How to predict a binding pose

- In a molecular simulation, every structure is different
- Every structure has the same statistical weight
- To predict a pose, we need to group together similar structures: clustering
- For pose prediction, I implemented a method based on
  - aligning every protein structure according to alpha carbons
  - calculating a symmetry-corrected RMSD matrix of the ligand atoms
  - hierarchical clustering according to the symmetry-corrected RMSD
  - selecting a representative based on the medoid - the point closest to all other points - of each cluster
  - ranking poses based on the population of each cluster

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