Leeds University Library Training Materials

SciFinder Scholar

Contents

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SciFinder Scholar

SciFinder Scholar includes:

Bibliographic databases:

- CAPLUS (Chemical Abstracts): Contains journal articles, patents, conference proceedings, technical reports, reviews etc. back to 1907. In addition to chemistry it covers geology, materials science, biology, medicine, food science, agriculture, polymer science, physics and engineering.
- MEDLINE: Covers biomedical sciences dating from 1951 to the present.

Chemical reactions database:

- CASREACT: Contains more than 8 million single- and multi-step reactions

Chemical substance databases:

- CAS REGISTRY: Contains data on more than 23 million substance and 43 million sequence records, the substances identified from the scientific literature from 1957 to the present with some classes going back to the early 1900s.
- CHEMLIST
- CHEMCATS

AIMS

This workbook contains a number of tasks and activities which will introduce you to SciFinder Scholar. By the end of this workbook you will be able to:

- Access SciFinder Scholar
- Explore the database to find references on a particular topic or by a particular author
- Perform searches of the database using substance information or structures
- Save or print your search results
- Find out if an article is available online and view that article

ABOUT THIS WORKBOOK

- Things that you need to type are displayed in **`Courier New bold`** font

1. Getting started

SciFinder Scholar is only available on computers where the software has been specially installed. It is already available on PCs in University clusters, departmental offices and labs with ISS machines.

In ISS-independent departments the software will need to be installed on each machine. If you need this done on your own computer, please contact your Departmental IT Rep who should be able to provide you with instructions. Alternatively you can download the software from the Library website at:

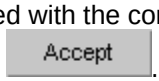
http://www.leeds.ac.uk/library/databases/indexguides/scifinder.htm

At present, only five people can use the database at one time, and you may find you can't access it at peak times. Off-peak times occur between 18:00 and 8:30 and at weekends.

Exercise 1a

From an ISS cluster, click **Start>Programs>Miscellaneous>Library services & remote databases>Library 'Chemical Databases' - SciFinder Scholar 2006**

On ISS-independent machines, double click on the SciFinder Scholar icon  which should appear on your desktop.

Before the software is opened completely, you are presented with the conditions of use. The first time you use SciFinder Scholar, you should read these terms. Then click 

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At this point the full Scholar screen loads and you are offered the option to explore the database using a number of different search options.

You can get help from within SciFinder Scholar at any time by clicking on 

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2. Searching by Research Topic

Exercise 2a

Click on the **Explore** button  and then on the **Research Topic** button 

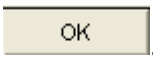
.

In the box type: **`OH radicals in the troposphere`**

Click on 

From here you can restrict your search to a particular **date**, **document type**, **language** or by a particular **author or company**.

In the **Publication year** box type: **`2000-2007`**
Select **Journal** as the **Document Type**

Now click 

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SciFinder Scholar makes various interpretations of the phrase you have entered and combines the terms in a way that allows you to choose exactly which search you wish to perform. These options are displayed in a box of topic candidates. You should check to see that the phrases in bold reflect accurately the phrase you entered.

The search will automatically truncate your keywords to search for related words, and will also automatically search for plurals. In the case above, this means that the database will find records containing the words:

tropospheric as well as **troposphere** and **radicals** as well as **radical**

The numbers of records that will be found if a particular combination is searched are shown and a check box is displayed next to each one so you can choose exactly which search you want to perform.

SciFinder Scholar generally produces the most interpretations when search terms are linked by prepositions (e.g. **in**, **of**). **SciFinder Scholar does not use Boolean logic, so there is no need to link your keywords with AND, OR, NOT as in many other databases. If synonyms are entered, they should be put in brackets after the word they are a synonym of.**

Exercise 2b

Click in the box by the entry:

