

Chemical Drawing & Word Processing Course Activity
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Purpose

Computer literacy is fast emerging as a “basic skill as important to daily life in the twenty-first century as reading is now. The purpose of this course activity is to give students practical experience in computer literacy by developing some general computer word processing and chemical drawing skills needed for this course. In particular, students should be able to draw chemical structures—perhaps using a drawing program like ISIS Draw or any drawing program of their choice—import and edit images, and save and insert images from web based sources into their reports. In the process, you will use search engines and chemical databases, (i.e., <http://www.google.com/image> “search image,”), to track down chemical data. An opportunity to learn these basics through the use of basic tutorials—to include but are limited to—learning simple basics for drawing chemical structure, and how to select, resize, and import chemical structure into a word document.

Getting Started

There are several drawing programs for drawing chemical structures available. Most drawing and word processing programs on the market generally have the same generic look and feel. If you are already accustomed to using a drawing program, good for you. In this course, use whatever drawing and word processing programs you are most familiar and comfortable using. Likewise, use any word processing program of your choice to word process this course activity and all future laboratory reports.

One chemical drawing program commonly used by students in our chemistry department is ISIS Draw. Another program is Microsoft Word, which most already use for general word processing. If you're new to ISIS Draw, you might be terrified. Once you watch the tutorial and get going, you'll see you can create professionally great graphics simply by clicking on your screen. ISIS Draw has a complete set of tools and templates for creating many different kinds of drawings, but we will use it mainly to draw chemical structures. Students can access ISIS Draw and a printer from our chemistry department computer laboratory across from MS401. Students can find access to other reliable computers and printers in our LRC. ISIS Draw, ChemSketch & Marvin Sketch are free downloads and can be installed on your own personal computer. The URL's to this Course Activity and a variety of chemical drawing programs are linked at

http://homework.sdmesa.edu/dgergens/chem231L/word_processing/frame_stub.html

Course Activity

Welcome to ISIS Draw. To start the learning process in learning the basics of drawing a chemical drawing program, find a computer with ISIS Draw loaded and that has Internet access. Open ISIS Draw and either Netscape or Explorer. Access the ISIS draw tutorial link and click on it. The ISIS tutorial at http://homework.sdmesa.edu/dgergens/chem231L/ISIS/isis_tutorial.html. I would suggest watching the tutorials first then mimic the same learning process using ISIS Draw. Resize your viewing screen so both ISIS Draw and your browser windows so they are both viewable at the same time. In this way, you can watch the tutorial and using the drawing program, you can draw mimicking the learning process being shown in the tutorial. The tutorial will answer most of your questions regarding the use of the program. Email your instructor immediately if have additional questions and/or suggestions regarding the tutorial.

Download the course activity drawing template shown on the next page.

The word document will be word-processed and turned in for grading. You can use any drawing program to draw (i.e., ChemSketch or Marvin Draw) complete this course activity but the tutorials only demonstrate the use of ISIS Draw.

NOTE: When importing images by copying and pasting an image from ISIS into a Microsoft Word document, select and copy the image in ISIS, then paste into Word by following these commands in order: <Insert>, <Paste Special>, and select <Enhanced Meta File>.

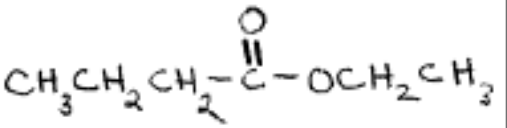
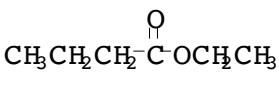
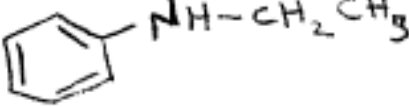
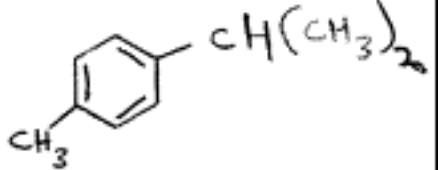
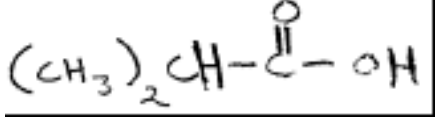
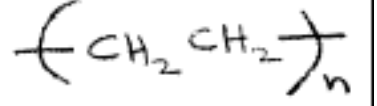
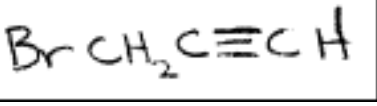
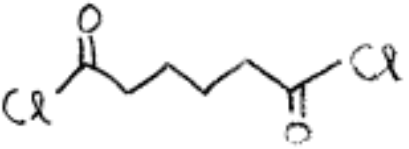
"A picture is worth a thousand (by a thousand) words"

