What are some ways to parameterize ligands?

- The generalized AMBER force field (GAFF) has long been the standard publicly available AMBER-compatible force field for small molecules [5]
- The Open Force Field Initiative (https://openforcefield.org)
  - is a nonprofit consortium that has partnered with the pharmaceutical industry to develop high-quality force fields that are compatible with biomolecular force fields
  - smirnoff99Frosst is comparable to the generalized AMBER force field [6]
  - The new Open Force Field 1.0 “Parsley” demonstrates improved comparison with quantum calculations and condensed phase properties
- I have demonstrations for parametrizing ligands with both GAFF and Parsley
  - In this presentation I will focus on GAFF, as the workflow is simpler
  - If you wish, your team may choose to set up your systems with Parsley

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