

- Sequence/structure database
- Atomistic simulations
- Experimental observations

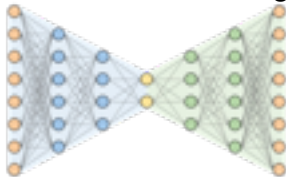


Statistical mechanics

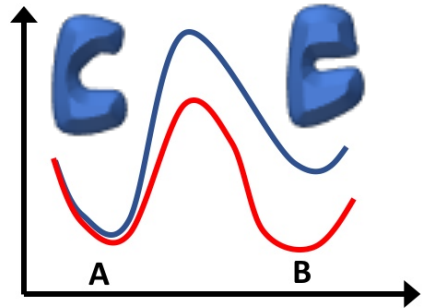
$$F = -k_B T \log Z$$



Machine Learning



Free energy



Conformational coordinates