PART 1 - Cleaning Up Hand Drawn Structures

In this course activity, you are being asked to **redraw exact duplicates** of these hand drawn structures by using any chemical drawing program of your choice. ISIS Draw is a good choice for drawing chemical structures as shown in the tutorial provided.

Download the word processing template and access the ISIS tutorials from the link

- http://homework.sdmesa.edu/dgergens/chem231L/ISIS/isis_tutorial.html
- THESE MOLECULES in this course activity will be seen again, as is in the FTIR course activity in your manual.
- **Don't Plagiarize your work—Our Academic Honesty Policies will be strictly enforced**
- Identify the functional group and correct molecular formula. An example, ethyl butanoate, an ester, is done for you.
- Add subscripts and/or superscripts where appropriate to all molecular formulas and ions
- Complete the template using the ethyl butanoate example as your guide.
- **Redraw exact duplicates** of these hand drawn structures.
- Copy and paste each drawing into the table cell on the right in this template.
- **Resize each image so all eight structures can fit on this page.**
- DON'T split this table between two pages; all of the below must fit on this page.
- Point deductions will occur if you plagiarize, don't draw exact duplicates of hand drawn, & split tables between pages

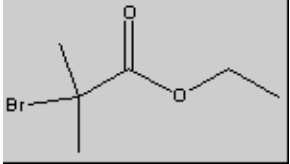
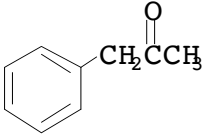
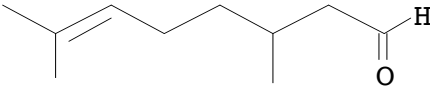
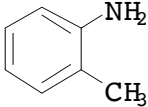
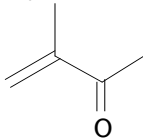
Hand Drawn Compound & Structure	functional group and formula	Re-Drawn Compound & Structure
<p style="text-align: center;">ethyl butanoate</p> 	<p style="text-align: center;">ester C₆H₁₂O₂</p>	<p style="text-align: center;">ethyl butanoate</p> 
<p style="text-align: center;">N-ethylaniline</p> 		<p style="text-align: center;">N-ethylaniline</p>
<p style="text-align: center;">4-isopropyltoluene</p> 		<p style="text-align: center;">4-isopropyltoluene</p>
<p style="text-align: center;">2-methylpropanoic acid</p> 		<p style="text-align: center;">2-methylpropanoic acid</p>
<p style="text-align: center;">polyethylene</p> 		<p style="text-align: center;">polyethylene</p>
<p style="text-align: center;">3-bromopropyne</p> 		<p style="text-align: center;">3-bromopropyne</p>
<p style="text-align: center;">adipoyl chloride</p> 		<p style="text-align: center;">adipoyl chloride</p>

PART 2 –Web Based Images - Copying and Pasting into Table Cells

In this course activity, we will use the internet as a resource for pre-drawn chemical structures. Searching for physical data (e.g., structure, mp, bp) on a compound using a database is very easy using the internet and in the process a chemical structure is often provided. Data bases, in general, will give the structure of the compound as an image. Images can be save to disk or can be inserted—copy and pasted—into a word document saving us time and effort in not having to re-draw each structure.

