

Finding Information for Research in Chemistry

Learning Objectives

After completing this section, students will be able to:

- Choose an appropriate resource to search for needed data and information in Chemistry
- Describe how to search for needed data and information in a specific resource
- Evaluate the validity of resources and sources identified
- Summarize the data and information discovered to answer the research question
- Cite the sources and resources used
- Make a tutorial of these steps in the format of text description (with screenshots), or video/audio, and other multimedia

1. Essential Information Skills for Productive Chemists

Getting along in the hybrid information environment of analog, electronic and digital formats and frameworks today involves some essential skills for chemists:

- Knowledge of chemical publication types and how to find data and information
- Good data and literature citation practices
- Informed data management habits
- Understanding of chemically intelligent and machine readable structures and identifiers
- Appreciation of information expertise and services

These skills have been applicable throughout the era of modern science. Chemistry is an information intensive field, typified in the magnitude, diversity, breadth, depth and detail of its documentation. The good news is there is a lot of information to 'mine' for research questions, and you will be learning various methods throughout the course. The challenge is staying organized in the deluge. Meeting this challenge is known as information literacy, breaking down research problems into discrete steps of critical inquiry.

1.1 5 Steps to Successful Critical Inquiry in Chemical Information

1. Scope and design the inquiry, and determine what information types are relevant for the need
2. Strategize where and how to look for the information
3. Evaluate validity and appropriateness of information sources

- Summarize, analyze and apply the information to the specific problem at hand, including revisiting the information search if needed
- Cite the sources and document the whole process and outcome sufficiently to communicate rationale and demonstrate validity of your approach

The sections in Module 1 will cover some basics of steps 1, 2, 3, and 5; the rest of this course covers step 4. There are a variety of methods and techniques available in practice for approaching each step:

Inquiry Steps	Types of Information Tools
Step 1: Scope the need	Structure of chemical information; common publication types; core resources
Step 2: Search strategies	Access to specific sources; general search methodologies; specific search tool functions
Step 3: Evaluate sources	Evaluation criteria; adequacy indicators
Step 4: Analyze and apply to problem	Organization; visualization
Step 5: Cite, document and communicate	Citation format; publication/communication practices

There are many information steps and tools involved in rigorous chemistry research! Guides to getting started, specific resources and advanced searching techniques can be very helpful.¹ More are always needed, especially for local institution resources and services. In this section you will be asked to create a guide for your peers based on your own 1-5 step research process.

2. Structure of Chemical Information

Published scientific information generally appears in various types of sources, depending on their intended role in the discovery of the information, primarily by other scientists. For example, a patent is designed to establish the first disclosure of a novel, protected technology, while a general chemistry textbook is designed to introduce core, well established chemical concepts to uninitiated students. These information types are organized in libraries and guides around common characteristics, which can be loosely categorized according to the point they are in the timeline of knowledge, from experiment to regulation and education.²

	Characteristics	Publication Types	Examples
Primary	first formal disclosure, usually peer reviewed	journal articles, data sets, patents	

Secondary	compiled, collections, structured, curated for scope, content, indexing, classification	compiled databases (literature, data)	SciFinder, Reaxys, Scopus, Web of Science, PubMed, PubChem, ChemSpider
Tertiary	expert synthesis	textbooks, guides, standards, review articles	
Gray	not community formalized	raw data, report, social media, chemical vendor's documentation	

3. Accessing and Searching Chemical Information Databases

Access to chemical information databases has been primarily subscription-based due to the large amount of manual labor needed for curating high-value chemical data and information as well as their often proprietary nature. In recent years, some open access databases such as PubChem and ChemSpider have emerged with the advance of cheminformatics techniques. However, chemists still need to rely on subscription-based databases for accurate and efficient searches. The table below summarizes some major databases we often use in chemistry research, their scopes, and major functionalities. Please choose the ones available through your institution to explore. The tutorials linked in the last column will help you get started with using these databases. For more information on databases covering chemical substance data, please consult Ben Wagner's book chapter³ and the poster presented by Ye Li and Leena Lalwani.⁴

