Chem 322a/325a: Chemical Information Literacy for Organic Chemistry

Links and tutorials for this assignment can be found on the Chem 322a/325a Course Guide: http://libguides.usc.edu/chem322a

Introduction

Technology plays a major role in today's understanding of chemistry. Chemists utilize different electronic and online resources for research and laboratory work. It is important to be aware of these tools and keep up-to-date on the most recent and relevant research, databases, and data.

In this lab you will explore chemical resources important for future lab assignments and research. Each section has questions that should be answered in your lab notebook. By the end of this lab, you should be able to determine what resource is best suited to answer a question and how to use that specific resource to determine a viable answer.

Materials Needed

Lab notebook, pencil, calculator, and computer/laptop*

*This assignment will not work on a tablet. If you do not have a personal computer, please use the software provided in one of the three ITS managed computer labs (SAL, WPH, and KOH). If you use a personal computer, you will be required to install ChemBioDraw onto your computer. If you do not want to install the software, please use one of the ITS managed computer labs.

Part I: Chemical Data and Laboratory Safety

Before stepping into a lab, it is imperative to know physical data, safety information, and other guidelines regarding any of the chemical or procedures you will be carrying out. In a teaching lab, most of the information is provided to you by a teaching assistant or by your instructor. In research labs, this responsibility falls onto the shoulders of the researcher.

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.

Chemical dictionaries and databases will provide a great deal of reputable and reliable information. On the Chem 322a course guide, go to the tab labeled **Reference Tools**. Click on *The Merck Index*.

1. Perform a Quick Search for "naproxen." Put the following information in your lab notebook: drawn structure, CAS registry number, CAS name (formal chemical name), molecular formula, molecular weight (assume g/mol), and percent composition.

2. Scroll to the bottom of the page and enter a chemical, medication, or drug you are interested in finding more information about in the Quick Search box. Using *The Merck Index* provide the following information: name, drawn structure, CAS number, CAS name (formal chemical name), molecular formula, molecular weight (assume g/mol), and percent composition.

Other resources are available to find chemical information including the *CHEMnetBASE* suite.

Some chemical dictionaries provide safety and hazard information, but they are not complete or thorough. One of the most reliable places to look for this information is a chemical manufacturer's website. By law, a company must provide a Material Safety Data Sheet (or MSDS) for every chemical that company produces and sells. Most companies have made this information free and open on their respective websites.

Sigma-Aldrich is one of the largest chemical manufactures in the world. Click on the link for Sigma-Aldrich and answer the following questions.

3. In the top right corner, search for "naproxen." You will see multiple entries under acetaminophen. Find the entry and MSDS for the naproxen that meets the **USP testing standards**. Click on the link for the MSDS and scroll through it. You will see there is a lot of available information including first aid information and handling instruction. Find the section labeled **Toxicological Information**. What is the oral LD50 for naproxen? LD50 stands for the lethal dose of the chemical such that 50 percent of the sample population, in this case rats, to die.

4. Using the LD50 provided, calculate how many tablets of acetaminophen must be ingested by an average human to potentially die. Assume an average human is 68 kg and a tablet of naproxen is 220 mg.

5. Using the chemical from question 2, search for the MSDS of that chemical. Perform the same oral LD50 calculate on your chosen chemical. If your chemical from question 2 does not appear in Sigma-Aldrich, use dimethylamine.

6. Look through your MSDS and note down anything interesting, new, or confusing.

Part II: Finding Spectra

When performing laboratory experiments, characterizing your compounds is extremely important. The process of characterizing proves the compound you created is the compound you intended to create. One way to determine if you have created the correct compound is through spectra. The spectra from NMR, IR, UV-Vis, Raman, MS, etc. can be compared to a reference spectra (a spectra that is verified as correct).

Find 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. Go to the **Databases** tab in the course guide.

7. Click on SDBS and agree to the disclaimer. Search for naproxen in SDBS (hint: search by CAS registry number). What spectra is available for this compound? Print any one spectra and staple it to the end of this assignment. Label this spectra as "spectra #1."

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 question 8. Follow these instructions to find spectra in Reaxys:

To find details regarding a compound, when you have the name or CAS number, click on "Substance, Names, 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.