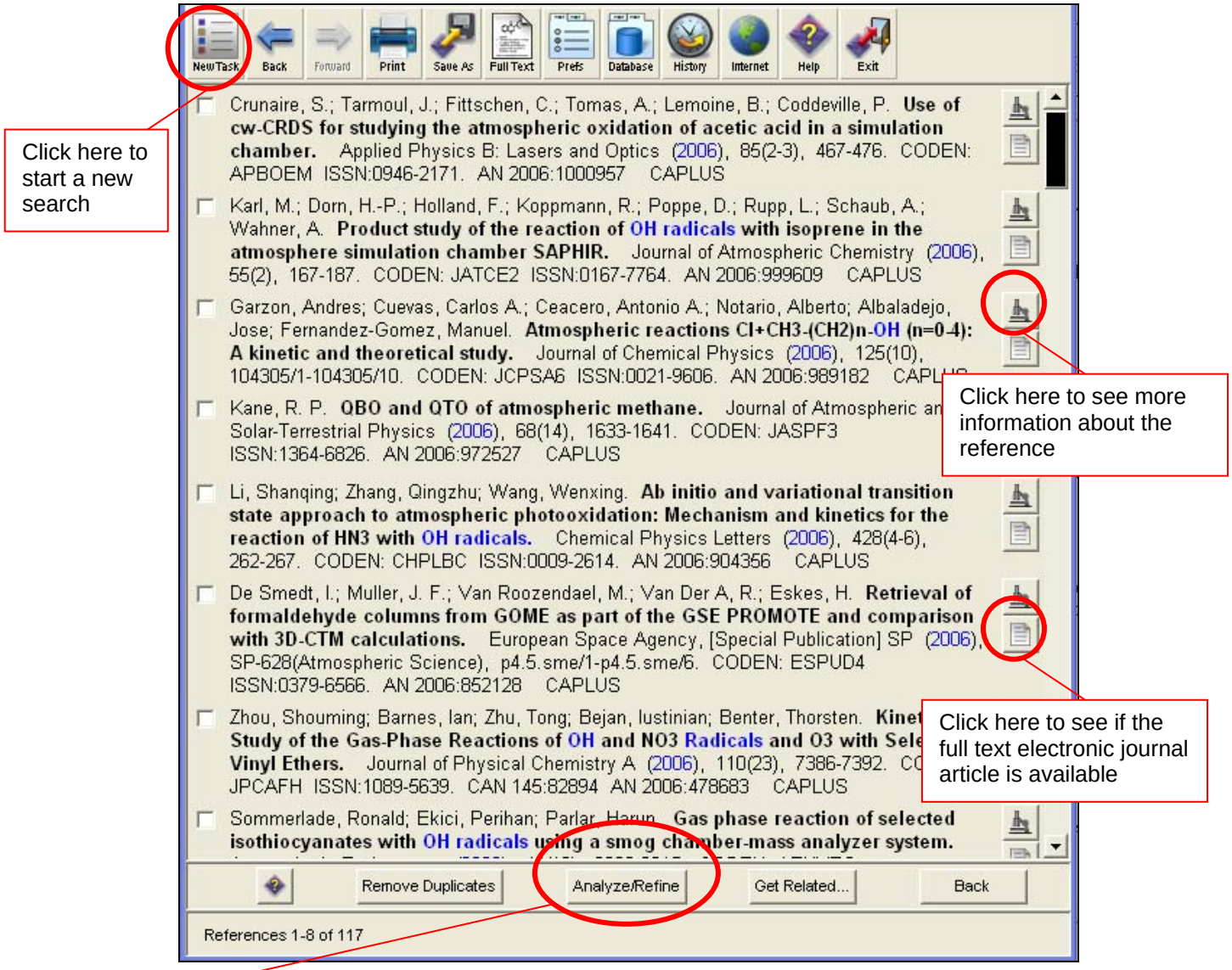
[number] references were found containing the two concepts "OH radicals" and "troposphere" closely associated with one another.

so that a tick appears in the box.

Now click 

.

The screen should look similar to the one below, displaying details of all the references SciFinder Scholar has found.



Limits

To limit the results to particular authors, dates, languages, or document types, or to reduce the results to a more specific subject, you can choose to **Analyze or Refine References**.

- Choosing to **Refine** the results allows you to add more limits and narrow your search
- Choosing to **Analyze** the results allows you to see what proportions of the records are found in a particular journal, are by a particular author, or are from particular organizations and you can then choose to display records using one of these criteria. This is useful if you want to search in a particular journal or you want to combine an author's name search with a topic search.

Exercise 2c

To see what options are available:

Click on Analyze/Refine and then on the Analyze button 

Use Back to return to your results.

Now limit the results you have already obtained to material published in English.

Click Analyze/Refine and then  to refine the search

Click on the Language button  .

Check the box next to **English** and then click OK.

Any records for articles not in English will have been removed.

Click 

at the top of the SciFinder Scholar screen. The task history describes what you have done to get to where you are now and will state the number of references found after refining by Language. Close this task history window when you have finished looking.

