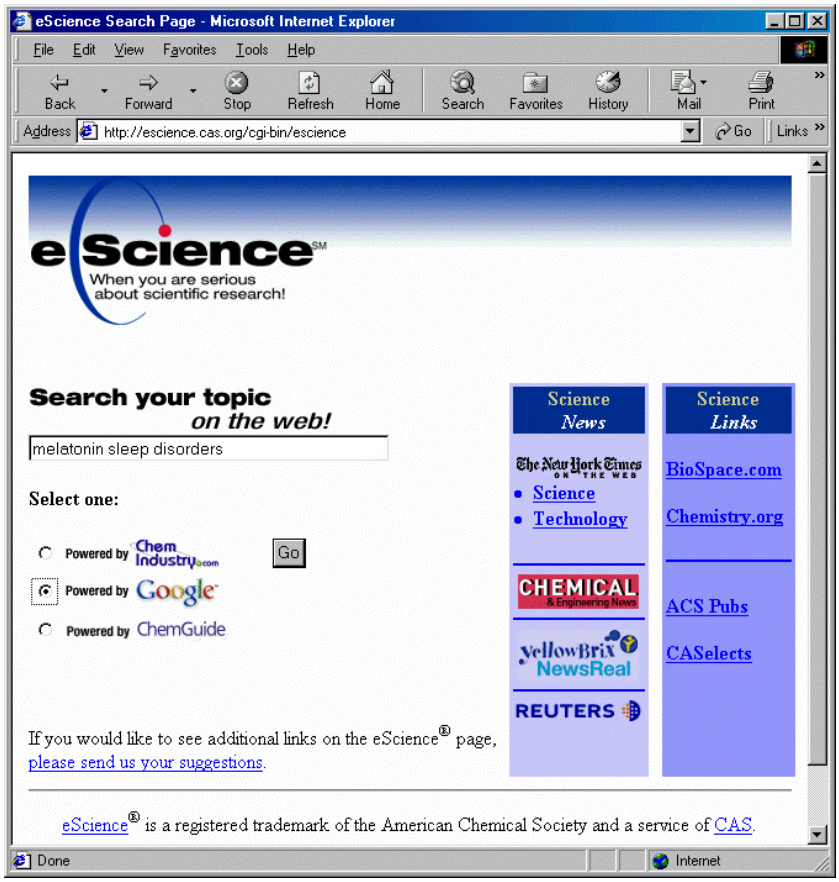
Linking to eScience®

eScience is a dynamic web resource from CAS. After viewing your SciFinder Scholar results, you can quickly and easily extend your search to the Web via the Google™, ChemIndustry.com, or ChemGuide search engine. eScience also provides convenient links to respected news services, science-related portals, and electronic publications. For more information about eScience, visit http://www.escience.org.

eScience can be accessed from any answer set created with Explore by Reseach Topic, Author Name, or Company Name/Organization. First, create a reference answer set with one of these Explore features.



Click the **Get Related** button. Then click **eScience**. Your web browser is launched, and the eScience web page is displayed.



The search box is prefilled with the search terms from your SciFinder Scholar Explore. You may edit these terms as appropriate. To search the Web, select the ChemIndustry.com or Google search engine. Then click **Go**.

Note: When answer sets are created with Explore by Author Name, SciFinder Scholar prefills the search box with all variations of author names selected in the **Author Candidates** dialog. If you receive a message that the search string is too long, shorten the string and try the search again.

Your results are displayed by eScience.

Accessing Full-Text Documents

Use SciFinder Scholar to access full text of articles and patents via your Internet browser and the ChemPort Connection. ChemPort offers several options for retrieving full documents for references of interest, some with no additional charge and some with additional charges.

Full-text options provided at no additional charge:

- View e-articles at publisher web sites (requires a separate subscription with journal publisher). Lists of participating publishers and journals are available at http://www.chemport.org.
- View e-articles using subscriptions with a third-party agent, e.g., a subscription agent (requires a subscription to the agent's service).
- Direct document requests to your in-house library system (requires separate setup; for details, see http://www.chemport.org/html/english/inhouse.html).
- View patents at the USPTO and EPO web sites and via MicroPatent (restricted to MicroPatent Global TOPS subscribers).

Full-text options with additional fees:

- Buy electronic articles and patents
- Order paper copies via a document delivery service

In the **SciFinder Scholar** window, **e-document** icons are placed to the right of individual articles or patents from sources that have electronic full text available via ChemPort. The **e-document** icon appears just below the **microscope** icon. Documents from sources that do not have electronic full text available do not have this icon. An **e-document** icon also appears in the top right corner of the **Detail of Reference #** window for documents available via ChemPort.

If your Site Administrator has worked with CAS to set up a list of your library journal holdings, a **house** icon will appear in the place of the **e-document** icon for journals on your in-house list. **House** icons work similarly to **e-document** icons. However, they help you quickly identify documents that are available via internal sources.

Accessing Single Documents

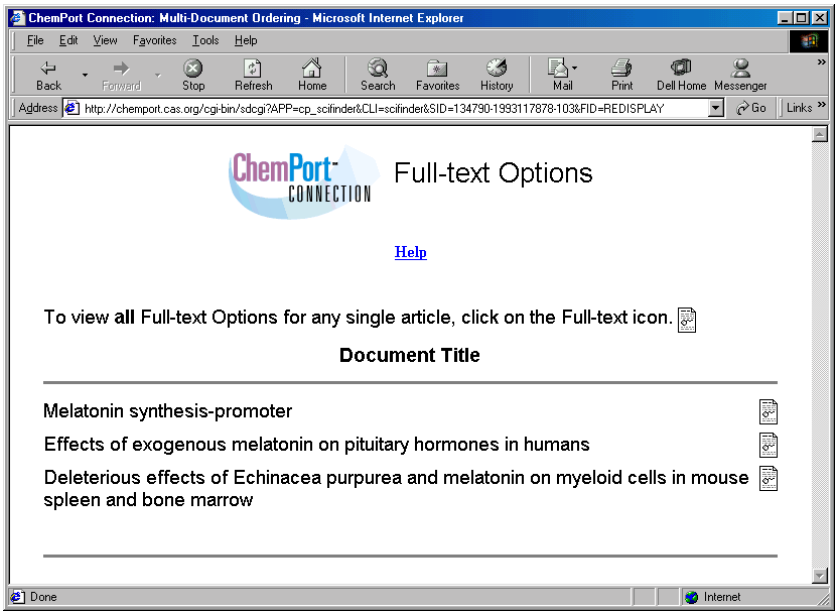
To access a single document, click the **e-document** icon for the document, if present. Or, click the check box to the left of the document. Then click the **Full Text** icon on the **Main Menu Toolbar** or select **Full Text Options** from the **File** menu.

Your Internet browser opens, and ChemPort retrieves information on the document you selected. You are then given options for accessing the document. Options that are grayed out are not available for the document you have selected. Help for these options is available at http://chemport.cas.org/html/english/fts_help.html.

Accessing Multiple Documents

To access more than one document, click the check boxes to the left of those documents. Then click the **Full Text** icon on the **Main Menu Toolbar** or select **Full Text Options** from the **File** menu.

Your Internet browser opens to the **Full-text Options** page, and ChemPort retrieves information on the documents you selected.



Titles of the documents are listed on the ChemPort page. To display all of the full-text options for an individual document, click the full-text icon to the right of the title. Options that are grayed out are not available for the document you have selected. Help for these options is available at http://chemport.cas.org/html/english/fts_help.html.

When you are finished viewing the full-text options, select **Close** or **Exit** from the Internet browser's **File** menu to return to SciFinder Scholar.

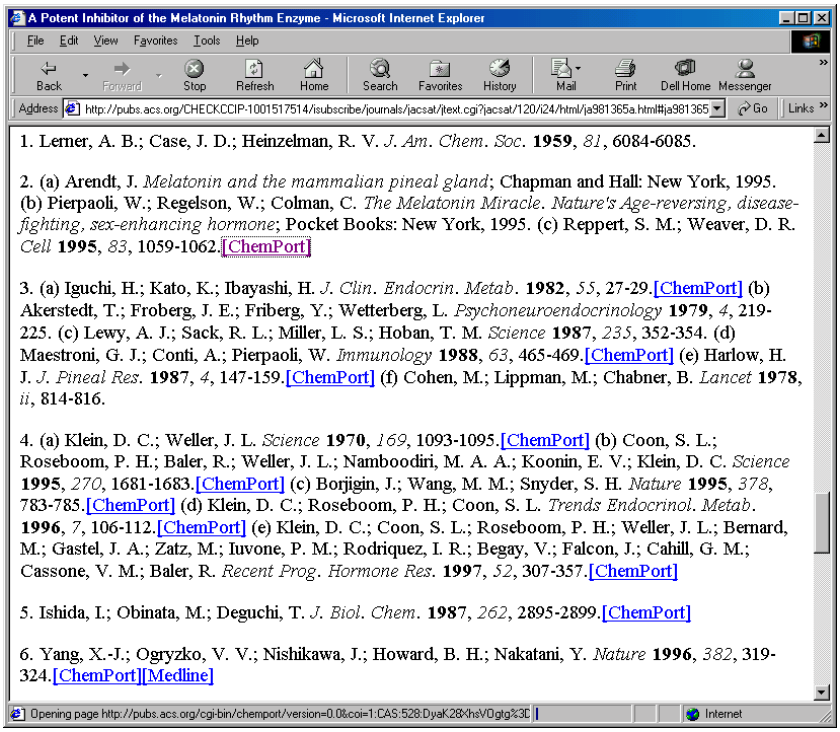
Linking from e-Articles to SciFinder Scholar

Through ChemPort Reference Linking, several publishers provide links from cited references within e-articles to SciFinder Scholar. In SciFinder Scholar, you to easily explore for information related to the reference of interest.