Resource	Access	Link to about page	Coverage and Scope				Chemical data indexed?	Structure search enabled?	Link to tutorials
			Discipline	Years	Type of reference indexed	Cited reference included?			
SciFinder	Subscription based	http://www.cas.org/products/scifinder	Chemistry related areas	Early 1800's - present	Journal articles, patents, conference proceedings, books	Yes	Yes	Yes	https://www.cas.org/training/scifinder
Reaxys	Subscription based	http://www.elsevier.com/online-tools/reaxys/training-and-support#faq	Organic, inorganic, organometallic Chemistry	1771 - present	Journal articles and patents	Partially cross linked to Scopus	Yes	Yes	http://www.elsevier.com/solutions/reaxys/learn-and-support#video

Web of Science	Subscription based	http://wokinfo.com/	General in science, social science, and humanities	1898 - present	Journal articles, books, conference proceedings	Yes	No	With additional subscription	http://wokinfo.com/training/support/training/web-of-science/
Scopus	Subscription based	http://www.elsevier.com/solutions/scopus	General in physical sciences, life sciences, health science, and social sciences	Varies; as early as 1823;	Journal articles, books, conference papers	No	No	No	http://help.scopus.com/Content/tutorials/sc_menu.html
PubMed	Open access	http://www.ncbi.nlm.nih.gov/books/NBK3827/#pubmedhelp.FAQs	Biomedical research	Varies, as early as 1809	Journal articles and books	No	No	No	http://www.nlm.nih.gov/bsd/disputed/pubmed.html
PubChem	Open access	https://pubchem.ncbi.nlm.nih.gov/help.html	Biological activities of small molecules	Unclear	Chemical substance, property, biological activity and associated literature	No	Yes	Yes	https://pubchem.ncbi.nlm.nih.gov/help.html
ChemSpider	Open access	http://www.chemspider.com/Helpstory.aspx	Chemical structure and associated data and literature	Unclear	Chemical substance, property, spectra, and associated literature	No	Yes	Yes	http://www.chemspider.com/Help.aspx

Please note: most of these databases index the citation and abstracts of articles; fulltext of the articles are often linked with the database records through your institutional citation link resolver to journals your institution have access to. Occasionally, you may discover articles that your institution does not have access to online. You can consult with your institution's library for access to the print source or through interlibrary loan service.

3.1 Search Techniques for Databases in Chemistry

Most of the databases, especially the subscription based ones, provide useful tools to refine your search. You may use the advanced search features and/or filter options in these databases to optimize your search strategy. Here are a few useful tips in general for searching databases in Chemistry.

- Use Boolean logic (AND, OR, NOT) to connect your search terms instead of typing in a full sentence ⁵
- Pay attention to subject terms (standard terms a database used to index literature) and use them for more accurate search ⁵

- Track down publications by a specific author through author name search or author ID such as ORCID ⁵
- Search for references cited in a chosen article and search for other publications cited a chosen article to expand your findings ⁵
- Learn structure, substructure⁶, and reaction⁷ searching through practice and understanding how chemical structures are indexed (covered more in later modules)

3.2 Search Techniques for Physical Properties and Spectra of Chemical Substance

Searching for physical properties and spectra of chemical substances is an important skill for chemists to master. Physical property data and spectra data are often indexed around chemical substances in databases and handbooks with referencing to the primary literature published the data. ³

- Databases such as SciFinder, Reaxys, PubChem, and ChemSpider listed in the above table index physical properties, spectra, and bioactivities and can be searched through chemical substances. When you locate the interested substance in these databases, you can navigate to the particular physical property data or spectra under various sections in the substance record. Please note: you may need to go to the linked primary literature from the database to obtain the actual spectra or the conditions of how a piece of physical property was measured. There is another type of databases which function as repositories of spectra, such as the [Spectral Database for Organic Compounds, SDBS](#). In SDBS, you can download the spectral data directly.
- Handbook examples include CRC Handbook of Chemistry and Physics and ASM Handbooks. You may either browse the handbook by property categories or use the index to search for a specific substance. Online versions for many of these handbooks are available and will allow you to search for property data and spectra with keyword searching. Some handbooks available through the Knovel platform may even allow you to download and interact with individual tables and graphs containing substance property data.

Depending on the database and handbooks available for you, you can explore more of the search techniques specific to the resource using their guide or help. Also, you may learn more about them from Ben Wagner's book chapter. ³

When you use physical properties and spectra discovered from literature in your own writing or presentation, the condition of how the data were measured are often important to include; because different conditions can generate very different data from the same substance. Without the original context, the audience of your writings will not be able to interpret the data you cited and evaluate your research based on the data.

