Anaconda and Jupyter Notebook Basics

1. Anaconda

- a. Download link: https://www.anaconda.com/download/
- b. Creating an environment: conda create --name chemoinformatics python=3.6
- c. Deleting environment: conda remove --name chemoinformatics --all
- d. Updating Anaconda:
 - i. conda update conda
 - ii. conda update anaconda
- e. Activating environment:
 - i. Linux and Mac: source activate chemoinformatics
 - ii. Windows: activate chemoinformatics
- f. Installing ipython kernel: python -m ipykernel install --user --name chemoinformatics --display-name "Chemoinformatics"
- g. Installing packages:
 - i. pip install package name
 - ii. conda install package_name
- h. Installing from requirements file
 - i. pip install -r requirements.txt

2. Jupyter notebook

- a. Starting: jupyter notebook
- b. Two views in jupyter:
 - i. Press Enter to move to Edit Mode
 - ii. Press Esc to move back to Command Mode
- c. Executing code in cell: Ctrl + Enter (Command Mode) or Shift + Enter to automatically move to the next cell
- d. A variety of other shortcuts available, look under Help -> Keyboard Shortcuts