Publishers currently participating include:

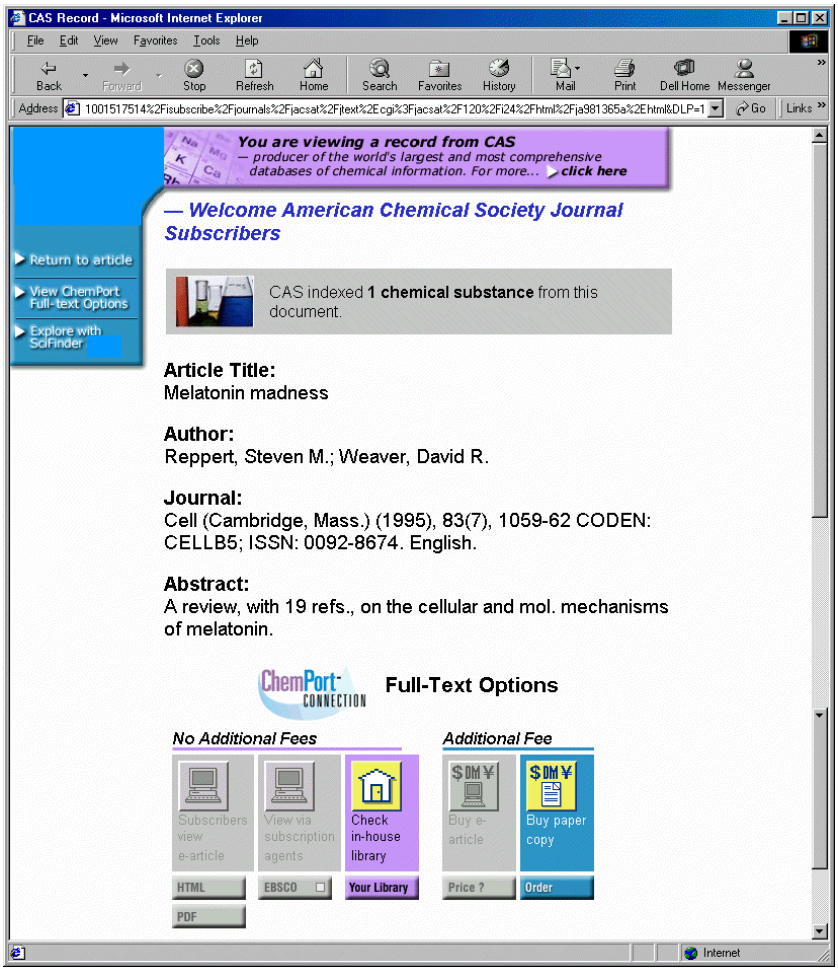
- ACS Publications
- International Union of Crystallography
- Institute of Physics
- Academic Press
- CatchWord (STM Journal Host)

Links to ChemPort appear with references that have records in CAS databases. Links to Medline and ACS Publications full text may also appear.



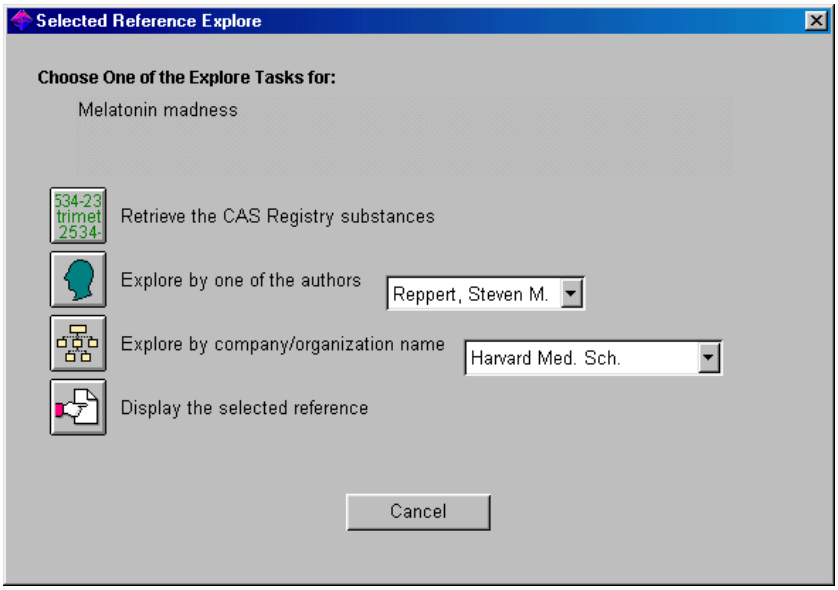
Click the **[ChemPort]** link for a reference of interest.

The CAS record for the reference is displayed by ChemPort.



To search for information related to this reference, click **Explore with SciFinder Scholar** from the blue bar on the left. You must be logged on to SciFinder Scholar for this feature to work.

SciFinder Scholar displays the **Selected Reference Explore** dialog box, where you can request information related to the reference.



You may explore in several ways:

- **Retrieve the CAS Registry substances** – Click this icon to obtain CAS Registry records for the substances discussed in the reference.
- **Explore by one of the authors** – Select an author from the drop-down menu of author names. Then click the **Author** icon to start an Explore by Author Name task.
- **Explore by company/organization name** – Select a name from the drop-down menu of company/organization names. Then click the **Company/Organization** icon to start an Explore by Company Name task.
- **Display the selected reference** – Click this icon to view the reference record in SciFinder Scholar.

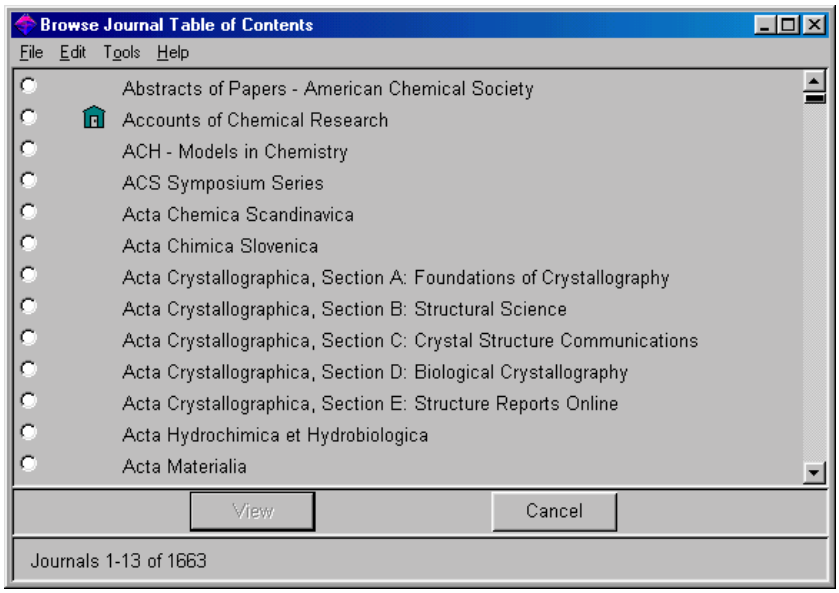
9 Browse Journal Table of Contents

The Browse Table of Contents feature delivers tables of contents for over 1600 key journals in the scientific world directly to your desktop. This feature lets you view the journal's table of contents page, the detailed record of the articles, and, for some journals, the full text of the articles. You may browse each table of contents and view, print, and/or save it.

Chapter 9 demonstrates how to browse journal contents in SciFinder Scholar to find articles of interest.

Accessing Browse Table of Contents

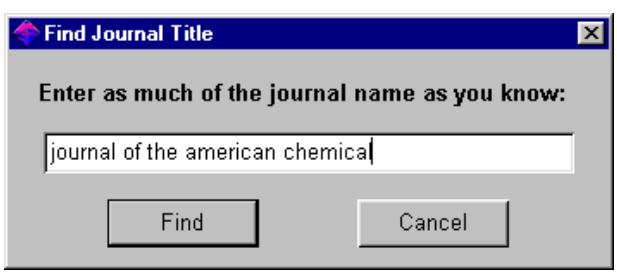
To access the Browse Table of Contents feature, click the **Browse Table of Contents** icon in the **Explore** dialog box. The **Browse Journal Table of Contents** dialog box is displayed.



The complete set of journals is listed by journal title in alphabetical order. This list updates automatically to reflect the journals that are available.

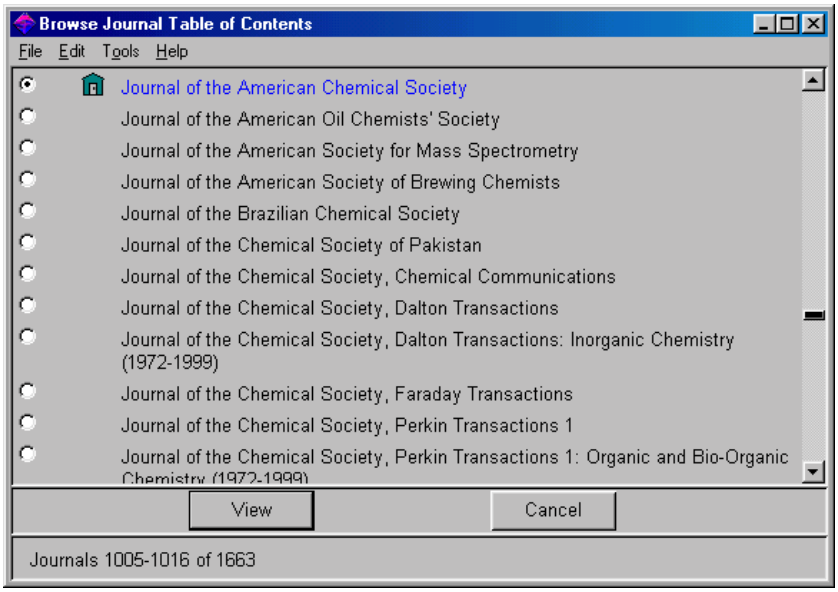
If your Site Administrator has worked with CAS to set up a list of your library journal holdings, a **house** icon will appear next to the journal.