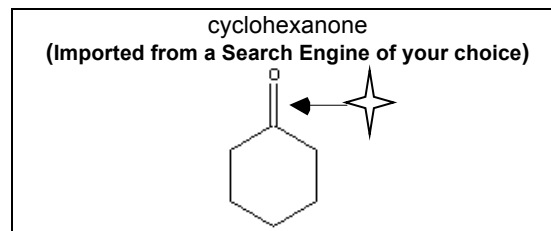
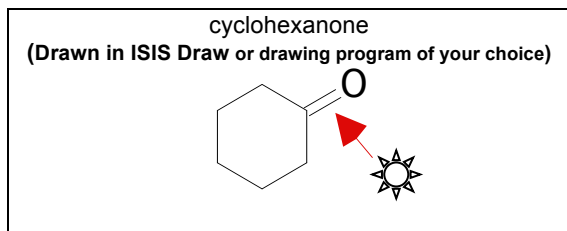
- Using a search engine of or database of your choice (i.e., <http://www.google.com/image> “search image,” search by molecular formula, search by molecular formula first, then match the name to its structure. Add subscripts and/or superscripts where appropriate to all molecular formulas and ions
- THESE MOLECULES in this course activity will be seen again, as is in the FTIR course activity in your manual.
- Molecular formula searches will afford you a much broader search result especially if you misspell a substance’s name.
- Check to see the number of atoms—and hydrogens—are added up correctly in your formula before searching
- **All eight structures need to be resized to fit on this page.** Don’t split this table between two separate pages

Once an image is found, copy the image from the internet by placing your cursor on the image, mouse click and hold, select <Save Image As> and save the image to disk or <Copy Image>. Find the saved image and insert it into the table cell in the left column. When inserting a saved image into a Microsoft Word document, select <Insert>, <Picture>, <From file>, select the <file name>. If the image does not go into the desired cell in the table, you may have to copy the image then paste back into Microsoft Word by selecting <Insert>, <Paste Special>, and select <Enhanced Meta File>. If you need additional help, please contact your instructor and we’ll be glad to help. We would like the image to fit into the box at the left without having the box expanding larger than what it is currently. The first one the substance, the ester, ethyl–2-bromo–2–methylpropionate, is done for you.

Web Base Image	functional group and formula	Compound & Structure
	<p>ester C₆H₁₁BrO₂</p>	<p>ethyl 2-bromo-2-methylpropionate</p> $(\text{CH}_3)_2\underset{\text{Br}}{\text{C}}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OCH}_2\text{CH}_3$
		<p>1-phenyl-2-propanone</p> 
		<p>3,7-dimethyl-6-octenal</p> 
		<p>3-methyl-1-butanol</p> $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{OH}$
		<p>2-aminotoluene</p> 
		<p>3-methyl-3-buten-2-one</p> 

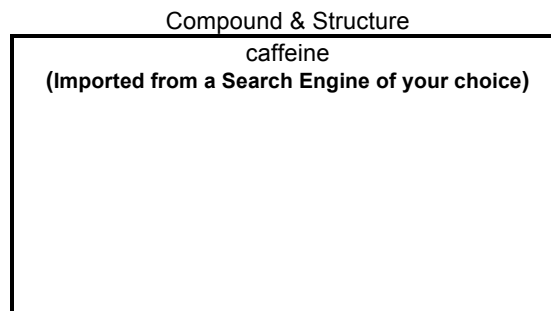
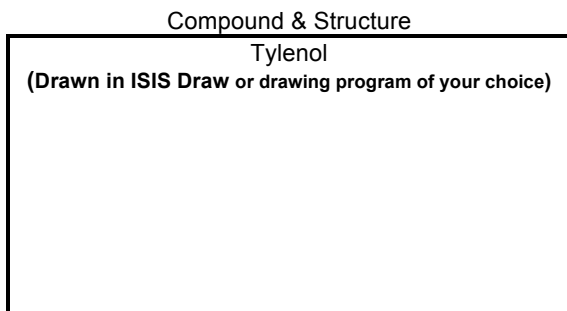
PART 3 - Editing a Chemical Structure

In this course activity, you are being asked to draw and import structures, followed by doing additional edits by adding some graphics to each structure. For example, cyclohexanone was drawn in ISIS Draw, and its structure was found using ChemSpider. Both were copied and pasted into their corresponding table cells. In Microsoft Word, the image was edited by using the drawing tools found in the Microsoft Word application. To each image, (1) a arrow and (2) a star were added to each image.



