

Markov State Models

- MSMs
 - are similar to chemical kinetics models, where there are states and rates of transitions between states
 - there are states and *transition matrices* - which describe the probability of transitions to other states after a certain amount of time
 - are based on Markov chains, which assume that the future of a system only depends on its current state
- They can be used to calculate
 - the rates of transitions between any pair of states
 - the most probable pathways between any pair of states
 - the equilibrium probability of any state
- MSMs are useful because they
 - can combine information from short MD trajectories
 - piece together local equilibria into a global picture

MSM of T4 lysozyme