Finding Related Articles

It is possible to do citation searches, either finding articles that cite a particular reference, or all articles cited by the reference. **Citation searching is a very good way to find material on the same or similar subject.**

To do this use the **Get Related** option on the results screen. This option also enables you to retrieve substance data on the substances indexed in a reference.

Exercise 2d

Scroll down the list and click on the box next to any article published **before 2003** then click Get Related....

From the options box that appears, click  , "Citing References".
The articles which appear will be those that have cited the reference you chose.

3. Viewing Records

Results list: SciFinder Scholar displays the authors, title (in bold) and source information (e.g. journal, patent, conference details) for each item. Terms matching your search and further limits are highlighted in blue. Journal titles are presented as abbreviations. Year of publication, volume numbers and page numbers are also provided. The most recent articles are shown first.

Full record: A full SciFinder Scholar record contains the bibliographic information that you can already see and also an abstract describing the paper and indexing terms used when you perform a search within the database. These indexing terms can help you find out the focus of the paper and help you decide if it is relevant to your work.

Exercise 3a

Click on one of the **Detail Viewer** buttons  next to one of the records on your results screen. A new window should open containing the full record.

Scroll down the record to see what it contains. Very recently added records don't yet contain the full information but in some of those towards the bottom of the screen you should see some of the Registry Numbers for substances mentioned in the article and the article's citations (bibliography) included. The Registry Numbers (three groups of hyphenated numbers) are linked to the Registry record for that substance. Some of the bibliography items are linked to their own SciFinder Scholar records.

Click on one of the purple Registry Number links. Another new window should open containing the Registry record for that substance.

Close the Registry record window by clicking Close.
Then close the full record window.

4. Searching by Author Name

When you know the name of an author, it is best to enter the surname and initials; if this gives too many hits, enter as much details of the first names as you know. SciFinder Scholar automatically looks for the initials as well as expanding any initials you enter. It will also look for abbreviated forms of the first names you enter. You can then choose which of the various options presented you want to search.

If you are not sure how to spell a surname, enter the name as you think it might be spelt and ensure there is a tick in the box **Look for alternative spellings of last name**. SciFinder Scholar will look for variations in the spelling including international variations.

Exercise 4a

Start a new search by clicking on the **New Task** button 

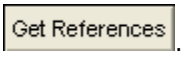
at the top of the SciFinder Scholar screen then on **Explore** 

Now click on the **Author** button  .

In the **Last name** box, type: `Pilling`
In the **First name or initial** box, type: `M`
In the **Middle name or initial** box, type: `J`
Now click 

.

SciFinder Scholar will then display a list of option it thinks you might be interested in searching. The number of references for each of the names is displayed.

Check the boxes next to **Pilling M**, **Pilling M J**, **Pilling Michael J** and **Pilling Mike** and then click 

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Records containing theses author's names are now shown.

5. Searching by Chemical Substance or Reaction

It is possible to search for articles on particular substances in SciFinder Scholar using several different methods. You can search using the substance's name, its molecular formula or CAS Registry Number, or you can draw a structure diagram or reaction.

Chemical Name

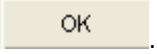
Exercise 5a

Click on 

at the top of the SciFinder Scholar screen and then on **Locate** 

Now click on the **Substance Identifier** button 

.

In the box, type: `aspirin`
Click 

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The record for the substance is retrieved; this includes the Registry Number, a small structure diagram and the number of references within the database.

Click  to see a fuller record containing alternative names, physical properties and registry numbers. There are also 4 icons above the structure drawing - move the cursor over each to see what they are for.

Click on the **Commercial Sources** icon  .
A number of companies selling the substance are listed.

Click on  next to one of the company records to see more details.

Now close this window, then close the window showing the commercial sources list.

To find articles containing references to substance you must first ask SciFinder Scholar to retrieve the references.

You can retrieve all the references contained in the database that contain information about the substance or you can specify what information you want to look for.

Exercise 5b

Click 

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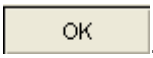
In the **Get References** box that appears, under **For each substance, retrieve:** click on the radio button next to **References associated with:** and then click in the box next to **Preparation**.

Now click 

. The list of articles that now appears contains information on the preparation of aspirin.

Note: Remember, the number of references you have now retrieved is shown at the bottom of the window. You can further refine or analyze to reduce the set of results to more relevant references.

Molecular Formula

When searching on formulas, you should enter each element and number and follow it with a space. The order you enter them in is not important, e.g. thymine (C_5 H_6 N_2 O_2) can be entered as **C5 H6 O2 N2** or **C5 O2 H6 N2** and will still be found.