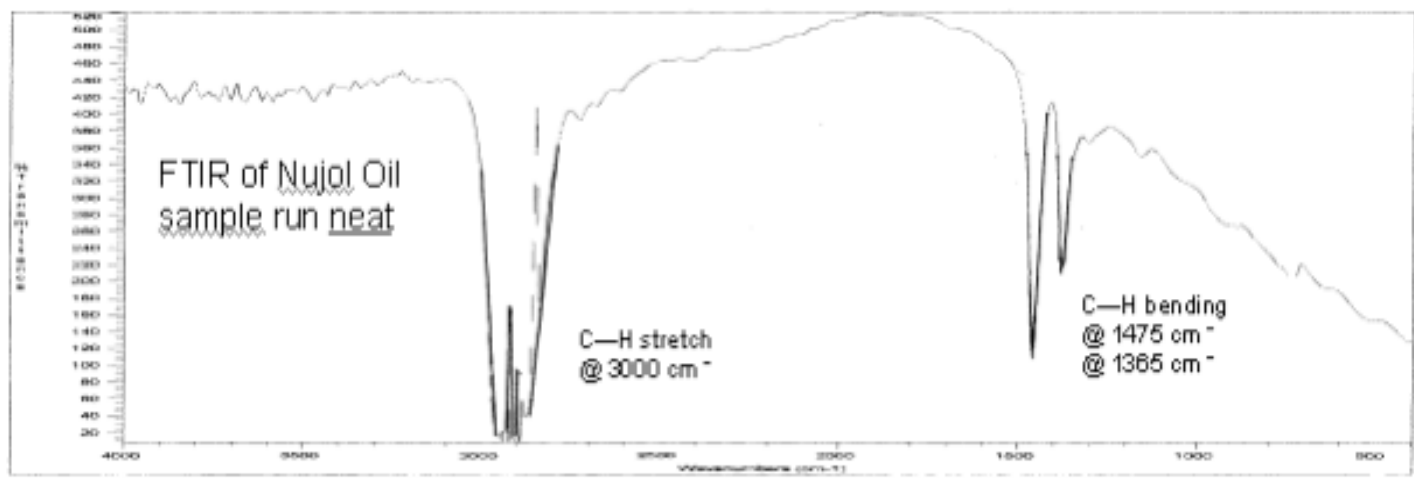
Using the cyclohexanone example above as a guide, complete the following for Tylenol and caffeine

- A. Draw the structure of Tylenol
- B. Using a search engine or data base of your choice (i.e., <http://www.google.com/image> "search image," search for the molecular formula of caffeine.
- Import both structures (A) and (B) into their corresponding table cell of our template.
- Finally, edit both images by adding (1) an arrow and (2) a star to each.
- Double clicking **images and graphics while in MS Word often opens the graphic editor in MS Word.**



PART 4 - Editing a Scanned Image (**SKIP THIS SECTION**) -

In this course activity, you will be asked to scan an FTIR spectrum of Nujol oil and save it to disk. Afterwards, you will be asked to recall that image and insert it into a word document. Finally, you will be asked to edit the image in Microsoft Word. For example, the scanned spectrum of Nujol oil was imported and then edited by adding the labels C-H stretching and C-H bending, and a title was given.



Have available a disk with this assignment document file on it. You will scan an image to this disk.

