4/7/2020 Week 12 Module 1
Analysis of Binding Free Energy Calculations

- This module will consist of
  - a mini-lecture describing how YANK does free energy calculations
  - a description of how to analyze free energy calculations with YANK
- At the end of this module, you should also be able to analyze a binding free energy calculation with YANK

How does YANK work?

- YANK performs alchemical binding free energy calculations
- The thermodynamic cycles
  - include
    - complex phase: decoupling the ligand from the receptor and solvent
    - solvent phase: coupling the ligand with bulk solvent
  - are described here: http://getyank.org/latest/theory.html
- It uses several specialized algorithms
  - Thermodynamic states are coupled by replica exchange: configurations from different thermodynamic states are periodically exchanged
  - Equilibration time is automatically estimated based on the sum of potential energies in all states. http://getyank.org/latest/algorithms.html#automated-equilibration-detection
  - Free energies are computed with the multistate Bennett acceptance ratio (MBAR). http://getyank.org/latest/algorithms.html#analysis-with-mbar
  - These and others are described here: http://getyank.org/latest/algorithms.html