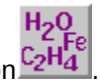
To search for polymers, put the component formula in parentheses and follow with **x**, e.g. polypropylene would be **(C3 H6)x**.

Use upper and lower case for elements having two letters, i.e. Si for silicon rather than SI.

To enter molecular formulae for multicomponent substances, specify each component, separated by a full stop. If SciFinder Scholar does not understand what you have entered it will ask you to enter it again.

Exercise 5c

Click 

. Now click on the **Chemical Substance or Reaction** button  then on the **Molecular Formula** button 

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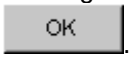
Enter the following formula into the box: `C21 H15 N O6 S. Na`
Then click 

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Click on  next to each record and find out what colour dye this substance is (close the window for each record after you have looked at it). Note some of the records are for substances that are incompletely defined.

Structure

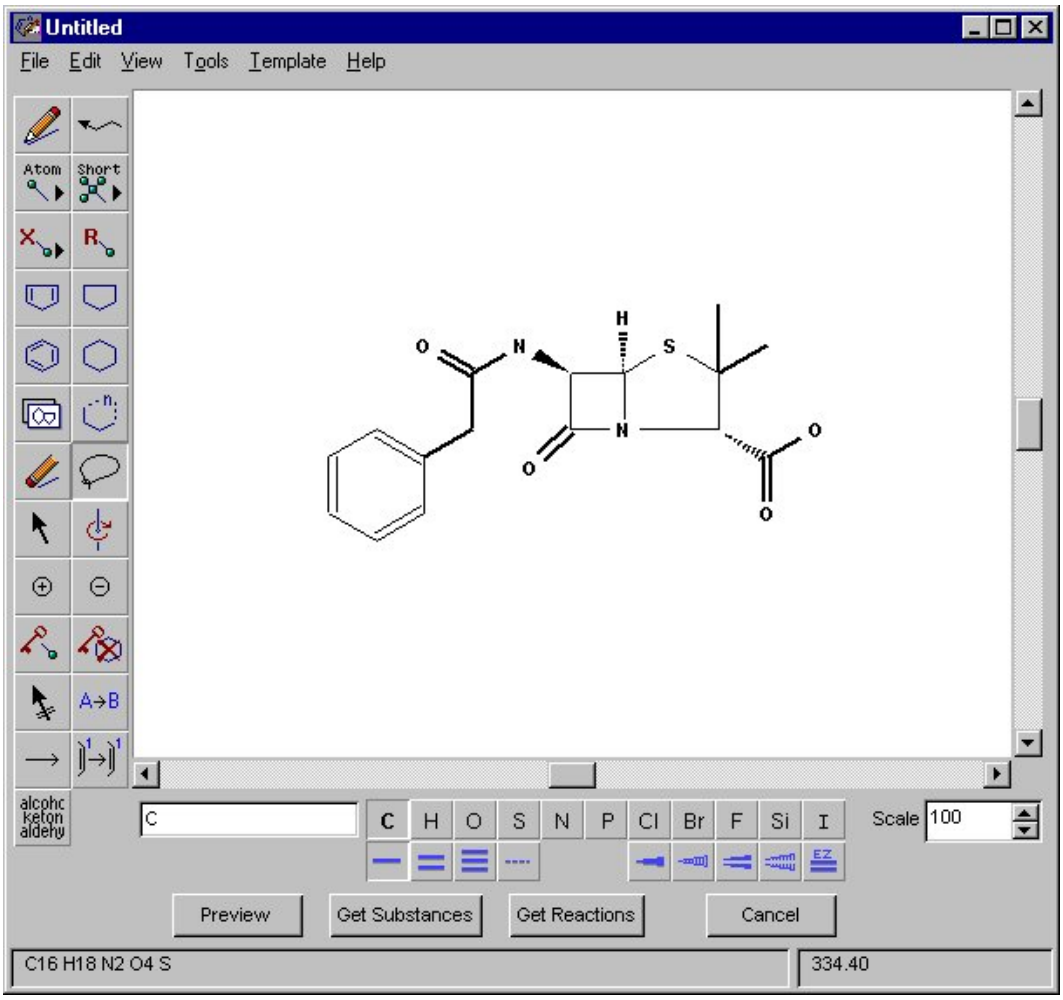
Within SciFinder Scholar there is a structure drawing palette. Structures can be drawn completely from scratch, or there are methods of pasting in information from which structures can be created.

