

SEARCHING THE CHEMICAL LITERATURE

Learning to search the scientific literature effectively and thoroughly is nontrivial and requires much practice. As you continue your scientific pursuits and begin doing lab research, you will need to know everything that is known about a certain compound or topic. After defining a problem, the first step in beginning a research project is to find out such information. If your literature search is not done well, you may spend weeks or months doing work that has already been determined to be fruitless, or you may redo work that has already been published. Of course, sometimes you may purposely want to reexamine previously done work, but that too requires knowing what has been done previously. Spending a day searching the literature can save you days, weeks or much longer in the lab.

Books and monographs are the main hardcopy printed information sources that library collections provide to chemists at present. Journals and data collections, however, have a paradigm shift in the past 20 years, becoming exclusively electronic access capable. Much of what was done manually 30 years ago is now preferred to be done electronically, as more chemical databases and literature are digitized and made available via the Internet. Even if what you want is not available to you at your institution, there is a loaner program that is worldwide. You still need to know how to use the library for books (this is actually becoming more and more obsolete), but primary chemistry research information from journals now is available from the Internet in most cases. Even journal articles that are 100 years old have been digitized!!

This exercise is a small example of how to search the literature. You must gain more expertise in this area as you do research. Electronic searches can change very rapidly so it is worth using electronic search methods frequently, to keep up with the latest methods. It is always worth checking a subject of interest or need to you, by doing a quick literature check. The Integrated Sciences and Engineering Library (ISEL) in the Lederle Lowrise Building (2nd floor) and the Chemistry Resource Center in the Integrated Sciences Building (ISB) have all the software interfaces you need to for an expansive literature search. Also, some sources (such as Web of Science) can be accessed from any computer on the UMass-Amherst campus, without special interface software. Also, research groups in the Chemistry Department have these software resources, so be sure to use them when you join a research group.

Remember, information = efficiency = success!! Remember also that the reference librarians at the Integrated Sciences and Engineering Library (ISEL) in the Lederle Lowrise Building (2nd floor) are founts of knowledge and are there to help you with using the library and its electronic resources.

BACKGROUND INFORMATION – HOW TO DO LITERATURE SEARCHES

(A) Perform an online search by directly accessing one of the following chemistry electronic journals: Journal of Organic Chemistry (J. Org. Chem., AKA JOC), Organic Letters (Org. Lett.), Journal of the American Chemical Society (J. Am. Chem. Soc. AKA JACS), or Angewandte Chemie International Edition (out of Germany, Angew. Chem. Int. Ed.) For an overview of carrying out a literature search go to <http://guides.library.umass.edu/chemistry>.

Link your browser to <http://guides.library.umass.edu/chemistry>. This takes you to the UMass Library Chemistry portal. This page is a good starting point for accessing online journals and other online information available to the UMass community. This does not allow access to all online information that exists, because having all electronic subscriptions is beyond our budget limits. The most common and useful journals are available electronically to the UMass community. *Note that accessing most of these journals requires that it be done on a UMass computer account or via a computer on campus. Note that sometimes you may get a message that too many people are using a resource at once, meaning you will need to try again later. So, do not wait until the last moment to do this assignment. You may also use a computer off campus but you must sign in to the library proxy server. For information on this, see the library website off-campus login.*

Try to find the “*Journal of the American Chemical Society*” or “*Journal of Organic Chemistry*.” These will be helpful to this exercise. Some other examples of journals that include organic chemistry related chemical articles are *Organic Letters*, *European Journal of Organic Chemistry* (Wiley-VCH), *Tetrahedron Letters* (Elsevier), *Chemical Communications*, *Organic & Biomolecular Chemistry* (Royal Society of Chemistry) and *Angewandte Chemie International Edition, In English*. These are just some examples. Many other journals also contain articles, communications and reviews that relate to organic chemistry. Journals that provide extended review articles on specific topics include *Accounts of Chemical Research*, *Chemical Reviews*, and *Chemical Society Reviews*. Links to the journal offerings of some of the major chemistry publishers (American Chemical Society, Royal Society, Wiley, Elsevier) can be found at the *Information*

Useful online databases for chemistry include but are not limited to *SciFinder Scholar* and *Web of Science*. Using the search engines at these sites provides a way of looking for specific information. See information below for a description on how to search with *SciFinder Scholar*.