To locate a journal title, scroll through the list using the vertical scroll bar at the right. Or, select the **Find** command from the **Edit** menu to locate a specific journal quickly. The **Find Journal Title** dialog box is displayed.



Type a journal title string in the entry box. Titles may be entered in upper- or lowercase. Click **Find**.

When the title string is found, that title is listed first in the **Browse Journal Table of Contents** dialog box and is highlighted.

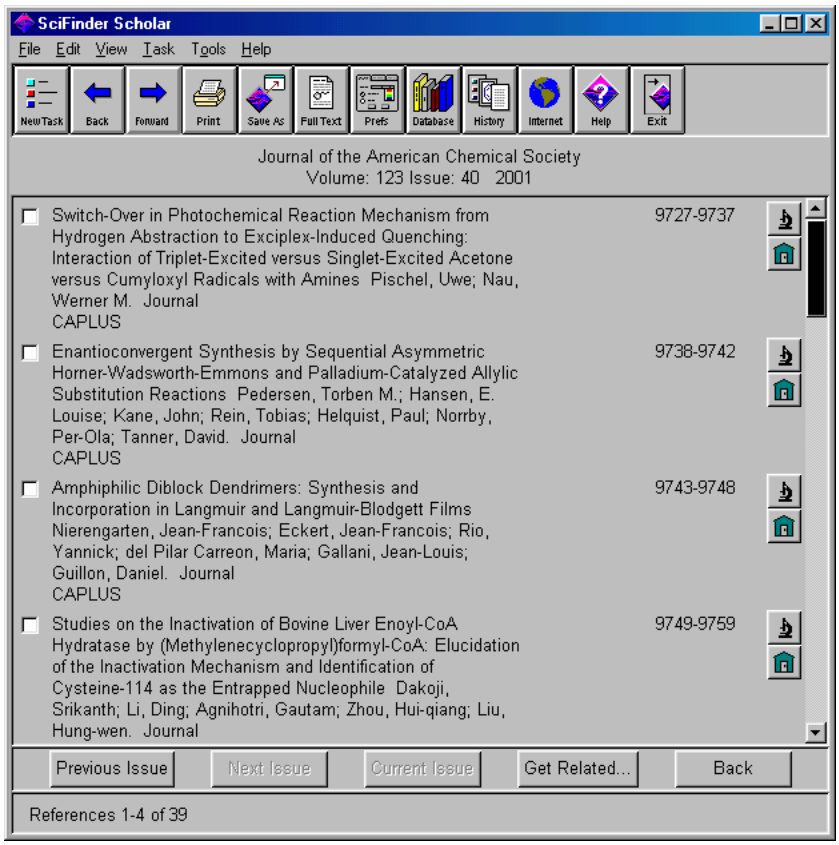


If the search string produces no results, SciFinder Scholar displays a dialog box informing you that the search string was not found. Click **OK**. You are returned to the **Browse Journal Table of Contents** dialog box.

Viewing a Table of Contents Page

To view the table of contents of a journal, click the radio button next to the title. Then click **View**. Only one journal may be selected at a time.

SciFinder Scholar displays the full table of contents page for the most current issue of the journal title you selected and includes the journal title, volume number, issue, and publication year in the header. The titles, authors of articles, and inclusive pagination are listed.



To view details for a reference, click its **microscope** icon. Details are displayed in the **Detail of Reference #** dialog box. For more information, see *Viewing Details of References* in Chapter 7.

You may also retrieve the full text of a document, if available. For details, see *Accessing Full-Text Documents* in Chapter 8.

Click **Previous** Issue to see tables of contents for previous issues. Click **Next Issue** and **Current Issue** to view later issues and the current issue, respectively.

Click **Get Related** to retrieve related information for the articles. See Chapter 7 for details.

Journal article references may be saved and/or printed. To do so, click check boxes next to references of interest. Then select **Save** or **Print** from the **File** menu. For details, see Chapter 2.

Click **Back** to return to the **Browse Journal Table of Contents** window.

Ending Your Browse Session

To leave Browse Table of Contents, click the **Back** button while viewing the list of journals. Or, select **New Task** from the **File** menu or **Main Menu Toolbar**.

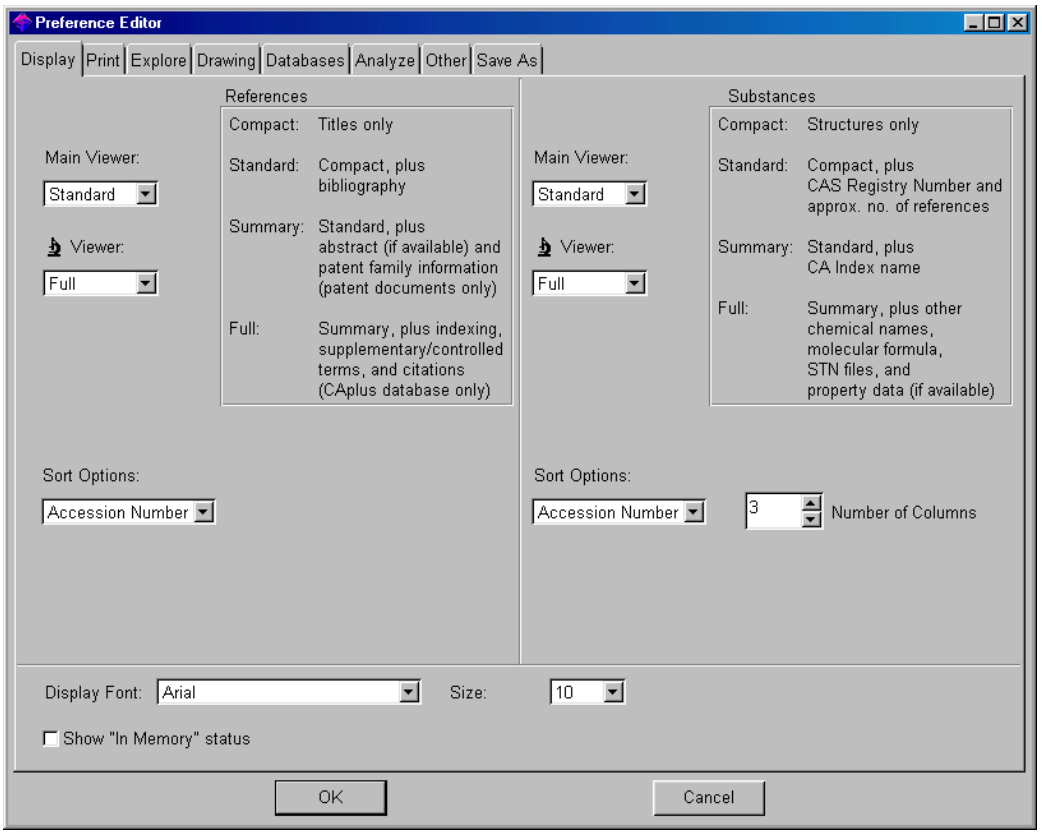
To exit SciFinder Scholar, select **Exit SciFinder Scholar** from the **File** menu or click **Exit** on the **Main Menu Toolbar**.

A

Preferences

Appendix A describes the Preference Editor, which can be used to customize your SciFinder Scholar session. Preferences are reset to the system defaults when you exit.

To change default settings, select **Edit Preferences** from the **Tools** menu or click the **Prefs** button from the **Main Menu Toolbar**. The **Preference Editor** dialog box is displayed.



The Preference Editor includes options for **Display**, **Print**, **Explore**, **Drawing**, **Databases**, **Analyze**, **Programs** (Macintosh only), **Save As**, and various **Other** preferences.

The contents of the **Preference Editor** change to reflect the settings currently stored. To customize options in any area, click the appropriate tab. Modify the appropriate options. When you have completed your changes, click **OK** to close the **Preference Editor**. Or, click **Cancel** to disregard the changes.

Display Preferences

Click the **Display** tab in the **Preference Editor** to customize display options. The Display preferences are displayed. (See the dialog box on the previous page.)

You may customize the display format of references and/or substances. Formats may be changed in the **Main Viewer**, i.e., the **SciFinder Scholar** window, and/or the **Viewer**, i.e., a "microscope" window.

You may also change the display of text by modifying the font and point size.

Reference Formats

Available reference formats for both the Main Viewer and the Viewer, as well as their definitions, are shown in the following table. The default reference format for the Main Viewer is *Standard*. The Viewer reference default is *Full*.

Menu Item	Definition
Compact	Displays the title of the article or patent
Standard	Displays the bibliographic information with the author names listed first
Summary	Displays the bibliographic information with the title listed first followed by the abstract, and, if applicable, patent family information
Full	Displays the entire record, listing the bibliographic information (title first), followed by the abstract, and, if applicable, patent family information, indexing, supplementary terms, controlled terms, CAS Registry Numbers, chemical names, and citations

To change the default for either viewer, select a different format from the appropriate drop-down menu.

Substance Formats

Available substance formats for both the Main Viewer and the Viewer, as well as their definitions, are shown in the following table. The substance default for the Main Viewer is *Standard.* The Viewer substance default is *Full*.

Menu Item	Definition
Compact	Displays the chemical structure
Standard	Displays the chemical structure, CAS Registry Number, the approximate number of references citing the substance, and, if available, links to additional information
Summary	Displays the chemical structure, CAS Registry Number, CA Index Name, the approximate number of references citing the substance, and, if available, links to additional information
Full	Displays the entire record including the chemical structure, CAS Registry Number, chemical names, molecular formula, a list of STN files that contain information about the substance, property data, the approximate number of references citing the substance, and, if available, links to additional information

To change the default format for either viewer, select a different format from the appropriate drop-down menu.