In the laboratory there is a scanner. (**We can just use a photo to do quick scanning of images in today's world**) You will need to save the scanned image to the same disk that has this assignment document file. Obtain a sample FTIR spectrum of Nujol oil from your instructor. Scan the image of FTIR spectrum of Nujol oil following the procedures "How to Scan" posted near the scanner. Name the scanned image file <Nujol.doc> and save the image and file to disk. Is the <Nujol.doc> image file on the same disk with the file for this assignment? If so, open the <Nujol.doc> and the file for this assignment. From the <Nujol.doc> document, select and copy the FTIR spectrum. Do a <Insert>, <Paste Special>, <Enhanced Meta File> to insert the FTIR spectrum for Nujol into box below for this assignment.

Finally, edit the FTIR spectrum for Nujol by double clicking on the image and adding the labels C—H stretching and C—H bending, and by giving the spectrum a title. We would like the image to fit into the box below without having the box expanding larger than what it is currently. Your scanned image should remain on this page.




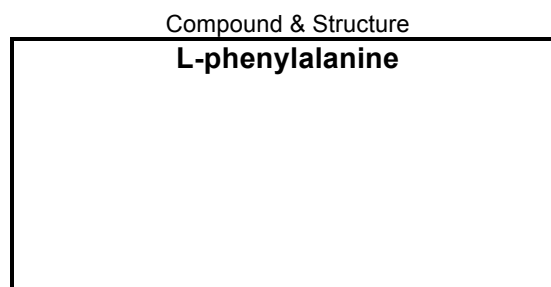
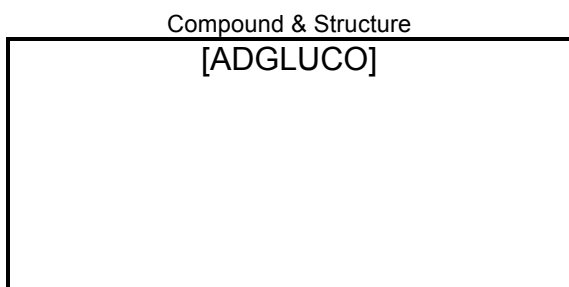
PART 5 - Use of Chemical Drawing Program Templates

In this course activity, you will be asked to insert pre-drawn images from templates available in ISIS Draw.

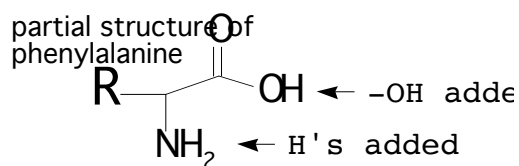
- **ChemSketch & Marvin Beans DOES NOT have the appropriate templates.**
- You may have to complete this section on campus if you do not have ISIS draw on your computer since some drawing programs may not have the needed templates given below.

Open ISIS Draw and select <Templates> in the menu bar. Select <Alpha-D-Sugars> and a menu of several alpha-D-sugar structures appear. Place the cursor on one of the bonds in the structure for the sugar [ADGLUCO], which is for alpha-D-glucose,

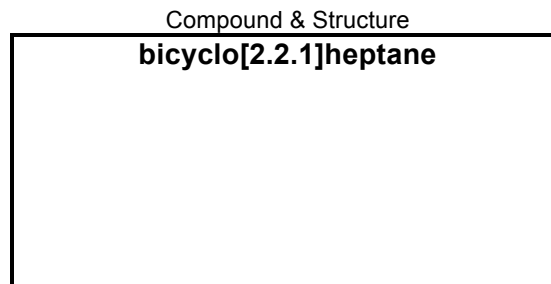
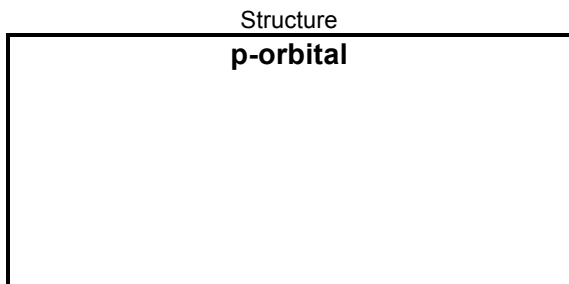
and mouse click. After mouse clicking, the structure should appear in ISIS Draw. Using the atom tool , add hydrogens to all the oxygens except the one in the ring. Import the structure into this document in the box below.



