4/7/2020 Week 12 Module 2
Analysis of Binding Free Energy Calculations 2

- This module will consist of
  - a mini-lecture describing the rationale behind binding pose prediction
  - a description of how to predict binding poses with YANK
- At the end of this module, you should also be able to predict a binding pose with YANK

Why use YANK for binding poses?

- Molecular docking scores are based on potential energy and don't include entropy
- The free energy of a pose depends on both
  - the enthalpy (proxy is potential energy) and
  - the entropy
- Molecular dynamics simulations of the bound pose are often trapped in a single minimum
- YANK is
  - likely to sample multiple bound conformations, due to Hamiltonian replica exchange
  - accounts for entropy