Reaction Formats

For reactions, only the Full display format is available. See *Viewing Reaction Candidates* and *Viewing Additional Hit Reactions* in Chapter 6 for details.

Sort Options

Reference answer sets can be organized in Accession Number Order; Title Order; or Title, Year Order. Substance results can be organized in Accession Number Order or Similarity Order, i.e., similarity to each other as opposed to the query structure.

For a definition of each sort option, see *View Menu* in Chapter 2.

Number of Columns

The **Number of Columns**, i.e., the number of substances placed side by side across your screen, may be set from 1 to 6 columns. The default number of columns is *3*.

Text Options

To change the default font, select a different font from the **Display Font** drop-down menu.

To change the default point size, select a different font from the **Size** drop-down menu.

Show "In Memory" Status

Select the **Show "In Memory" status** box to display a memory message at the bottom of the **SciFinder Scholar** window. This message indicates the number of answers that can be listed and read.

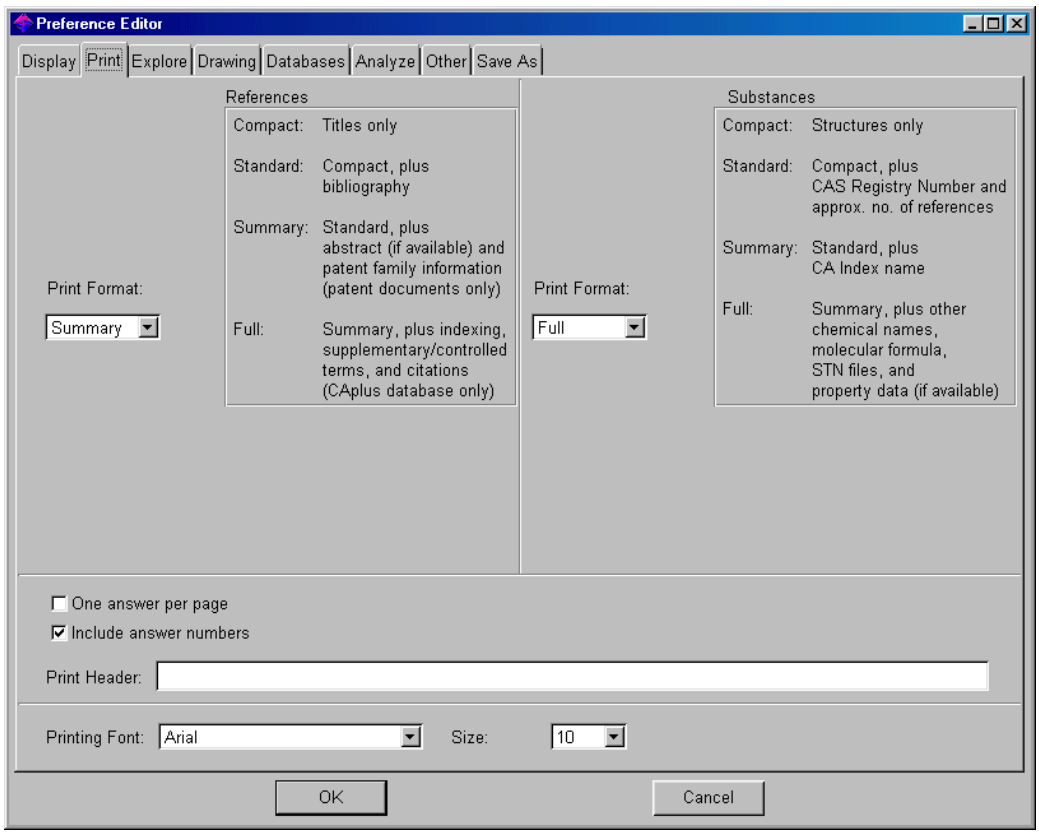
This number is system-dependent and relates to the number of answers your system can hold in its memory.

Setting Display Preferences

After modifying your display options, click **OK** to store your settings and close the **Preference Editor**.

Print Preferences

Click the **Print** tab in the **Preference Editor** to customize print options. The Print preferences are displayed.



You may customize print formats for references and substances. You may set some special features as well. Refer to the *Special Print Features* section for details.

Reference Formats

The **Print** formats for references are identical to those for Display. Refer to the tables in the *Reference Formats* section of the *Display Preferences* for Display formats and their definitions. The default for printed references is *Summary*.

Substance Formats

The **Print** formats for substances are identical to those for Display. Refer to the table in the *Substance Formats* section of the *Display Preferences* for Display formats and their definitions. The default for printed substances is *Full*.

Special Print Features

To activate these special print features, select one or both of the following options:

- **One answer per page** – automatically inserts a page break between two or more printed answers
- **Include answer numbers** – inserts answer numbers in your printed answers (selected by default)

To help identify your printed items, type a header in the **Print Header** box. Headers may be of any length, and is displayed at the top of each printed page.

To change the default font for printing, select a different font from the **Printing Font** drop-down menu.

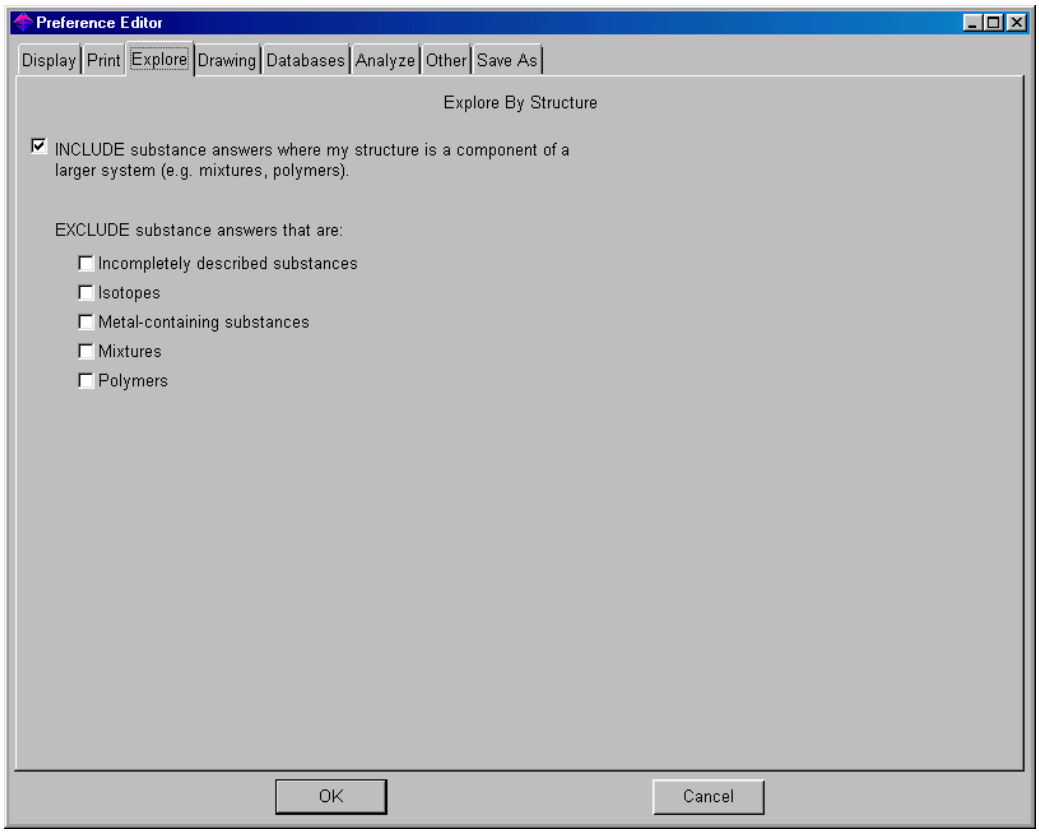
To change the default point size for printing, select a different size from the **Size** drop-down menu.

Setting Print Preferences

After modifying your print options, click **OK** to store your settings and close the **Preference Editor**.

Explore Preferences

Click the **Explore** tab in the **Preference Editor** to customize the explore and retrieval features of structure searches. The Explore preferences are displayed.



The default, **INCLUDE substance answers where my structure is a component of a larger system (e.g. mixtures, polymers)**, retrieves all substance records that contain the structure that you drew, including multicomponent chemicals, such as mixtures, in which your structure is one of the components. This increases the number of substances retrieved. If you are looking for a specific structure that is very common in multicomponent substances, you may want to deselect this option.