3.3 Learning to Become a Power Searcher While Doing Research

You can always consult publications and learning materials from chemical information professionals for advanced search skills like those can be found in XCITR.¹ It takes practice and patience to become a power searcher in the chemical information world. In reality, you may

need to balance the comprehensiveness of results and the time spent to seek for them. Please never hesitate to consult with your librarians and experienced researchers around you for suggestions and tips. Further more, with what you will learn in this class, you will be able to see the chemical information world from an insider point of view. For example, in module 5 of this class: Comparing and Searching Chemical Entities, you will learn more about how databases like PubChem and ChemSpider are organized and updated in order to understand the advanced methods to retrieve chemical information from them.

Nowadays, search engines like Google and Google Scholar and collaborative references online like Wikipedia can often provide quick and easy access to chemical data and literature online. They can be used to get started with a topic as long as you pay attention to the true source of the data and information discovered and evaluate the sources carefully as described in the next section. For comprehensive research on a topic and finding credible sources, these quick tools are usually not sufficient. Using the databases mentioned above will ensure you perform effective and efficient searches to identify data and information for your research.

4. Evaluating Chemical Information Sources

The primary goal of evaluating sources is to determine if they are acceptable to use for your purpose. Underlying acceptance is a decision about reliability, which may be influenced by a number of factors including the origination of the information, the level of the review, the adequacy of the citation, additional description and recommendation and/or use by authorities or peers. It is important in some fields, such as chemical safety, to distinguish where the information came from, the commercial, academic research, government, education or general public sectors. It may also be helpful to know how the information has been previously analyzed, particularly if it has been certified or correlated with other authoritative sources.

Some general questions you can ask yourself as you are reviewing sources include^{2-3, 8}:

- Is the purpose of the source and specific study or information clearly described?
- Are the methods used in the study or to generate the information adequately described?
- Has the technique been repeated? independently? validated by models?
- Are the results consistent with other similar published studies?
- Is the source reviewed, by peers? by authoritative experts?
- Is the author identified? is the study clearly traceable by citation?
- Does the source include references to other relevant literature?

With answers to these questions, you will have a good idea on the provenance of the data or information you are using, which will help you to determine how much you can trust it. Once you accumulated sufficient experiences in reading and evaluating sources, your judgment about a particular source may become more intuitive. However, keeping these questions in mind will help you to stay objective. The answers to these questions will also help you determine the additional information you want to include with your own writing when citing the sources so that the audience is aware of the context from which you draw your conclusions.

5. Citing Information Sources

5.1 Reasons for Citing and Citation Style

Citing the sources of information that you consulted and used in research is critical and plays several roles, it:

- lends validity to your own research approach
- links your contribution to its provenance
- gives the original creator credit
- directs the reader to more information

Accomplishing this across millions of publications by hundreds of thousands of researchers in thousands of sources requires consistent practice. Standard formats specify the critical information components needed to identify a definitive information source. The standard style most commonly used in chemistry is published by the ACS⁹ and you will be asked to use this format for the assignment.

The approach to articles generally includes the following components⁹:

Author 1; Author 2; Author 3; etc. Title of Article. Journal Abbreviation Year, Volume, Inclusive Pagination. DOI and/or URL (access date).

Please consult the *Reference* chapter of the ACS Style Guide for the format of different types of citations⁹. This guide from Pennsylvania State University could also serve as a quick guide of styles (<http://www.library.wisc.edu/chemistry/research-help/write-and-cite/acs-style-guide/>) .

5.2 Citation Management Software

Citation management tools are often used to help researchers organize citations, annotate references, and automatically format bibliography while they write. Starting to use a citation management software in early in your education will help you save your time when you work on class projects or writing an article, and organize an accumulation of interesting references for future use. The table below lists a few popular citation management software products.¹⁰ You may choose one or two to explore based on availability at your institution and your preference of functionalities. Reference records can be transferred among many of the tools below. If you cannot decide which one to use, start with any of the free ones and you can always transfer your references to another tool later. More detailed comparison and information about specific software can be found at the Research Guide page from the University of Michigan Library.¹⁰ You will have an opportunity to explore one or more of these tools in the next few weeks through another module: Collaborative Citation Management.

