Installing “Parsley”

- Parsley parameters
  - can be applied using a Python package
  - are designed for use with OpenMM

- To install the openforcefield software and force fields
  - conda activate openmm
  - conda install -c omnia openforcefield openforcefields

- To install a program that outputs OpenMM to AMBER format for YANK
  - conda install parmed

  - conda install --yes -c conda-forge -c omnia openmmforcefields

Parsley parameterization

- After completing the installation of “Parsley”, I wrote and executed the jupyter notebook in 3cl-pro/YANK/ligands/0-build/buildSystems.ipynb
- This creates AMBER files of the ligand in solvent
  - prmtop - describes the forces between atoms
  - inpcrd - coordinates of the atoms
- The positions in the inpcrd file look like the pdbqt and sdf input files, except that there are additional hydrogen atoms

```
(openmm) Minh-IIT-MBP2018:[~/Documents/GitHub/Chem456/static_files/tutorials/3cl
-pro/YANK/ligands]: ls
ParselyParameters.ipynb ZINC000001714738.sdf    ZINC000003951740.prmtop
ZINC000001542916.inpcrd ZINC000002015152.inpcrd ZINC000003951740.sdf
ZINC000001542916.prmtop ZINC000002015152.prmtop ZINC000013985228.inpcrd
ZINC000001542916.sdf    ZINC000002015152.sdf    ZINC000013985228.prmtop
ZINC000001714738.inpcrd ZINC000003951740.inpcrd ZINC000013985228.sdf
ZINC000001714738.prmtop ZINC000003951740.mol2
```