You may exclude the following substance types:

- **Incompletely described substances** – The composition and structure of the parent and substituents are known, but positions of the attachments are not known, e.g., trichlorobenzene.
- **Isotopes**
- **Metal-containing substances**
- **Mixtures**
- **Polymers**

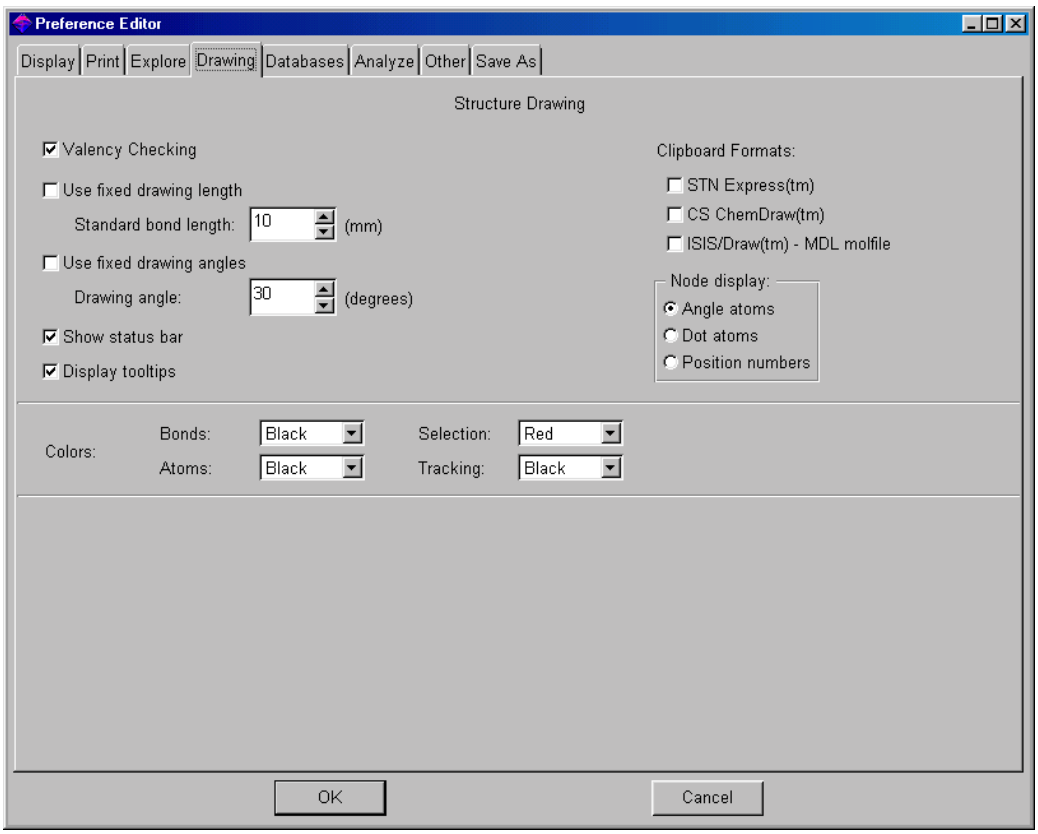
Eliminating one or more of these substance types reduces the number of substances retrieved. If you do not exclude a substance type, SciFinder Scholar will retrieve any substances in these categories that match your structure.

Setting Explore Preferences

After modifying your Explore options, click **OK** to store your settings and close the **Preference Editor**.

Drawing Preferences

Click the **Drawing** tab in the **Preference Editor** to customize your Structure Drawing environment. The Structure Drawing preferences are displayed.



You may select one or more of the following options:

- **Valency Checking** – warns you about the presence of an abnormal valence
- **Use fixed drawing length** – sets bond lengths between 5 and 50 mm
- **Use fixed drawing angles –** sets bond angles between 1 and 90 degrees
- **Show status bar** – displays the molecular formula and the molecular weight at the bottom of the **Horizontal Tool Palette**
- **Display tooltips** – displays definition boxes for items in the Structure Drawing window when the cursor is placed over them
- **Node display** – displays atoms as either angles, dots, or numbers at the node positions in your structure. Only one selection is permitted at a time. Selecting one deselects the previous choice. The default node display is *Angle atoms*.

You may also select one or more connection table **Clipboard Formats** for structures placed on the clipboard with the **Copy** command from the Structure Drawing window. Structures may be copied to the clipboard in the following formats:

- STN Express
- CS ChemDraw
- ISIS/Draw – MDL molfile

See Appendix B for more information on using the clipboard for exporting structure queries.

Color Preferences

To change the default color for **Bonds**, **Atoms**, **Selection** (selected bonds and atoms), or **Tracking**, select a different color from the appropriate drop-down menu.

Setting Drawing Preferences

After modifying your drawing options, click **OK** to store your settings and close the **Preference Editor**.

Database Preferences

Click the **Databases** tab in the **Preference Editor** to choose databases searched with an Explore task. Database selections may only be made before you begin a task.

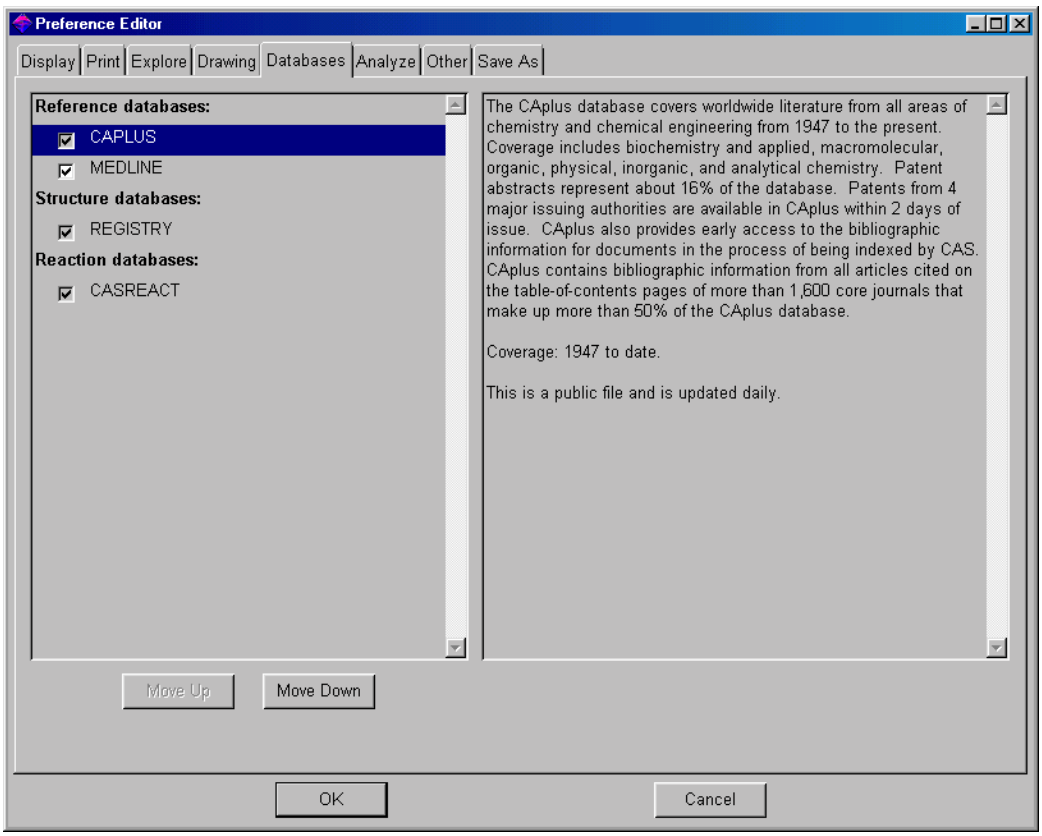
Reference databases offers two choices:

- CAPLUS (cannot be deselected)
- MEDLINE (can be selected or deselected)

If the default order for references is Accession Number Order, the order that the databases are listed determines the order that references are displayed. To change the order, click the name of a database and then click **Move Up** or **Move Down**.

The **Structure database** is REGISTRY.

The **Reaction database** is CASREACT.

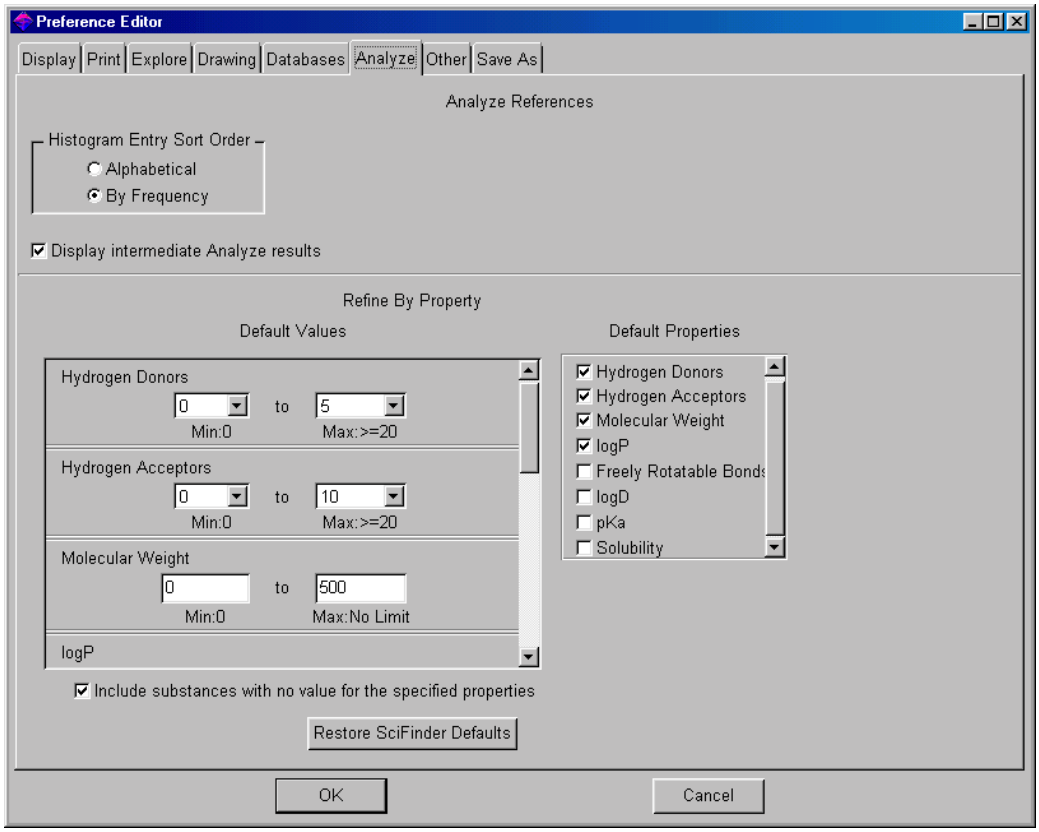


Setting Database Preferences

After modifying your databases options, click **OK** to store your settings and close the **Preference Editor**.

