Additional Resources

- Resource for alchemical binding free energy calculations (http://www.alchemistry.org/wiki/Main_Page)
- Thermodynamic cycle in YANK (http://getyank.org/latest/theory.html)

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