Chem 300: Chemical Information Literacy for Analytical Chemistry (Part 1)

Introduction

This is a self-guided tutorial of important resources provided by the USC Libraries applicable to upper-division chemistry courses. Before answering any questions, please go to http://libguides.usc.edu/chem300. This online course guide will serve as a starting point for this assignment. Each section below is tied to a tab on the course guide. First start by reading the information on the course guide tab and then read and answer the questions below. Repeat this for all four tabs. Once you have answered all of these questions, submit your answers to your instructor and download part 2 of this assignment.

A. Reference Sources

Reference sources provide physical data, safety information, and other key details needed for carrying out labs and experiments. There are many different places with this information, but what is important is to use a reputable, accurate, and well respected resource. This is **not** the time to use Wikipedia. In turn, scientists turn to one of many chemical dictionaries and references to find information to prepare for experiments.

Answer the following question by using the links provided under the **Reference Sources** tab.

A-1. Often solvents are chosen based on particular chemical properties a researcher needs to highlight. If an experiment calls for a solvent that would not boil when heated to 95.0°C, which of the following solvent(s) would meet this requirement: hexane, heptane, and/or octane?

B. Spectra

Finding spectra for compounds can be extremely challenging. For organic compounds, the first place to look is SDBS, or the Spectral Database for Organic Compounds. This database is managed by the National Institute of Advanced Industrial Science and Technology, or AIST, in Japan. Click on SDBS link and agree to the disclaimer.

B-1. When performing a ^{13}C NMR on an unknown compound, there are peaks located at roughly 120 and 150 ppm. Which of the following compounds could fit this description: 1,2-cyclohexanedione, 1,3-cyclohexanedione, and/or 1,4-cyclohexanedione?

B-2. Using SDBS spectra only, how could you tell the difference between furan and tetrahydrofuran (THF)?

For more complex organic compounds or non-organic, SDBS will not have any spectra. The next best place to look is Reaxys. On the course guide, click on Reaxys.

Read the section below before first before answering the question. Follow these instructions to find spectra in Reaxys:

To find details regarding a compound, when you have the name or CAS number, click on Names and Formulas. Enter your search. On the results page, find the compound that matches your search and find the link to Spectra (it should be in the right hand column). The page will load with available spectra, a citation to where the article the spectra is from, and a link to the full-text article.

B-3. Search for zirconium tetrachloride in Reaxys (hint: use CAS number 10026-11-6). Which of the following spectra are available for this compound: NMR, IR, UV-vis, MS, and/or Raman?

C. Literature Searching

Web of Science allows researcher to not only search for literature, but also to see the impact of one article in research. You will search for an article and discover how to trace backwards and forwards in time the impact of one single article.

Web of Science has many different search parameters from author, topic, DOI, publication name, etc. You can use just one parameter or several, it is completely up to you. Just be aware that basic topic searches, like "nanoparticles," can yield 250,000+ results. Many times you will need to construct searches using Boolean terms: AND, OR, and NOT. These operators will allow you to combine, expand, or eliminate and ignore other ideas. In Web of Science, you will see the default AND operator to the left of the search boxes.

C-1. Perform a basic topic search for "bioinformatics." You will notice that there are over 20,000+ results. On the left side, there are Refine Results tools. You can use these tools to help narrow the number of results based on parameters like document type, language, and year. Limit your results to only the publication year of 2011. How many results do you have?

You will see under each article link there is a field that says **Times Cited**. This means the number of times this article is used in subsequent articles.

C-2. Find an article with a value of at least 40. Click on the article title. Write down the article citation in ACS format. Refer to the **ACS Style Guide** link for creating a journal article citation.

On this page in the right column you will see several boxes, one says Times Cited, and the other says **Cited References**. This means the number of articles that were used and cited in the article you have selected. Cited references are extremely important in research when you need to go back and find background information or additional information on a topic.

C-3. How many cited references does this article have?

Now, click on the link that says **Citation Map**. A citation map is a visual representation of cited references and the subsequent articles that have cited your article. Click around and become familiar with the interface.

Web of Science also has the ability to search for articles written by one unique author. For example, the problem with basic author searches is the name John Smith is so common that you would get inapplicable results. Instead of finding the chemist John Smith, you may so get results about a computer scientist, doctor, or even a fiction writer named John Smith. Web of Science has an Author Search tool that will help eliminate this issue.

Under the tab that says Web of Science, click the link that says **Author Search**.

C-4. Chemistry Professor and Nobel Laureate Ariel Warshel has published over 400 articles during his tenure here at USC. Can you create a comprehensive list? How many articles has he written in his time here at USC? (hint: search by his full last name, but only put in A for his first initial, choose

All Research Domains, and under organizations scroll and select the University of Southern California)

D. SciFinder

On the main interface of SciFinder you will see you can perform many of the same searches in this assignment in one place. SciFinder connects reference sources with article searching and databases. One strength of SciFinder is the ability to search by molecule or reaction.

To use the reactions tool, click on Reaction Structure. Then open the structure editor (either Java or Non-Java will work). Here you can draw molecules or reaction schemes.

D-1. Find the most efficient* way to make tetrahydrofuran (THF). Draw THF using the structure editor and then click on the "Add a Reaction Role" button (it looks like an arrow above the letters A and B). Highlight your structure and choose the role of "product." What is/are the starting material(s), reagent(s), solvent(s), and reaction conditions?

*In this case, efficient refers to the fewest number of steps with as close to 100 percent yield as possible.