Analyze Preferences

Click the **Analyze** tab in the **Preference Editor** to customize the Analyze and Refine features. The Analyze References and Refine by Property preferences are displayed.



Select an option from the **Histogram Entry Sort Order** section to customize the order of Analyze results. You may choose to arrange the results in **Alphabetical** order or **By Frequency**. The default is *By Frequency*.

Select **Display intermediate Analyze results** to view results as they are processed. This is selected by default.

In the **Refine by Property** section, you may set Default Values and Default Properties for the Refine by Property feature described in Chapter 5.

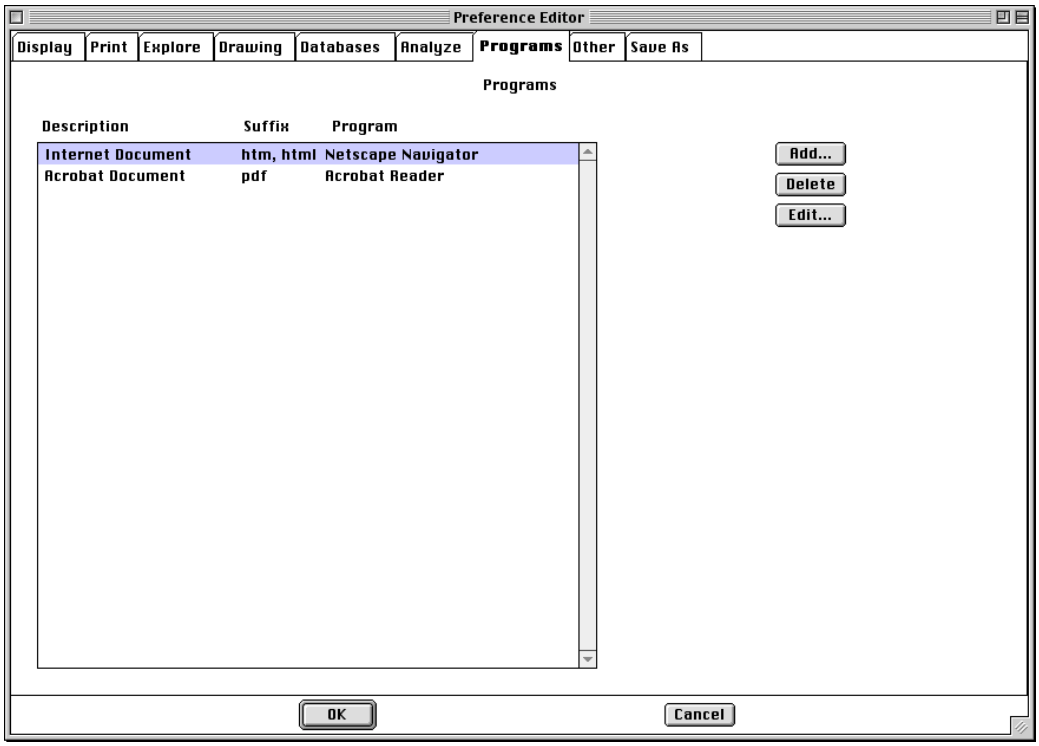
Enter or select ranges of interest for the properties listed in the **Default Values** box. In the **Default Properties** list, select the properties you would like to have selected by default for the Refine by Properties feature. Select **Include substances with no value for the specified properties** to ensure that substances without values available are retained in your answer set. Click **Restore SciFinder Defaults** to return the values to their original settings.

Setting Analyze Preferences

After modifying your Analyze and Refine options, click **OK** to store your settings and close the **Preference Editor**.

Programs Preferences (Macintosh only)

Click the **Programs** tab in the **Preference Editor** to customize applications to launch automatically when specific file types are accessed within SciFinder Scholar. The Programs preferences are displayed.



At present, Acrobat and Internet documents are the only file types that can be found within SciFinder Scholar data.

To add an application to your Programs preferences, click **Add**. The **Add Program** dialog box is displayed, where you can enter the appropriate information. Click **OK** to save the information and insert the application into your program list.

To edit information about a application, select it and click **Edit**. The **Edit Program** dialog box is displayed, where you can make the appropriate changes. Click **OK** to save the changes.

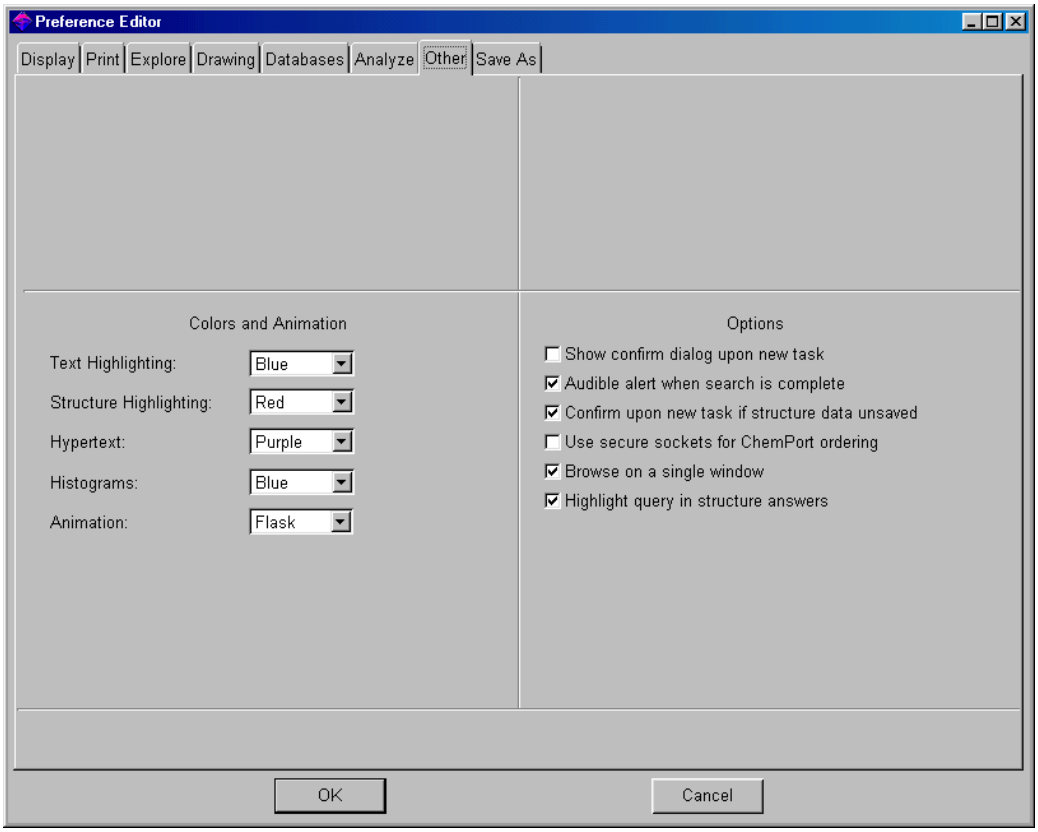
To delete an application from the list, select it and click **Delete**. You are not given a confirmation dialog box for deleting applications. If you change your mind, click **Cancel** to retain your previous list.

Setting Programs Preferences

After modifying your Programs settings, click **OK** to store your settings and close the **Preference Editor**.

Other Preferences

Click the **Other** tab in the **Preference Editor** to customize Colors and Animation and other Options. These preferences are displayed.



Colors and Animation

To change the color of highlighting, hypertext, or histograms, select a different color from the appropriate drop-down menu. The default colors are *blue* for text highlighting, *red* for structure highlighting, *purple* for hypertext, and *blue* for histograms.

To change the animation that displays while SciFinder Scholar retrieves information, select a different option from the **Animation** box. You may select from three different animations. These are shown in the bottom right-hand corner of all applicable windows. The default animation is a *Flask*.

Color and animation changes take effect immediately.

Options

The **Show confirm dialog upon new task** box is used to automatically display a message when you begin a new task that will remind you that the task you are leaving has not been saved. This option is *off* by default.

The **Audible alert when search is complete** option sounds an alert when your SciFinder Scholar search has finished. This option is *on* by default.

The **Confirm upon new task if structure data is unsaved** option should be selected if you want SciFinder Scholar to notify you that the structure task you are about to leave is not saved. This is *on* by default.

The **Use secure sockets for ChemPort ordering** option is available if you want to use secure measures when ordering documents via the Web through ChemPort. This is *off* by default.

The **Browse on a single window** option allows Windows users to use the same browser window for all Internet link requests. If deselected, a new browser window opens for each request. This option is *on* by default.