To import phenylalanine derived from the **L-phenylalanine** template, use the select <Templates> in the menu bar in ISIS Draw, the <L-Amino Acids>. Place the cursor on one of the bonds in the structure for the amino acid **L-phenylalanine** and mouse click. After mouse clicking, the structure should appear in ISIS Draw. Using ISIS Draw, add a hydroxyl group to the carbonyl carbon and add hydrogens to the nitrogen to form a complete structure of L-phenylalanine, then select all and import the entire image of L-phenylalanine into the box on the right above.

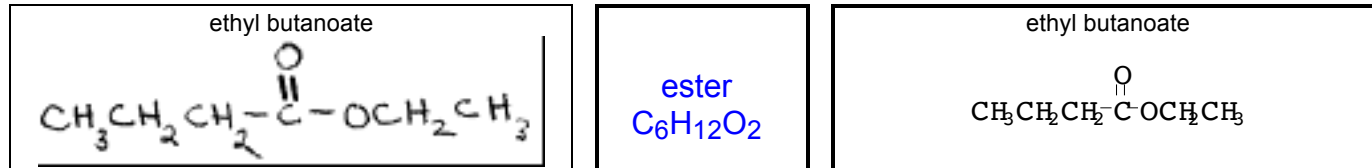


In ISIS Draw, do the same by adding a **p-orbital**, and **bicyclo[2.2.1]heptane** found under their corresponding templates into the table cells, below:



PART 6 - Copying and Pasting Data from a Data Base

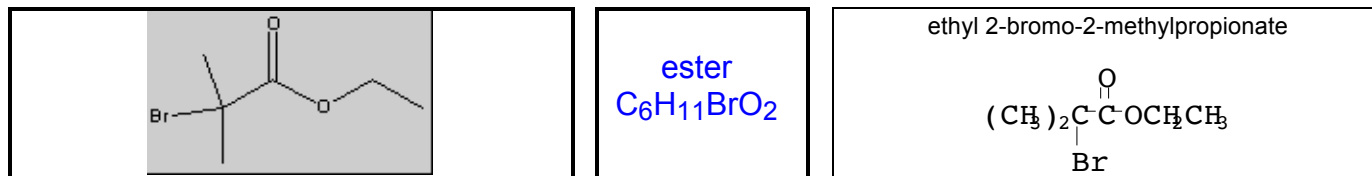
In this course activity, you are being asked to search on a compound using the internet followed by copying pasting that data into this template. For example, physical data for ethyl butanoate was found in ChemSpider, then copied and pasted into the box below.



Ethyl butyrate [105-54-4] Synonyms: Ethyl Butanoate; Butyric Ether; Butanoic acid ethyl ester; Ethyl n-Butyrate; natural ethyl butyrate; BUTIRATO DE ETILO; formula: $C_6H_{12}O_2$ molar mass: 116.1596 melting point: $-135.4\text{ }^\circ\text{C}$ density: 0.878 g/mL boiling point: $252\text{ }^\circ\text{C}$ at 0 mm refractive index: 1.392 solubility in water: 0.68 g/100 mL. Insoluble Flash point: $26\text{ }^\circ\text{C}$ Comments: Colorless liquid with pineapple odor. Used in perfumes, rum

Now do the same for the ethyl 2-bromo-2-methylpropionate. Use the internet to search on the compound. Searching by molecular formula will give a much broader search result for the given compound. To do a molecular search, be sure that you total the number of atoms—and hydrogens—correctly.

- Paste the data into the table cell below.
- Make the data presentable like the example data table above.



ethyl 2-bromo-2-methylpropionate Synonyms: _____ Formula: _____ molar mass: _____ melting point: _____ $^\circ\text{C}$ density: _____ boiling point: _____ $^\circ\text{C}$ refractive index: _____ solubility in water: _____ Flash point: _____ Comments: _____
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