Parameterizing the ligand

- Why do we need ligand parameters?
- I am assuming that you docked the ligand using AutoDock Vina or AutoDock 4
- Parameters from docking programs
  - are not carefully assigned, e.g. charges have minimal dependence on environment
  - are not compatible with biomolecular force fields like AMBER

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