Virtual Screening Scripts

- I wrote a few scripts to manage the virtual screening
  - <u>sync_virtual_screen.sh</u>, to transfer files back and forth between my computer and XSEDE's Bridges
  - <u>create_vina_sh.py</u>, a python script to create a shell script, script0.sh, to run vina on every ligand file in a directory and use a specified number of cores
  - <u>vina_multithread.job</u>, a SLURM batch script to
    - run create_vina_sh.py based on the number of cores that SLURM provides
    - run the resulting shell script0.sh

```
Minh-IIT-MBP2018:[~/Documents/GitHub/Chem456/static_files/tutorials/hivpr-dockin
g]: more sync_virtual_screen.sh
rsync -Cuavz virtual_screen/ dminh@bridges.psc.xsede.org:~/virtual_screen/
rsync -Cuavz dminh@bridges.psc.xsede.org:~/virtual_screen/ virtual_screen/
```

Virtual Screening Procedure

- First, I transferred the files to Bridges using sync_virtual_screen.sh
- Then, I logged onto Bridges and executed the command `sbatch vina_multithread.job'
- Next, I transferred the results to my own computer using sync_data.sh
- Finally, I performed some preliminary analysis on an ipython notebook, AnalyzeVS.ipynb, also exported to html format.