Other ways to calculate ΔG

- The Bennett Acceptance Ratio (BAR) [3] uses data from two states
- The Multistate Bennett Acceptance Ratio (MBAR) [4] uses data from a series of states
- BAR/MBAR are proven to be statistically optimal
- Thermodynamic integration is based on the fundamental theorem of calculus, integrating one the derivative of the free energy with respect to a parameter
- All of the methods require thermodynamic states with configuration space overlap, meaning that
  - similar configurations have similar energies
  - the most relevant configuration space is similar

Alchemical Pathways