	EndNote	Zotero	RefWorks	Mendeley	Papers 2
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Cost	Discounted price for affiliates of educational institutions	Free	Institutional subscription based	Free, additional fee for advanced accounts	Discounted price for affiliates of educational institution
Access and sharing	EndNote desktop software. Collections can be accessed and shared online through EndNote Web.	Must be installed through the Firefox browser. Collections can be accessed and shared online.	Must be accessed online. Collections can be shared online.	Must be installed on the computer. Collections can be accessed and shared online.	Must be installed on the computer. Collections can be accessed and shared through Livefe feature
Linking to PDFs and other attachments	Yes	Yes	Yes	Yes	Yes
Annotate and index PDFs	Yes	No	No	Yes	Yes
Import citations directly from PDF	Yes	Yes	No	Yes	Yes
Compatibility with Word Processing Programs	MS Word, OpenOffice, Mathematica, Pages, LaTeX through BibTex	MS Word, OpenOffice, Google Docs,	MS Word, OpenOffice, LaTeX through BibTex	MS Word, OpenOffice, BibTex	MS Word, OpenOffice, BibTex
Citation Style Modification	Can add new styles, modify existing styles	Most popular styles available, difficult to modify styles	Most popular styles available, cannot add styles, but can modify existing styles	Most popular styles available, difficult to modify styles	Most popular styles available, difficult to modify styles
Tutorials	http://endnote.com/training	https://www.zotero.org/support/screrecast_tutorials	https://www.refworks.com/tutorial/	http://community.mendeley.com/guides/videos	http://support.mekentosj.com/kb/tutorials

6. Presentation Dos and Don'ts

Communicating your research with peer students and researchers can take many forms. It can be a research article you write for publication but can also be an oral presentation or a poster you present at the end of your class or at a professional conference. You may also choose to communicate through social media if you have a good crowd of targeted audience there.

Preparing a research poster is a good start point for you to explore your own style of communicating science.

6.1 Components of a Research Poster and How to Plan for Making One

Microsoft Powerpoint is a good tool for the task and you may also use more advanced tool such as Adobe Illustrator if you have access to it. No matter what kind of tools you use, the most important idea is to tell your research story with a clear and easy to follow visual guide. The suggested components of a research poster include:

- Title
- Authors and affiliations
- Conference/program details (optional)
- Abstract (optional)
- Introduction
- Materials (if any) and Methods
- Results
- Conclusion
- Future Research Directions (optional)
- Reference (optional)
- Acknowledgement (optional)

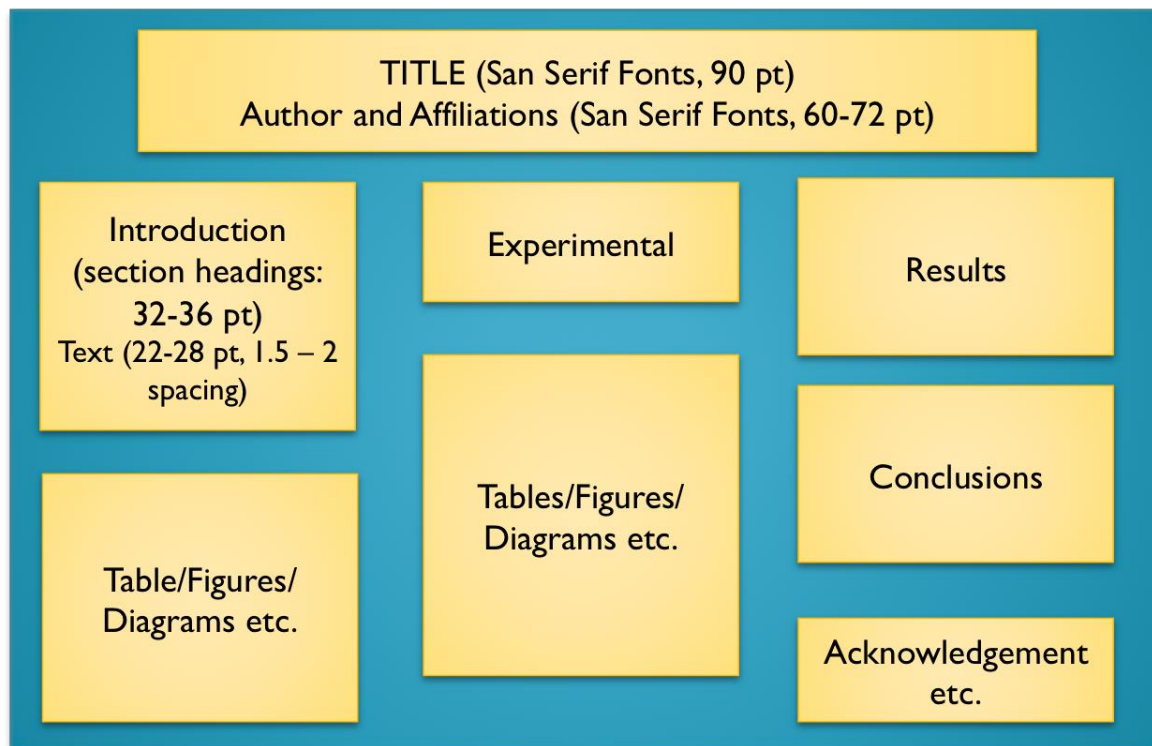
Before you start, ask yourself the following questions:

