

## Lesson Plan: Chemical Information Search

**Objectives:** Emphasize the importance of thorough literature research when planning any experiments or programs. Practice chemistry-oriented searching using key internet search engines.

**Overview:** Science today is built on generations of research. There are many stories in which work was undertaken and concluded only to find out that the same questions had already been answered. In too many cases, the information was already published and the new investigators either improperly searched for it or, most likely, never looked at all. There is a strong urge simply to jump in and solve the problem in one's own lab. This typically results in a wasted effort and often embarrassment when it is realized that the work cannot be patented or utilized. The discovery of existing information comes when a proper search is done in preparation for commercialization. Experiments described in publications may be duplicated to insure validity, but all available information must be made available before any lab work is done.

Activity: The Internet has become an extremely valuable tool for locating information quickly and easily. There are many sources of online information, including journal archives (e.g., Nature, Analytical Chemistry). In this activity we will explore the use of three internet tools for researching information.

### 1. Google

The leader in general internet search engines is Google ([www.google.com](http://www.google.com)). As most students already know, this engine offers surprising speed and utility when searching for any general topic. What may be less well understood is how to search for data using the "advanced search" function which is available via the link just to the right of the data entry box. The most useful feature on the advanced search menu is the entry box labeled "this exact wording or phrase." This alone can reduce the number of irrelevant hits by insuring that any 2- or more word phrase is correctly targeted.

Try searching for the compound calcium anhydride by searching using both the standard and advanced search options. In the advanced search engine be sure to enter calcium hydroxide in the "this exact wording or phrase" box. Note the differences in the responses returned using the "exact phrase" option and summarize the value of utilizing the advanced search features of Google.

### 2. Wikipedia

Wikipedia represents much of what can be achieved with the internet and the willingness of the internet community to jointly build on useful ideas. Wikipedia is a compilation of user-generated definitions and explanations of almost any topic imaginable. Each entry can be modified and corrected by the end-user. It is built on a spirit of cooperation and trust and can often serve as a good first source of information for any topic. However, the results from Wikipedia may contain misinformation and errors and information used from this site should be correlated with a more traditional source. Wikipedia may be reached via their top portal at <http://www.wikipedia.org> which offers the choice of language. The English version is at [http://en.wikipedia.org/wiki/Main\\_Page](http://en.wikipedia.org/wiki/Main_Page).

One aspect to Wikipedia that may not be as well known is their effort to tailor their database to specific areas. A link is provided on Wikipedia's main page under "Wikipedia's Sister Projects" that is labeled "Wikiversity." Follow this to [http://en.wikiversity.org/wiki/Wikiversity:Main\\_Page](http://en.wikiversity.org/wiki/Wikiversity:Main_Page) which is a portal to a collection of educational resources. In the panel to the right labeled "Explore Wikiversity" there are a number of options

that lead to content-specific educational content. This can be by level, subject, type, and other options. Under “School subjects” options are provided for chemistry, biology, mathematics, and other subject areas. Select “Portal:Chemistry” which will lead to <http://en.wikiversity.org/wiki/Portal:Chemistry>.

The chemistry site is dedicated to the study of chemistry and offers a number of subject areas for exploration. It is not designed to be a search site in the same context as Google. Rather, it pulls together resources to address certain topics, much as a book might do. Browse the section labeled “Guide to Chemistry” and explore some of the links. An example is “Mass relations in chemistry and stoichiometry” at [http://en.wikiversity.org/wiki/Mass\\_relations\\_in\\_chemistry\\_and\\_stoichiometry](http://en.wikiversity.org/wiki/Mass_relations_in_chemistry_and_stoichiometry). Look at this site to understand the nature of what Wikiversity is trying to accomplish. The essence of this content is an explanation of a chemistry unit called the “mole” which is used to determine the mass of compounds needed for a balanced chemical reaction. It is an instructive guide.

Explore a content area of your choice and write a short paragraph of what you found and how the type of information compares to a Google search or the traditional Wikipedia site.

### 3. **Wolfram Alpha**

Wolfram Alpha at <http://www.wolframalpha.com/> is a more recent addition to the internet. Wolfram Alpha is called a “Computational Knowledge Engine.” This is an exciting and unique addition to the internet community that has set high ambitions as a source of useful “computational information” to anyone. This explanation is not easy to understand at first and is best explained by some trial and error on your own. Navigate to the site and take advantage of the “New to Wolfram Alpha?” box on the right. Try a few of their suggestions and you will see why this is such an exciting idea. Wolfram Alpha is focused on providing “computable” data for a wide variety of subject areas. The word computable infers largely numerical data that the company accesses via their own databases and manipulated using their own algorithms. It is still under development, but you will be amazed at what it can already do and enthusiastic for what it could become, especially if you work with numerical data.

