

File formatting

- ZINC provides the library in a file format that AutoDock Tools is unfamiliar with, SDF
- To convert to the format that AutoDock uses, I used Open Babel with the command
 - ``obabel dbfda-world.sdf -O dbfda.pdbqt -m``
 - -m means that the molecule is split into multiple files
- This generated 1657 pdbqt files in the same directory

Virtual Screening Scripts

- I wrote a few scripts to manage the virtual screening
 - sync_virtual_screen.sh, to transfer files back and forth between my computer and XSEDE's Bridges
 - create_vina_sh.py, 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
 - vina_multithread.job, 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/
```