- Who is my audience? How much do they know about my topic?
- What is my research question?
- What is the take-home message I want to deliver?
- What materials do I have or will I have for each section of my poster?
- How can I use visual ways to show my work?

The answers to these questions will help you determine the content and design of your poster.

6.2 Poster Design Tips

This figure below shows a popular way to design your research poster.



Here are a few tips on preparing a good poster.

- Start with figures, visual communication
- Images should be fairly simple, no ambiguous or meaningless features
- Use of color and form to guide the eye
- Consistent overall formatting but clearly distinguish and set off different components
- Flow of information important, clear path, from top left to bottom right
- Clearly identify what is the main point, front and center
- Use heavy lines and oversized labels for chemical structures, bring the area of interest to the front view
- Use flow chart to show your methodology instead of long paragraphs
- Use text wisely and concisely with a font size allowing people to see from at least 3 feet away
- Always cite references used during your research in a consistent style
- Prepare a 1-minute story and a 5-minute story to talk about your poster before presenting it for audience having different levels of interests

You can learn more about making posters and other means of communicating chemistry from Marin Robinson¹¹. For examples of good poster presentations, see: Compound Interest (<http://www.compoundchem.com/>)

7. Assignment / Exercises

Description: Create your own guide, based on your experience answering one of the research questions below (Note: You may also choose a research question you are currently working on). Use a flow-chart model for the guide, based on inquiry steps and post it in the OLCC course platform for others to benefit.

Instructions:

1. choose one of the questions
2. using one or more of the recommended sources in the list below, search for chemical data and information to answer the question
3. evaluate the validity of the data and information you used
4. cite the source properly using the [ACS style](#).
5. make a tutorial style guide to teach your peers using the resource you used to search for the needed data and information
6. post the tutorial on the course platform

Research questions:

1. What is the melting point of the drug Lipitor?
2. Which solvent is greener, Benzyl Alcohol or Toluene?
3. Which common organic compounds are incompatible with Acetone and in what condition?
4. Trace the research pathway that lead to the ring-opening metathesis polymerization technique through reference and citation linking.

You may use one or more secondary resources listed below based on the availability at your institution. Please consider how well these resources could provide data and/or information and if the data and/or information you identified there would be considered scholarly?

- Google or any other search engine
- Google Scholar
- SciFinder
- Reaxys
- ChemSpider
- PubChem
- Web of Science
- Scopus
- PubMed

The tutorial can be text description (with screenshots), or video/audio, and other multimedia.

The tutorial should guide your peers to:

- Access the secondary resource(s)
- Perform a search or searches relevant to answering the research question
- Narrow down the search results with tools provided by the resource

- Locate the fulltext where the data and/or information needed were presented

Make sure the tutorial includes:

- Your answer to the research question based on data and/or information you find.
- Evaluation of the validity of the data and/or information you use
- Citations to the data and information sources and resources used (ACS style recommended)

Tips and tools for making a tutorial:

- To take screenshots,
 - on a PC, use Print Screen → paste to Paint. (Read more at <http://windows.microsoft.com/en-us/windows/take-screen-capture-print-screen#take-screen-capture-print-screen=windows-8>)
 - on a Mac, use Command + Shift + 4 and then drag to select the area to shot. Image saved on desktop as .png file. (Read more at <https://support.apple.com/en-us/HT201361>)
- Free screencasting software
 - Jing/ (<https://www.techsmith.com/jing.html>)
 - More options and comparisons at https://en.wikipedia.org/wiki/Comparison_of_screencasting_software
- An example of tutorial with screenshots
 - <http://guides.lib.umich.edu/c.php?q=282993&p=1885552>
- See examples of video tutorials in the tutorials linked in the Database table under the section Accessing and Searching Chemical Information Databases.

References

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