ChemDraw Tutorial and Practice

The goal of the experiment is to expose all CHEM 113B students to ChemDraw, the most commonly used drawing program for organic molecules. ChemDraw is available on computers in the Chemistry Computer Lab (DH 503). As a CHEM 113B student, you may also download a copy to your personal computer. To do so, go to http://sitesubscription.cambridgesoft.com/, scroll down to "San Jose State University," and follow the appropriate link to download either version 16 or 17. In you lab reports, you will be required to use ChemDraw for your chemical schemes and figures. Please always use the "ACS Document 1996" format (File > Apply Document Settings from... > ACS Document 1996).

This lab has no prelab and no post-lab quiz. You will submit your completed tutorial (15 pts) as a pdf, doc, or docx file to Canvas. Please include heading for each section (e.g., "A. Freehand Models and Schemes"). Note – any sharing of structures between students will result in a score of a zero on the lab.

ChemDraw Basics

- 1. Choose the "ACS Document 1996" format (File > Apply Document Settings from... > ACS Document 1996) to set the proper template.
- 2. By default, you have a 1 page document. You will need to change the document settings to give yourself enough room to draw. Choose File > Document Settings. In the Document Settings window, change the "Height" of the document to 5 pages (or more if you need it).
- 3. Sometimes crosshairs are helpful to check alignment. To view them, select View > Show Crosshair. You can change the position of the crosshairs by clicking and dragging the center of where the bold crosshairs meet.
- 4. Drag the tools bar window to the left side of the screen to lock it outside the document. The tools bar contains all of the drawing tools needed for today's lab.
- 5. Refer to Chapter 6 in the User Guide (available on Canvas) for details on how to use the drawing features.
- 6. We will get started by drawing DABCO (1,4-diazabicyclo[2.2.2]octane) together.



7. Note – to insert a degree symbol (°), you need to use the keyboard command: PC – Alt + 0176 (keep Alt depressed while you enter the numbers)

Mac – option + shift + 8 (all depressed at the same time)

Practice

Provide an accurate ChemDraw rendering of each of the structures below. Make sure to pay attention to bond angles, bond lengths, conformation and stereochemistry. For part B, reproduce the schemes as exactly as possible with respect to the layout of the scheme, fonts, etc. Copy and paste your structures into a Word file for the Canvas submission.

A. Freehand Molecules and Schemes (6 pts)

1.
$$\frac{1}{\sqrt{N}}$$
 2. $\frac{1}{\sqrt{N}}$ 3. $\frac{1}{\sqrt{N}}$ 4. $\frac{1}{\sqrt{N}}$ 5. $\frac{1}{\sqrt{N}}$ 6. $\frac{1}{\sqrt{N}}$ $\frac{1}{\sqrt{N}}$

B. Published Schemes (6 pts)

MeO
$$_{6}$$
 $_{6}$ $_{7}$ $_{2}$ $_{2}$ $_{2}$ $_{3a}$ $_{3a}$

C. Models (3 pts)

Represent one of the models in ChemDraw. Make sure to indicate which one you drew as well as the proper stereochemistry. ChemDraw also has helpful features to determine the molecular weight and molecular formula of a structure. Go to View > Show Analysis Window. Highlight your compound for part C. Select "Formula" and "Mol. Wt. on the analysis window and then click Paste. The formula and molecular weight should now appear below your structure. Note, the values will update if you change the structure.

D. Extra Credit (up to 3 bonus pts)

If you have extra time, draw a self-portrait using ChemDraw.