The UNIX operating environment and its variants (Linux, Mac OS X) are the language of scientific computing as well as data management and information technology. This workshop will provide instruction and hands-on experience in programming and data analysis on your own laptop, ultimately leading up to topics in drug discovery such as molecular visualization and drug binding and its scientific basis in thermodynamics.

Online Tutorials:  http://sites.google.com/a/une.edu/unix

Monday, Jan. 5
9-12  Intro to UNIX (with Mac OS X); Installation for PCs (Cygwin)
1-4p  Hands-on Laptop Session: UNIX terminal commands and VI text editor

Tuesday, Jan. 6
9-12  Lecture Tutorial: Scripting in C Shell, Awk
1-4p  Hands-on Session: Simulation data analysis

Wednesday, Jan. 7
9-12  Lecture Tutorial: Introduction to scientific programming in C and Python
1-4p  Hands-on Session: Program construction, compilation and execution; histogram analysis

Thursday, Jan. 8
9-12  Lecture Tutorial: Introduction to protein modeling using the Foldit game (group: uneRx)
1-4p  Hands-on Session: Structure prediction competition for scientific discovery

Friday, Jan. 9
9-12  Lecture Tutorial: Molecular visualization with VMD
1-4p  Hands-on Session: Ligand docking and alignment of PDB structures