Optional exercise 5d

Click 

. Now click on the **Chemical Substance or Reaction** button  then on the **Chemical Structure** button  . The palette window will open.

Build the structure of penicillin G. The completed structure is shown below, followed by basic instructions for using the structure drawing palette.



How to draw structures

Bonds:

Use  to draw bonds and specify the atoms that are linked. The default is set to a single carbon bond, but you can change the bond type by clicking  ,  or  for double, triple and undetermined bonds respectively, or

 for stereo up bonds,  for stereo down bonds, and  and  respectively for stereo up and down double bonds.

Atoms:

To change the atom to be drawn, click on the letters above the bond buttons, e.g.  ,  ; or click and hold down  which will bring up a periodic table to choose an element from. Keeping the mouse button held down, move the cursor to the atom required then let go. The element currently chosen will be shown in the box to the left of the element buttons - you can also type the letter(s) corresponding to the element you want directly into here. Clicking and holding down  will bring up a list of commonly used groups, e.g. SO_2, NH_3, Me (methyl), which can be selected in place of single elements.

- If you make a mistake click **Edit** on the menu bar then **Undo**. This will 'undo' the last change made.
- You can 'rub out' areas using the erase tool  . For larger areas it may be easier to remove them by clicking the lasso button  then drawing round the area you wish to delete. Clicking on **Edit** from the top menu then **Cut** will remove the area.
- To change a bond that has already been drawn to another type, click on the required bond button along the bottom of the window; then click on the bond in the diagram to change it.
- To change the element found at a node, click on the button along the bottom corresponding to the element required, or type the symbol into the box to the bottom left of the screen, then click on the node where you wish the new element to be placed.
- Draw rings by clicking on one of the ring symbols (e.g. ) then clicking in the drawing palette.
- To make a bond between two nodes that are already drawn, click  then move the cursor over the node until it is highlighted red. Click and hold the mouse button and move the cursor over the second node until that is also red, then let go of the mouse button.

There are various templates for more complicated structures (e.g. multiple ring compounds) available. Click **Template** in the menu bar then choose one of the types of molecule templates available, e.g. amino acid, carbohydrate, polycarboxylic, steroid. A selection of available templates for that molecule type will then appear. Click on the template required then click  . Click on the drawing palette to draw the structure.

To add a ring to one already drawn, click on one of the ring icons (from the right hand side menu) then move the cursor on the target ring until the bond you want to attach to is highlighted red (make sure the whole bond is highlighted and not just one of the end nodes), then click to draw the ring.

A quick way to draw a structure is to copy the CAS Registry Number from another record within SciFinder Scholar. The Registry Number is usually at least 5 digits long and is usually shown with hyphens. Once you find a record for a substance, you can highlight the Registry Number by clicking and dragging your cursor over it, then when it is highlighted, click on the **Edit** option in the menu bar and choose **Copy**. Go to the structure drawing palette and click on **Edit** and **Paste** from the top menu bar. Once you have a structure in place you can edit it as required.

Alternatively**,** you can take a structure from another drawing package and save it as a .str, .cxf or .mol file, and then open the file in the SciFinder Scholar drawing palette. In ISIS/Draw choose **Export** from the **File** menu and then choose **molfile**.

- When searching by structure, it is useful to be able to 'lock' or 'unlock' parts of the structure for substructure or reaction searching. Unlocking a node allows for substitution at that node; locking a node

prevents any substitution at that node. Lock and unlock using the  and  buttons respectively. It is also possible to search for a reaction by drawing two structures and then drawing an arrow between the two. It is useful to be able to combine this with the mapping of atoms and/or the specification of the role of the structure. To specify a role, click on 

and then on one of the structure drawings. A box will appear asking you to define a role for that structure.

Finding substance information using structures

Once you have a structure drawn in the window of the palette, you can run a search for an exact match to the structure or a related structure or you can search for a substance where the structure drawn is part of a bigger structure (these are the two options you are presented with after clicking 

). You can also search for reactions in which the structure you have drawn takes part - after clicking 

you are presented with various choices as to the structure's role in the reaction.

You can run a preview of the database which means that a test search will be run which will give you an idea of the number of records that might be located. It also offers the possibility of checking that the structure you have entered will give the correct kinds of records.

If you choose 

you will be asked where in the reaction you wish the structure to be found. You could click on this button to see what options there are.

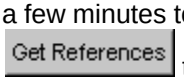
Exercise 5e

Once the structure drawing of Penicillin G is complete, click 

, then click on 

to search for an exact match or related structure.