(B) Doing an electronic Chemical Abstracts (CA) Search with SciFinder: *Chemical Abstracts* is the most commonly used, all-encompassing, and useful resource for searching the chemical literature. A searchable electronic version is available to UMass-Amherst faculty and students via *SciFinder Web* (<http://guides.library.umass.edu/chemistry>), which is available free to anyone who registers using a UMass email account. There is a limitation on the number of people who can log onto the *SciFinder* database at any one time, so it is a good idea to get together with a few friends, log on, and do your literature searches together from the same computer logon, to avoid “logjam” problems.

To use *SciFinder Web*,

After registering, go to the main *SciFinder* page. At the top you will see buttons labeled “Explore References”, “Explore Substances”, and “Explore Reactions”. You may also simply type a topic into the search function. There are other ways to access information and you should definitely explore and become familiar with them, but the description below will be limited mainly to describing a structure search.

Click on “Explore Substances”. On the new window, click on the structure palette. Draw the structure of a molecule for which you wish to do a search then hit “ok”. You may choose to do an exact structure search, substructure, etc. Choose “exact” then “search”. The next window shows all references that include the structure you drew. Note that if the structure is very common, the number of references will be very large. Clicking on “Substance Detail” and then “References” will lead to another window in which you may refine your search to include only those topics of interest to you, for example “Properties” or “Spectral”. Click on that and “Get References”. This would lead to a link to a publication. Various buttons allow you to view the abstract or the full paper, depending upon whether or not UMass has access to that particular journal.

UMass-Amherst does not have electronic subscriptions to all journals, and not all journals are available electronically: the abstract may be your main record if the journal is hard to get, or in a foreign language that you do not know. A few examples of the more important journals that publish organic-related papers and that our library subscribes to are *Journal of the American Chemical Society* (*J. Am. Chem. Soc.*) AKA “JACS”, *Journal of Organic Chemistry* (*J. Org. Chem.*), *Organic Letters* (*Org. Lett.*), *Tetrahedron* (no abbreviation), and *Tetrahedron Letters* (*Tet. Lett.*).

ASSIGNMENT – WHAT TO DO

As an online literature search, (1) choose a topic dealing primarily with synthetic organic chemistry or methodology (a paper dealing with a newly discovered/invented organic synthesis reaction). An author, research topic, or a specific molecular structure are good places to start your search. This is a good opportunity for you to explore a synthetic chemistry chemical topic of interest to you. (2) Use *SciFinder Web* to locate a specific abstract that is appropriate for your topic, as described immediately above. Check the direct connection to see if the article you are considering is available at UMass-Amherst in an e-journal. To help ensure that the article will be mainly about organic chemistry, **you must choose an article from one of the following journals**: JACS, JOC, Org. Lett., Angew. Chem. Int. Ed., or Eur. J. Org. Chem. We have electronic access to all these. JACS is an outstanding journal, but keep in mind there is a lot of non-organic chemistry articles there. It is an all-division type of journal. (3) Find the reference to the full article from the abstract and print out the full article. **The article must contain organic chemical structures and an “experimental” section that includes the synthesis and spectroscopic data for an organic compound.**

Your article must be approved by Dr. McDaniel. Send him your paper as an attachment and he will reply with an approval or denial. If your paper does not get pre-approved, you will not receive a score for this assignment.

In future research if you need an article that is not readily available electronically, you would need to check with the reference librarian at the Integrated Sciences and Engineering Library (ISEL) in the Lederle Lowrise Building (2nd floor) for help to get the hardbound journal that contains the article you want, and then photocopy the article.) Many articles now include Electronic Supplementary Material (ESI, for Royal Society journals), or Supporting Information (American Chemical Society). This information is usually available as a link from the electronic copy of the journal. You may decide to take a look at this material to help your understanding of the article.

In short: Topic of your choice → SciFinder Web → Find a Synthetic Article → Get Dr. McDaniel’s approval → Abstract of article, with reference to full paper → full organic paper (from one of the required journals).

Once you locate a copy of your article, print it or download a copy for reading. Do not expect to completely understand the material in the article that you choose, rather try to find an article that covers a synthetic chemistry topic that is at least somewhat readable to you or of interest to you. The introduction section of most papers is usually readable, even by someone who has taken only one semester of organic.