8. Search for pentamethylcyclopentadiene in Reaxys (hint: use CAS number 4045-44-7). What four main types of spectra are available? Download and print any one spectra. Label this spectra as "spectra #2."

Part III: Topic and Article Searching

Topic searching is an important tool in discovering articles and research materials. The most effective way to do a topic search is to use a database. Databases allow you to search across multiple disciplines, journals, and years. USC Libraries subscribes to thousands of databases. You will try out two different databases: PubMed and Web of Science.

A note about searching for articles: articles are only as good as your ability to find the full-text of an article. Without the full-text, you do not get the graphs, tables, references, and supplemental information. Usually the full-text article is not available in the database, but on a different website. USC Libraries has provided the "Find it @ USC" link to directly link to the full-text article, if available. Occasionally, USC Libraries does not have a subscription to the journal the article appears in. When clicking the "Find it @ USC" link, you will be told to request the article via interlibrary loan (ILL).

PubMed is a service provided by the National Institutes of Health and contains millions of citations of medically related research. All NIH funded research must ultimately be available through PubMed for free.

9. Click on PubMed in the course guide and search for "naproxen." Then start over and search for "naproxen delivery systems." How many articles appeared in each search?

10. On the left side, you will see a filter tool. Using the second search results, try limiting the number of results by only selecting articles less than five years old. Now how many articles appear?

11. Perform a PubMed search for the compound you chose in question 2. Find an article about it and write down the citation and a brief description of the research. If you need help formatting a citation, see the course guide for a sample citation.

Web of Science is one of the most broad science databases we have here at USC. This database covers resources from all fields of physical sciences, life sciences, and engineering.

12. Click on Web of Science and do a topic search on the "formation of peroxides" (quotes are not required). Like PubMed, you will see a filter tool on the left side. Experiment by selecting and deselecting various filters. Pick an article that seems interesting to you and find the full-text. Print the article and attached it to the end of this assignment. If you cannot find the full-text choose a different article.

Part IV: Chemical Drawing Software

Adapted from Experiment 1: Molecular Modeling, ChemDraw & Excel (U. Colorado Boulder)

Chemical drawing software assists chemists in representing both simple and complex chemical structures in 2D form. All professional correspondences, articles, and presentations use compounds drawn on this type of software. These drawings will be required for any formal lab report in future classes. This part of the assignment will allow you to become comfortable with ChemBioDraw and test your ability to draw organic compounds.

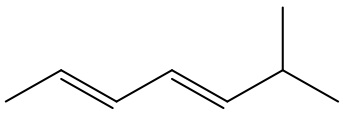
ChemBioDraw (PC and Mac) is available for download to personal computers for all current USC students, faculty, and staff. The download link and instructions are available on the course guide under the tab **Chemical Drawing Software**. If you do not want to download this software to your computer or do not have a computer, the software is available in the computer labs in SAL, WPH, and KOH. A demonstration of the software will be given during the lab lecture period.

After drawing your structures in ChemBioDraw, you will be exporting them to Microsoft Word to print and submit. Depending on your operating system and version of Word, you might encounter compatibility issues with inserting the drawing directly into Word. In these cases, the best workaround is to save your ChemBioDraw file as an image file (.gif, .jpg, .png, .tif, or .emf should all work) then insert them into Word as a picture.

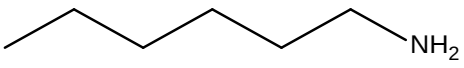
A quick warning, if you open your Microsoft Word document on a computer without ChemBioDraw, your structures will appear as gray boxes. Please make sure to print your document before you leave the computer lab.

When you launch ChemBioDraw, you will see various toolbars and a blank document. On the left side you will see the main toolbar including single, double, and triple bonds, hash marks, wedges, pre-drawn rings, and a text editor.

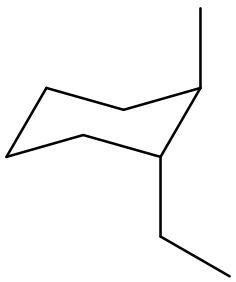
13. Draw the structure shown below. It does not have to be tidy. Copy the structure into a blank Word document. Label the structure as #1.

