

Converting AutoDock Vina results to mol2

- The docking results didn't really have a logical naming scheme. I decided to rename them based the ZINC identifier. I did this in a short jupyter notebook: [3cl-pro/ADVina/analyze/renameDocked.ipynb](#)
- The pdbqt formatted files from AutoDock aren't readily accepted by YANK. I converted the files into mol2 format using a short jupyter notebook based on OpenBabel: [3cl-pro/YANK_GAFF/ligands/0-build/convert_ADVina_to_mol2.ipynb](#)
- In the OpenBabel command,
 - the option ``-l 1'` means that the mol2 file will have one binding pose
 - the option ``-p 7'` means that hydrogen atoms will be added based on pH 7

Running YANK

- YANK parameters are described in YAML scripts, e.g. [3cl-pro/YANK_GAFF/yaml/MPro_ZINC0000001542916.yaml](#)
- Running ``yank script -y MPro_ZINC0000001542916.yaml'` will execute the code, but you shouldn't do it on the login node on Bridges
- On Bridges you can enter ``python submit_YANK.py --type shared --yaml MPro_ZINC0000001542916.yaml'`, which will create a script and submit it to the queue.