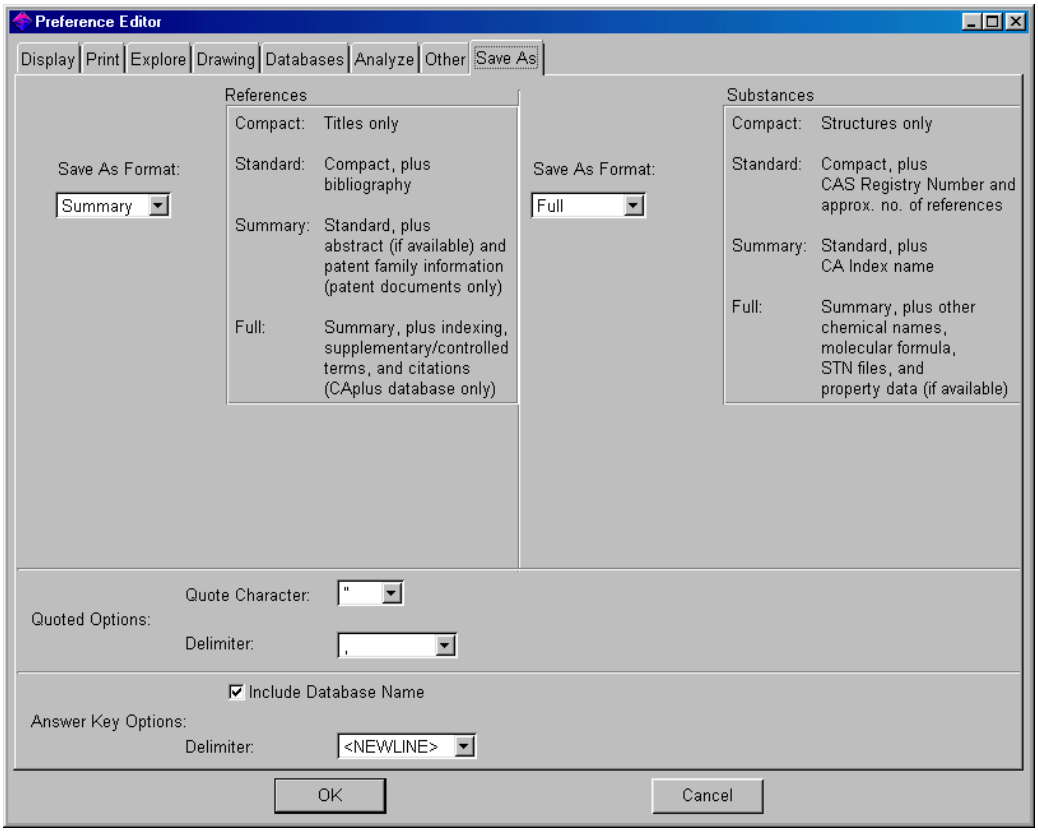
The **Highlight query in structure answers** option highlights the portion of a structure answer that matches the drawn structure. It is *on* by default.

Setting Other Preferences

After modifying your Other options, click **OK** to store your settings and close the **Preference Editor**.

Save As Preferences

Click the **Save As** tab in the **Preference Editor** to customize Save As options. The Save As preferences are displayed.



Reference Formats

The Save As formats for references are identical to those for Display. See the *Display Preferences* section at the beginning of this appendix for details. The Main Viewer default format is *Summary*. The Viewer default is *Full*.

Substance Formats

The Save As formats for substances are identical to those for Display. See the *Display Preferences* section at the beginning of this appendix for details. The substance default for the Main Viewer and the Viewer is *Full.*

Quoted Options

Select characters to define terms and to separate entries by choosing from the **Quote Character** and **Delimiter** drop-down menus, respectively.

The defaults (“ and ‘) are the most commonly used characters for the Comma-Separated Value (CSV) format that is used for input into spreadsheets, e.g., Excel, and database programs, e.g., Filemaker Pro. Numerous other options, including tab-delimited, can be specified with these settings.

Answer Key Options

Select **Include Database Name** to show the database from which that record was retrieved. This option is *on* by default.

Also select from the **Delimiter** drop-down menu to identify how you want to separate answers. (<*NEWLINE*> is the default.)

Setting Save As Options

After modifying your Save As options, click **OK** to store your settings and close the **Preference Editor**.

B Importing and Exporting Structure Queries

SciFinder Scholar allows you to use structure queries created in other Windows and Macintosh applications, including:

- STN Express® with *Discover!*
- ChemDraw®
- ChemIntosh®/ChemWindow®
- ISIS®/Draw

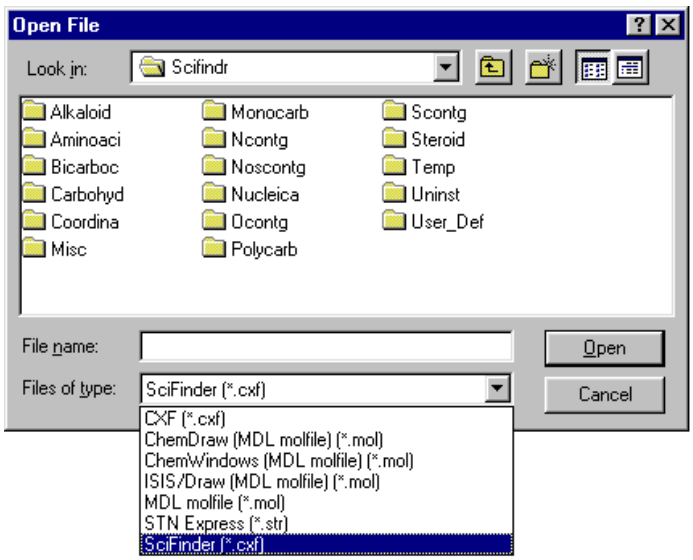
Structures may be saved in:

- STN Express format (.str)
- SciFinder format (.cxf)
- MDL molfile format (.mol).

In addition, SciFinder Scholar can save structure queries in these same formats for use in the above or other applications. This appendix discusses opening from and saving to these formats.

Importing Structure Queries

There are two ways to import a structure into SciFinder Scholar. One way is to save the structure in .str, .cxf, or .mol format in another application. The resulting file can be opened in the SciFinder Scholar Structure Drawing window. To do this, select **Open** from the **File** menu. The **Open File** dialog box is displayed. Choose the appropriate file type from the **Files of type** drop-down menu.



Select a file name and click **Open**. The structure is displayed in the SciFinder Scholar Structure Drawing window.

For ISIS/Draw users, structure queries are not typically saved as molfiles. To create a molfile in ISIS/Draw, choose **Export** from the **File** menu. Then choose **molfile**.

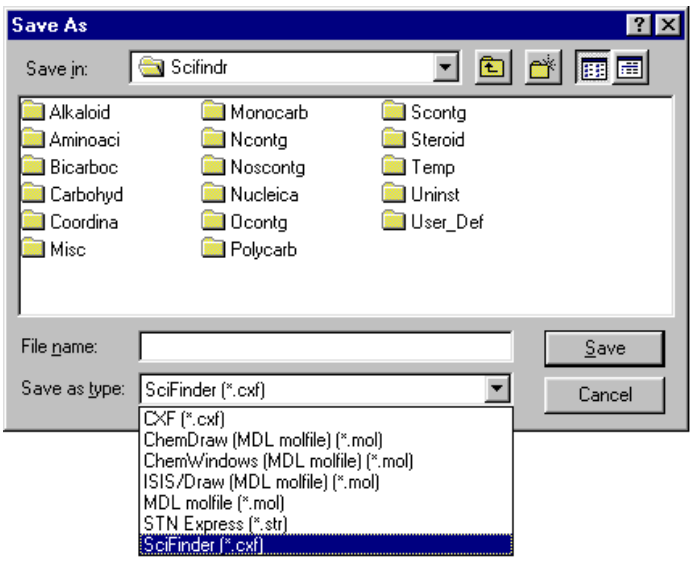
Alternatively, STN Express and programs using the MDL molfile format can copy one or more of the formats above to the clipboard. If this capability is enabled within the **Drawing** tab of the **Preference Editor**, select either the entire structure or the portion that you want to import into SciFinder Scholar. Select **Copy** from the **Edit** menu. Switch to the SciFinder Scholar Structure Drawing window. Then select **Paste** from the SciFinder Scholar **Edit** menu to display the structure.

For ISIS/Draw users, this capability must be turned on. In ISIS/Draw v2.1.3, choose **Settings** from the **Options** menu and then select the **General** tab. Click the check box next to **Copy Mol/Rxnfile to the Clipboard**. This procedure should be similar in other versions.

Depending on the chemical structure, there are significant convention differences between MDL molfiles and SciFinder Scholar structure queries. SciFinder Scholar translates these conventions as accurately as possible. When it is not possible to do a one-to-one translation, SciFinder Scholar broadens the query to the most precise common denominator.

Exporting Structure Queries

SciFinder Scholar can save structures in .str, .cxf., or .mol format. From the **File** menu in the SciFinder Scholar Structure Drawing window, choose **Save** if you have not already saved the structure as a SciFinder Scholar structure query. Alternatively, choose **Save As** if you have already saved the structure as a SciFinder Scholar structure query and you want to save it in multiple formats. The **Save** or **Save As** dialog box is displayed. Choose the file type from the **Save as type** drop-down menu.



Enter a name in the **File name** box and click **Save**. The structure is saved in the specified location. The resulting file can be opened by applications that can read that particular file type.

ISIS/Draw users must choose **Import** from the **File** menu and then choose **molfile** to read an MDL molfile.

To copy a structure using the clipboard, first verify in SciFinder Scholar that the appropriate clipboard format is selected in the **Drawing** tab in the **Preference Editor**. Then select either the entire structure or the portion that you want to export. Choose **Copy** from the **Edit** menu. Finally, select **Paste** in any application that can read the format from the clipboard.

When exporting to the MDL molfile format there may be significant convention differences between MDL molfiles and SciFinder Scholar structure queries. SciFinder Scholar translates these conventions as accurately as possible. When it is not possible to do a one-to-one translation, SciFinder Scholar broadens the query to the most precise common denominator. SciFinder Scholar structure queries have many attributes that bring greater precision when searching extremely large databases such as CAS REGISTRY. These attributes may not be as desirable when structures are saved for a purpose other than as a query or used in other structure-search applications that either do not need or possibly may not support this precision. In these cases, use the structure query editor for that format, e.g., ISIS/Draw, to modify the attributes that you want to change. In ISIS/Draw, many of these attributes are found within the **Edit Molecule** option in the **Object** menu when the entire structure is selected.

C

Smartsearch: Inside Explore by Chemical Structure

This appendix describes SciFinder Scholar's Smartsearch capability, which interprets your structure query for the maximum relevant retrieval of substance candidates. In this appendix, you will find tips and information to help you understand what is being done to maximize retrieval.

NOTE: This feature applies to exact and substructure searches, but it does not apply to reaction searches.

