3/24/2020 Week 10 Module 1
Free Energy Calculations

- This module will consist of
  - a mini-lecture describing free energies, various applications of free energy calculations, and how they are calculated based on molecular simulations
  - an exercise on setting up an alchemical binding free energy calculation with YANK
- At the end of this module, you should be able to answer the following questions:
  - What are free energies?
  - How are free energy calculations useful?
  - How can you calculate a free energy difference from a molecular simulation?
- You should also be able to run a binding free energy calculation with YANK

What are free energies?