Conformational clustering

Clustering

- MD simulations yield configurations in continuous space
- Clustering methods group together similar configurations (or, in a more general data science context, observations)
- Clustering is useful
  - interpreting simulation results
  - calculating thermodynamic and kinetic properties
    - predicted populations of conformations
    - predicted rates of transitions (e.g. Markov state models [1, 2])
  - selecting representative configurations for molecular docking [3]