The search will take a few minutes to complete.

Once complete click 

to view the article information.

Note: If you start a structure search by mistake, you can stop it by clicking 

which appears at the bottom of the screen.

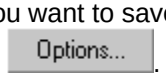
For more details of structure searching see CAS's SciFinder Scholar Solutions page at http://www.cas.org/SCIFINDER/SCHOLAR/SOLUTIONS/index.html

6. Saving and Printing

You can save references and substance information, including structures, from SciFinder Scholar into files.

The following file types are useful:

- ASCII (.txt) - this preserves the information in the form as you would see it if you printed it
- Rich Text Format (.rtf) - this is similar to ASCII but also preserves some of the formatting

Files of this type can be read in Word. Choosing one of the two options above allows you to specify how much of the information you want to save, and whether you want to save all of the records, or only those marked. After choosing **Save As...** from the File menu, click on 

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For downloading into database programs use one of the following:

- Quoted format (.txt) - allows you to create a delimited file which can be entered into a database like Excel. (Once in Excel, choose **File** then **Import**, then select your .txt file. Excel will want to know that it is a delimited file, and the delimiters are commas.)

- Tagged Format (.txt) - creates files for bibliographic database programs like EndNote and ProCite. Once in EndNote, import using the SciFinder (CAS) import filter.

Exercise 6a

Make sure you are on a screen showing search results. Check the boxes next to any two of the records to select them.

As soon as you select a record, SciFinder Scholar assumes you will want to save or print only the record(s) you have selected. However, at the stage of saving you will still be able to choose to use all the records.

Now click on 

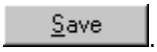
at the top of the window. The **Save File As** box appears.
Click on the arrow next to the **Save in** box at the top of the window and change this to the drive you use to save files (e.g. My Documents). Choose the folder where you want to save the file.

Click on the arrow next to the **Save as type:** box and change the file type to **Rich Text Format**. Type a name for the file into the **File name** box.

Now click on 

.

Check that the button next to **Selected answers** is highlighted and that you are saving the **Summary** - this will save the bibliographic information and the abstract of the articles you have selected. Details of the other save options are given in the box on the right hand side. Click 

.
If you wish to go ahead and save the records, click 

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Printing

When printing, you are also offered a choice of the amount of information you want to print out. If you click 

, the material will not print straight away, but instead, a box will appear allowing you to choose how much of the information you wish to print. Once you have chosen, if you want to go ahead and print, you can click on 

.

7. Locating the articles

Some of the references in SciFinder Scholar are available in full text on the web. If there is a little 'PC screen'  button next to a reference, this indicates that there is something on the web. **However, if you can't get through to the full text of the article by clicking on it, it doesn't necessarily mean you can't get access at all.**

To check definitively whether you have access to the electronic full text of an article in a journal, you should search for the journal title in the Library catalogue at http://lib.leeds.ac.uk/ and follow the links from there.

[Note: You should always search the Library catalogue using the full (i.e. not abbreviated) journal title. To find the full title of a journal from the abbreviation given in SciFinder Scholar, you could try looking at the list of "Core Titles Covered in CAplus" at http://www.cas.org/sent.html.]

If the journal article you need is not available electronically or in print you can order it through the Library's Document Supply service. If you are a member of staff, or a research postgraduate, you can sign up for a Documents Direct account and order the article online from the British Library. See the webpages at http://www.leeds.ac.uk/library/docdel/ for more information.

Exercise 7a

Search for articles by Dr Patrick C McGowan (refer to **Exercise 4a** if you can't remember how to search by author).

Find the reference to the article published in 2004 entitled **Formation and structural studies of iron(III) and ruthenium(II) complexes of 1,4,7-triazacyclononane and N-monofunctionalised 1,4,7-triazacyclononane.**

Click  next to the entry. The ChemPort screen will open in a new web browser window. From this page you can click on **HTML from the publisher** and the article will be displayed.

Further information

For further, online, training on SciFinder Scholar, see the SciFinder Scholar Interactive Tutorial at http://www.cas.org/SCIFINDER/SCHOLAR/interact/index.html

Further information can also be found SciFinder Scholar Solutions page http://www.cas.org/SCIFINDER/SCHOLAR/SOLUTIONS/

Note: When you have finished using SciFinder Scholar, click on the 'Exit' button.
At present, only five people can use the database at one time.

Maintained by: Sci-Eng Team