What is Smartsearch?

Smartsearch is a highly technical capability within Explore by Chemical Structure that allows you to draw a chemical structure in the way that is most familiar to you. Smartsearch takes your structure and makes appropriate adjustments to account for various conventions used by chemists. Smartsearch intelligently interprets the structure drawing to allow for the maximum relevant retrieval of substances that match your drawing.

What does Smartsearch Retrieve?

Smartsearch automatically finds all substances that contain the same arrangement of atoms and bonds that you draw. The retrievals may include:

- The structure exactly as you have drawn it
- Stereoisomers
- Tautomers (including keto-enol)
- Coordination compounds
- Charged compounds
- Radicals or radical ions
- Isotopes
- Polymers in which the structure is a monomer

Some examples where Smartsearch allows for special areas of interpretation are listed below:

Tautomers and aromatic bonds are automatically accounted for, including the keto-enol forms of a drawing. Smartsearch will intelligently retrieve the tautomers and aromatic systems on the basis of the single and double bonds you draw in your structure.

SciFinder Scholar may retrieve structures where double bonds are in different locations than in your drawing or where hydrogens are on different atoms than in your drawing.

For some substances, especially dyes, you may find a charge located on a different atom than where you placed it.

Structures that contain metals are automatically manipulated to allow for greater variations. Disconnected and ring forms are retrieved regardless of how you represent the structure. A metal is any element other than the following: H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, I, At, He, Ne, Ar, Kr, Se, Rn. All hydrates are automatically retrieved for metal-containing substances.

Phosphorus-halide and arsenic-halide type search queries retrieve variations where the halogen is a free ion, is bonded to the phosphorus or arsenic, or is bonded to another halogen, regardless of which way the query is drawn.

Both open (acyclic) and closed (cyclic) representations of fluorescein- and phthalein-type dyes are retrieved, if both have been registered, regardless of which way the query structure is drawn. This is also true for hemiacetals and simple sugars.

No special intelligence has been included to allow for polymers, complex carbohydrates, biosequences, alloys or tabular inorganics, stereochemistry, or radical ions. However, these substances are retrieved if they match your structure.

Because SciFinder Scholar favors retrieval over precision, you might receive some false hits in your answer set. However, for each answer, you can decide whether or not you want to view further information on the substance. Use of the Keep Substances, Refine Substances, and Analyze Substances tools will help you zero in on structures of particular interest. In particular, the Analyze by Precision feature can help you eliminate loosely related answers.

In the results, there may be times when more than one answer appears to be the same substance. The answers are not the same; they may differ by stereochemistry or other factors. Click the **microscope** icon and look at the names of the answers to find the differences.

Exact vs Substructure Searches

If your SciFinder Scholar package includes the SciFinder Substructure Module (SSM), when you click **Get Substances**, you are given the option to retrieve answers where your query structure is:

- an exact match or a related structure
- a substructure of a more complex structure

If you do not have SSM, your searches are conducted as exact searches.

The remainder of this appendix describes the differences in how exact and substructure searches are treated by Smartsearch.

Exact Searches

Exact searches retrieve answers such as those listed on the first page of this appendix. Families, e.g., polymers, mixtures, salts, are automatically retrieved. To eliminate particular substance types from future answer sets, adjust the options within the **Explore** tab of the **Preference Editor**. Or, use the Additional Options feature, available from the **Get Substances** dialog.

Answers retrieved with exact searches will not have additional substitution, beyond what you have drawn in your query structure. With exact searches, you cannot specify “open” sites. Structures are considered to be “closed,” so you do not need to draw hydrogen atoms on your structure. Smartsearch automatically includes them if you do not.

Substructure Searches

As with exact searches, answers such as those listed on the first page of this appendix are retrieved. To eliminate particular substance types from future answer sets, adjust the options within the **Explore** tab of the **Preference Editor**. Or, use the Additional Options feature, available from the **Get Substances** dialog.

Substructure searches, however, will provide answers with additional substitution. All nodes are assumed to be “open,” and ring systems are assumed to be “unlocked.” Use the tools described in Chapter 5 to adjust these substructure drawing defaults.

Additional variability can be added to substructure drawings with use of the **X menu** and **R Group** tools. See Chapter 5 for details.

D

Property Definitions

SciFinder Scholar's Refine by Property feature allows you to retrieve substances that possess a particular property or set of properties. In addition, properties are displayed in many SciFinder Scholar substance records.

Properties are calculated using an algorithm from Advanced Chemistry Development, Inc. (ACD). This appendix lists the ACD definitions for the properties currently available in SciFinder Scholar.

Hydrogen Acceptors

The sum of the number of nitrogen and oxygen atoms in the molecule. (These atoms are capable of forming hydrogen bonds with the hydrogen atoms attached to nitrogen or oxygen atoms.)

Hydrogen Donors

The total number of hydrogen atoms attached to the nitrogen and/or oxygen atoms in the molecule. (These hydrogen atoms are capable of forming hydrogen bonds with hydrogen acceptor atoms.)

Molecular Weight

The sum of the atomic weights of the atoms in a molecule calculated using the 1997 IUPAC atomic weights.

logP

The logarithm of the partition coefficient between octanol and water for the neutral form of a compound.

Freely Rotatable Bonds

The total number of single, nonring bonds about which rotation causes a significant physiochemical change in the relative position of the atoms in a molecule.

logD

The logarithm of the partition coefficient between octanol and water at a given pH for the mixture of the neutral and ionic forms of a compound.

pKa

The negative logarithm of the acid–base dissociation constant (in the range of 0 to 14) at 25 °C and zero ionic strength in aqueous solutions for the most acidic and/or most basic sites in a molecule. The pKa for the most basic site is the pKa of the molecule after the most basic site has been protonated.

Molar Solubility

The number of moles of a compound that dissolve in pure water at 25 °C to produce a liter of saturated solution.

Semiquantitative Ranges for Molar Solubility

Very Soluble	1 mol/L ≤ Solubility
Soluble	0.1 mol/L ≤ Solubility < 1 mol/L
Slightly Soluble	0.01 mol/L ≤ Solubility < 0.1 mol/L
Sparingly Soluble	Solubility < 0.01 mol/L

CA Sections

Records in the CAplus database are categorized by subject matter into CA Sections. CA Sections are organized into section groupings, shown in bold type in the CA Section list below.

With the Analyze References feature, you may analyze an answer set by CA Section Title. References are grouped by subject matter into appropriate CA Sections. Results of the analysis are displayed in a series of histograms. Refer to Chapter 7 for information on analyzing references.

Biochemistry Sections

1. Pharmacology
2. Mammalian Hormones
3. Biochemical Genetics
4. Toxicology
5. Agrochemical Bioregulators
6. General Biochemistry
7. Enzymes
8. Radiation Biochemistry
9. Biochemical Methods
10. Microbial, Algal, and Fungal Biochemistry
11. Plant Biochemistry
12. Nonmammalian Biochemistry
13. Mammalian Biochemistry
14. Mammalian Pathological Biochemistry
15. Immunochemistry
16. Fermentation and Bioindustrial Chemistry
17. Food and Feed Chemistry
18. Animal Nutrition
19. Fertilizers, Soils, and Plant Nutrition
20. History, Education, and Documentation

Organic Chemistry Sections

21. General Organic Chemistry
22. Physical Organic Chemistry
23. Aliphatic Compounds
24. Alicyclic Compounds
25. Benzene, Its Derivatives, and Condensed Benzenoid Compounds
26. Biomolecules and Their Synthetic Analogs
27. Heterocyclic Compounds (One Hetero Atom)

28. Heterocyclic Compounds (More Than One Hetero Atom)
29. Organometallic and Organometalloidal Compounds
30. Terpenes and Terpenoids
31. Alkaloids
32. Steroids
33. Carbohydrates
34. Amino Acids, Peptides, and Proteins

Macromolecular Chemistry Sections

35. Chemistry of Synthetic High Polymers
36. Physical Properties of Synthetic High Polymers
37. Plastics Manufacture and Processing
38. Plastics Fabrication and Uses
39. Synthetic Elastomers and Natural Rubber
40. Textiles and Fibers
41. Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers
42. Coatings, Inks, and Related Products
43. Cellulose, Lignin, Paper, and Other Wood Products
44. Industrial Carbohydrates
45. Industrial Organic Chemicals, Leather, Fats and Waxes
46. Surface-Active Agents and Detergents

Applied Chemistry and Chemical Engineering Sections

47. Apparatus and Plant Equipment
48. Unit Operations and Processes
49. Industrial Inorganic Chemicals
50. Propellants and Explosives
51. Fossil Fuels, Derivatives, and Related Products
52. Electrochemical, Radiational, and Thermal Energy Technology
53. Mineralogical and Geological Chemistry
54. Extractive Metallurgy
55. Ferrous Metals and Alloys
56. Nonferrous Metals and Alloys
57. Ceramics
58. Cement, Concrete, and Related Materials
59. Air Pollution and Industrial Hygiene
60. Waste Treatment and Disposal
61. Water
62. Essential Oils and Cosmetics
63. Pharmaceuticals
64. Pharmaceutical Analysis

Physical, Inorganic, and Analytical Chemistry Sections

65. General Physical Chemistry
66. Surface Chemistry and Colloids
67. Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms
68. Phase Equilibriums, Chemical Equilibriums, and Solutions
69. Thermodynamics, Thermochemistry, and Thermal Properties
70. Nuclear Phenomena
71. Nuclear Technology
72. Electrochemistry
73. Optical, Electron, and Mass Spectroscopy and Other Related Properties
74. Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes
75. Crystallography and Liquid Crystals
76. Electric Phenomena
77. Magnetic Phenomena
78. Inorganic Chemicals and Reactions
79. Inorganic Analytical Chemistry
80. Organic Analytical Chemistry