- 1) Explore the various suggestions and sample inputs to get a feel for what information can be retrieved. Try non-chemistry examples such as your birth date, a math formula or even something as simple as “32 gallons.” The algorithms try to make some sense out of your input and respond with information garnered from one of their databases. It is not designed to answer specific questions (at least yet). It is most valuable in cases where numerical data is either output or input, or for finding numerical facts about items such as birthdays.
- Try entering the equation  $4+7+x^2 = 9$ . The answer should be  $x = -i\sqrt{2}$
  - Enter your birthday and report a) one other person with the same birthday, and b) the time of sunset in Boston on that date. Be sure to select the “more” toggle to see the full extent of information possible.
  - Try the suggestion of typing two stock symbols or names. For example, Microsoft and Apple. The result represents an enormous amount of information that is valuable and easy to retrieve quickly. This has nothing to do with chemistry, but represents what you can do when investing your money when earning a chemist’s salary.
  - More examples are found at: <http://www.wolframalpha.com/examples/>

- 2) To move closer to the point of earning a “chemist’s salary” complete the chemistry-related exercises below:
- Assume that you need to plot the densities of the chemical elements found on the periodic table by atomic number. This would normally take a lot of time to compile and plot the information for over 100 elements. Try to find this information via either Google or Wikipedia. After trying some search strategies at these two sites, switch to Wolfram Alpha and try the same search. If you are having problems finding the best search terms, try “atomic number densities.”
  - To get a list of the above data, type “densities of the elements.”
  - Now experiment with chemical names, such as the following:
    - Aspirin
    - Hemoglobin
    - LSD
    - Pick any chemical compound on your own \_\_\_\_\_ .

In each case note the molecular weight and the structure of the molecule. In the case of a naturally produced compound, such as hemoglobin, note that the DNA coding sequence is also provided (the bases A, C, T, and G). An interesting plus is a 3D representation of the actual molecule that can be used in other software programs. What are your conclusions concerning the type and ease of data provided by Wolfram Alpha?

- 3) The next query will challenge Wolfram Alpha. Work is still in progress concerning the extent to which the “knowledge engine” will understand and be able to compute an answer. What we are trying next is to have the site produce some information about a chemical reaction.
- Go to the query box at [http://www.wolframalpha.com](#) and type in the following chemical reaction:  
$$\text{H}_2 + \text{O}_2 \Rightarrow \text{H}_2\text{O}$$
  - In this case we know that hydrogen (H<sub>2</sub>) reacts with oxygen (O<sub>2</sub>) to produce water (H<sub>2</sub>O). The symbol for “produce” is given by “=>.” Wolfram first assumes that the symbol “H<sub>2</sub>” is a mathematical symbol and produces an unexpected response. But immediately after the assumption is stated, it gives an alternative definition that you can select, which in this case is “chemical compound.” Select “a chemical compound” to change Wolfram’s definition.
  - The new response will show the reaction of hydrogen and oxygen to form water. Note that it displays both the common names and chemical names. Also note, and this is important, that Wolfram has also balanced the chemical equation for us. The formation of water combines 2 molecules of H<sub>2</sub> with one molecule of O<sub>2</sub> to produce 2 molecules of H<sub>2</sub>O. The balancing insures that we have exactly the right number of each atom to produce the products. Since water has only one oxygen atom but the molecule O<sub>2</sub> has two oxygen atoms, each time an O<sub>2</sub> is used it results in two water (H<sub>2</sub>O) molecules. Thus, 2 molecules of H<sub>2</sub> are required to provide the 4 H atoms in the products. This is called a “balanced equation.” This is a very innovative feature.

- d) After the balanced equation comes a table of thermodynamic information concerning this process. These values can be used to calculate whether the reaction is exo- or endo-thermic (exo- gives off heat, endo- adsorbs heat). A second table gives additional substance properties useful for the engineering of a full scale reaction.
  - e) Experiment with an equation of your own. Try collecting the same information via one of the other search engines.
- 4) The final query will question the properties of a solution, "0.4M potassium hydroxide." Type this into Wolfram Alpha and inspect the results. The 0.4M is a measure of the concentration of potassium hydroxide in water. The data should include such items as pH but it also includes a "preparation" which indicates how much KOH is dissolved into water to make a 0.4M solution. Very convenient way to check calculations when preparing solutions.
- 5) Note that Wolfram Alpha obtains its core data from established databases of known constants. The power of the engine is in assessing the question and providing the best answer based on real data. This distinguishes it from many other sites.

#### 4. Other Databases

The databases discussed in this lesson are freely available and, at most, only require registration. There are many databases for which access must be purchased. Most scientific journals has their articles archived and searchable for a fee. Some databases have been established to aid literature and patent searching. Industry organizations such as the American Chemical Society(ACS) and Chemical Abstract Services (CAS) also have dedicated databases that require purchase.

<http://www.cas.org/index.html>

Chemical Abstracts also offers a free database for simple compound lookup based just on a unique identifier number known as the CAS Registry Number, and vice versa. For example, try this site to identify the compound noted only as (CAS): 1310-58-3. It will return the compound potassium hydroxide.

<http://www.commonchemistry.org/>

#### Summary

The goal of this lesson is to demonstrate the power that is available from the internet when conducting technical studies, in this case chemistry. The arrival of new sites such as Wolfram Alpha makes this an evolving area and it suggests that even more powerful site is in development.

Please summarize your conclusions concerning these databases in terms of their potential usefulness and how their differences impact which one is best suited for a task.