CHEM 333 Session 1: Competence with Linux

Once familiar with the basics of unix, there are certain tasks that you should be comfortable doing, as they are representative of the sort of meta-work that computational chemists and structural biologists do on a routine basis. These include finding and editing files, translating file formats, comparing file contents, extracting data from files, and converting the output of one program into the proper format for input into another program. If any of the following tasks are difficult for you, you should spend time learning about basic unix tools until they are easy for you.

1) Examine the directory /sb/demo/

a) How much disk space is used by the files and subdirectories?

b) Which subdirectory takes up the most space?

2) Say you have a data file located somewhere under /sb/demo/chem233/ and you don't remember its exact name. You know that the name of the file is probably something like this: "HGHsomething.log"

a) What commands could you use to locate the file efficiently?

b) Within that file, you know that the third line of the log will show the precise command that was used to execute the program. This may be important for documentation or reproducibility later. How can you print just the first three lines of the file? (Here, "print" means display on the screen, not to a printer.)

c) If your calculation converged to a successful result, then the logfile will contain the message "Stationary point found". What command can you use to search the file for a given string of text? Did it converge?

3) Download 1DMO.pdb to your working directory. (If you are not familiar with pdb.org, then you should explore it a little.)

a) Is that the letter O or a zero? How could you tell? [If you got Shiga Toxin, it's the wrong one.]

b) How many lines in the file start with the word 'ATOM'?

c) Extract the first model from the NMR ensemble and save it as my_model.pdb

d) Compare it to /sb/demo/chem233/unix/test/one_model.pdb. Exactly how does it differ? Are the differences significant?