Chemistry 430 — Simulation in Chemistry & Biochemistry

Laboratory #1 — Unix Tutorial & Using Molecular Visualization Programs

In this introductory lab you will first work through tutorials on the use of Unix/Linux commands via a "shell" or terminal window. Then you will be introduced to the Chimera, ChimeraX, VMD, PyMOL, Tinker-FFE and Spartan programs, and learn how each of these can be used to visualize molecular structures and perform basic calculations.

Protocol

(1) Login to your account on one of the iMac workstations, using your chosen Username. Initially everyone's Password is set to **`ChEm430`**. After logging in for the first time, please change your password to something of your choosing that is not too simple or easy to guess. Do this by opening a Terminal window by clicking on the black, rectangular icon already in your dock at the bottom of the screen. Then use the **`passwd`** command in the Terminal window, and choose a new password.

(2) The six workstations in Louderman 454 for use in the Chem 430 course are named: "eggnog", "holly", "icicle", "ivy", "merry" and "noel". They all have a "full name" ending in "wustl.edu", so "eggnog.wustl.edu" for example. If you want to login remotely, issue the following command in a terminal window on your remote machine:

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username@machine.wustl.edu
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where "username" is replaced by your username for the course, and "machine" is the name of one of the workstations.

(3) Most of the visualization software packages can be freely installed on your own personal computers. Links to download software versions for Mac, Windows and Linux, along with information, manuals and tutorials, can be found in the "Software Resources" section of the course web site.

(4) The tutorial "Unix for the Beginning Mage" is a very good (if somewhat whimsical…) introduction to using Unix/Linux commands in a terminal window. The tutorial is located in the Reading & References section on the course website. If you are using a Macintosh, work through the tutorial using the macOS "Terminal" application. On Windows, use the "PowerShell" application as your command line window for the tutorial.

We will not have sufficient the time to go through this tutorial during the class lab session. But if you are not already familiar with simple Terminal commands, then you should find time outside of class to work through this tutorial. In addition, a small book titled "Macintosh Terminal Pocket Guide" available in the lab for you to consult as needed.

(5) Download the Tinker-FFE (FFE=Force Field Explorer) software package for Mac. It can be found on the course website under Software Resources. Double click on the .dmg file,

and then run the installer. This will install FFE in your Home area in the directory /Tinker-FFE. The FFE application is located in ~/Tinker-FFE/ffe, and can be dragged to your dock for easy access. *[This package may already be installed for your account. Check for the "water dimer" icon in your dock at the bottom of the screen. Note a single water molecule icon is used for a different application, the VMD molecular visualization program.]*

(6) Open FFE by double clicking on its icon, choose the "Download from NCI…" option under the FFE "File" menu, then enter ibuprofen in the text box to download the structure of this common NSAID from the National Cancer Institute database.

(7) Using FFE options under "Modeling Commands", run the "Analyze", "Minimize" and "Spacefill" programs on the ibuprofen structure. What is the value of the van der Waals surface area of ibuprofen in square Angstroms? How about the accessible surface area, and the "contact-reentrant" (smooth molecular) area?

(8) Open the Spartan Student program, and use its structure building menu to construct the ibuprofen molecule. You can then run a Hartree-Fock molecular orbital calculation using the STO-3G basis set for this molecule. Look at several of the highest energy occupied orbitals for ibuprofen. Save a picture of the highest occupied π-type orbital. Use the "Command-Shift-4" key combination to do a screen capture, drag the mouse over the screen area to be saved.

(9) Two visualization programs that are widely used for biomolecular structures are Chimera and VMD. We will use both of these packages later in the course. Both programs have online tutorials: "Chimera Getting Started" and "Using VMD Tutorial", which are found in the Software Resources area of the course website.

We will be using both Chimera and VMD throughout the course. They are very useful programs to learn, as they are standard "research grade" tools used in actual computational chemistry, molecular modeling and structural biology research labs. Before the next lab session, you should try to work through both of these tutorials to get a basic familiarity with these important and powerful programs.