

Example pose prediction

- To extract the bound state from YANK results and align the protein to the first frame: https://github.com/daveminh/Chem456/blob/master/static_files/tutorials/bromodomains-YANK/getBoundState.ipynb
- To predict the ligand binding pose: https://github.com/daveminh/Chem456/blob/master/static_files/tutorials/bromodomains-YANK/ligandPosePrediction.ipynb
- Results are in poses.dcd

