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.

Molecular Dynamics with Explicit Solvent

https://github.com/daveminh/Chem456/tree/master/static_files/tutorials/ubq_wat-md