Format. Your report needs no prelab, no copy of this handout (keep it for yourself!), and there is no postlab. It should indicate that the report is “Chemistry Electronic Literature Searching”, with your name, your TA’s name, and the data. **All of the following information must be reported for full credit:**

- (1) Basic information about the article in this format or something similar: Ishida, T.; Nogami, T.; Yasui, M.; Iwasaki, F.; Iwamura, H.; Takeda, N.; Ishikawa, M., "Ferromagnetism of pyrimidine-bridged copper(II) complexes", *Molecular Crystals & Liquid Crystals*, **1996**, 279, 87-96. The authors, the title of the article, the journal title, the year of publication, and volume number, and inclusive pagination are the data given in this particular example.
- (2) A brief (2-3 sentences) description *in your own words*, telling what the article is about. It is therefore a good idea to choose an article whose introduction is at least partly understandable, in order for you to be able to condense the general idea of the article into your words.
- (3) Tell whether the article is total synthesis, new reaction development, new catalysis development, new methodologies, etc.
- (4) Tell *how many* footnotes or references are given in the article (references to other work). This gives indication of how complex the article is. Often, the references are as important as an article

itself, so it is important for you to get some practice in locating where the references are found in different types of articles. Some footnotes have only one article per note, some have multiple articles per note ((a), (b), (c) ...). It is OK to count multiple-article footnotes as one footnote.

- (5) Tell whether or not the article has electronic supporting or supplementary material available from the Internet.
- (6) Tell what kinds of spectroscopic data are given in the Experimental section (Supporting Information in an ACS journal) of the paper (e.g., NMR, IR, UV-Vis, MS, etc)
- (7) Tell what the main point or points was (were) that you found interesting about the article. Tell whether you found the article quite difficult to understand, or relatively easier to understand; in either case explain why ("the article has a lot of physics that I did not understand", "the synthesis part of the article had a number of reactions that I recognize"). This is meant to be a "note" to yourself about what you actually get from the article – it is often hard to figure out what an article is all about from one reading, even for an expert!
- (8) In addition to the information given above for your report, attach copies of the electronic CA abstract, and of the first page (only) of the journal article.

ADDITIONAL POSSIBILITIES FOR LITERATURE SEARCHING – (NOT PART OF THIS ASSIGNMENT)

This practice exercise is just the tip of the iceberg for modern electronic data searching. For this project, it was not necessary to learn how to do a complete literature search. In the future, however, when you do research, you will have to do searches that are more detailed, so it is in your interest to learn at least the basics now. Save this handout for use in future courses or research. Below is more information on doing searches of the chemical literature. This too is only a partial description. To provide a complete survey of the chemical literature, there are numerous other sources that have to be searched. These will be learned from necessity and through experience. You may find that even for this project you wish to explore some of the methods described below. Feel free to do so.

General Reference Works. There are many interesting and very useful sources of information in the Reference section of the Physical Sciences Library. Take some time to explore this area.

A nice summary for searching the chemical literature can be found at the following URL at Yale:

<http://www.library.yale.edu/science/help/cheminf.html>

Many references at the Yale site require subscriptions and therefore are not available to non-Yale students, but the general pages are useful and interesting, since Yale has an enormous library collection. Many other universities offer similar comprehensive links. It is worthwhile to explore some.

Other useful online literature databases.

A Science Citation Index search is extremely useful and well worth learning. This type of search allows you to take a key article from say 1985 that you may have found by your CA search, and find every paper that has referred to (cited) that article since then. This allows you to learn what other research has been done on that topic since the original work. This and more is found by clicking through to the *Web of Science* link found at <http://guides.library.umass.edu/chemistry> (under "Cited Reference Search")

Beilstein is a very useful compilation, available in both print and electronic versions. The print version is not recommended for the novice or the weak of heart. Using the online version is also a bit challenging. The electronic version of Beilstein allows one to draw a chemical structure and to use that to search the very extensive Beilstein database of organic compounds. UMass-Amherst has a subscription to this database, but its use requires download and installation of a software interface. Graduate research groups use Beilstein, but we will not consider its use in this course.

ChemFinder is a free online source of mainly physical properties of chemicals (<http://www.chemfinder.com>). With ChemFinder, one can search on a chemical name, or using a free plug-in for your web browser, one can draw a structure and do a search on that.

The National Institute of Standards and Technology (NIST) Web-book is an excellent site for finding physical properties and spectra: <http://webbook.nist.gov/chemistry>.

The Spectral Database for Organic Compounds (SDBS) in Japan is an *excellent* resource for many types of spectra for many molecules: http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng.

A caveat: note that web sites that are active today can quickly become cobweb sites. If you find an outdated link please inform me and I'll make a change in this handout.

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