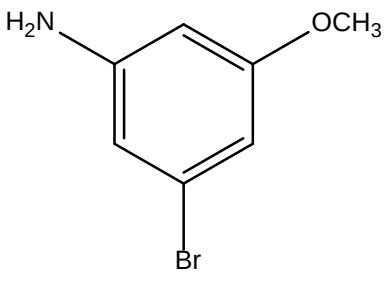


14. Draw the following molecule and copy it into your Word document. Label the structure as #2.



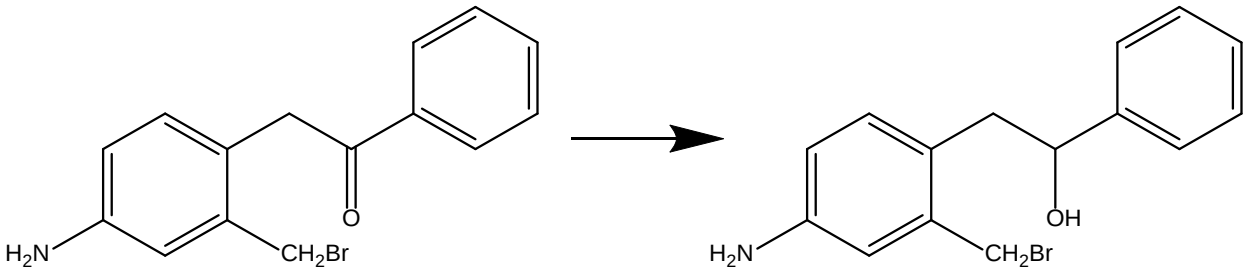
15. Draw the structures shown below and copy them into your document. Label the rings #3 and #4 respectively.





ChemBioDraw also allows drawing a reaction mechanism so you can visually show someone how you got from reactant A to product B. On the left side you will see a tool that looks like an arrow.

16. Can you duplicate the reaction drawing below? It does not have to be tidy. Hint: draw the reactant and copy and paste it as the product and make the change to the double bonded oxygen. Copy and paste the completed reaction into your Word document labeled as #5.



Sometimes the drawings can get messy. The bond lengths are different, the angles can look funny, and the proportions are off. ChemBioDraw has several tools to help clean up your drawings.

Structure → Clean Up Structure (Ctrl+Shift+K): when your structure highlighted, this feature will align bonds, adjust angles, and make the drawing neater. You may need to repeat this several times.

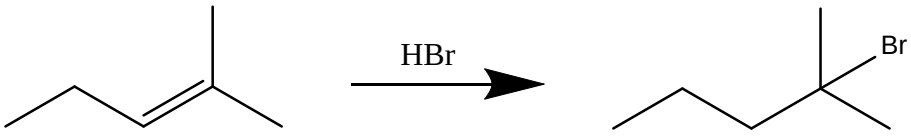
Object → Align: when multiple drawings are selected, this tool aligns the highlighted drawings one of six different ways. Most often you will use align T/B (top/bottom) centers.

Object → Distribute: when multiple drawings are selected, this tool evenly spaces out the drawings either horizontally or vertically.

17. Take the drawings from questions 13-16 and use the cleanup tools on them. Then copy and paste these cleaned up drawings into your Word document. Label the set of drawings as #6.

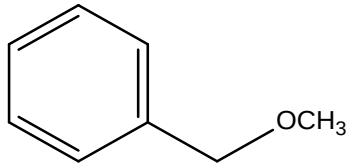
The grouping features allows you combine multiple drawings into one. This makes copying and pasting the drawing much easier. Usually you will use grouping only after you have used the cleanup tools on your drawings.

18. Draw the reaction scheme below. Make sure to clean up each individual drawing first, then align, and finally group the drawings together. Copy and paste into your Word document and label the drawing #7.



ChemBioDraw has the ability to analyze certain properties of a drawn molecule. Go to View → Show Analysis Window.

19. Draw the following molecule and open the analysis window. Copy and paste the drawing into your Word document and include the information provided on the analysis window. Label your drawing as #8.



Print out your Word document and attach it to your lab assignment.