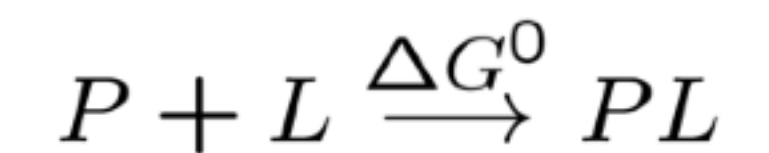
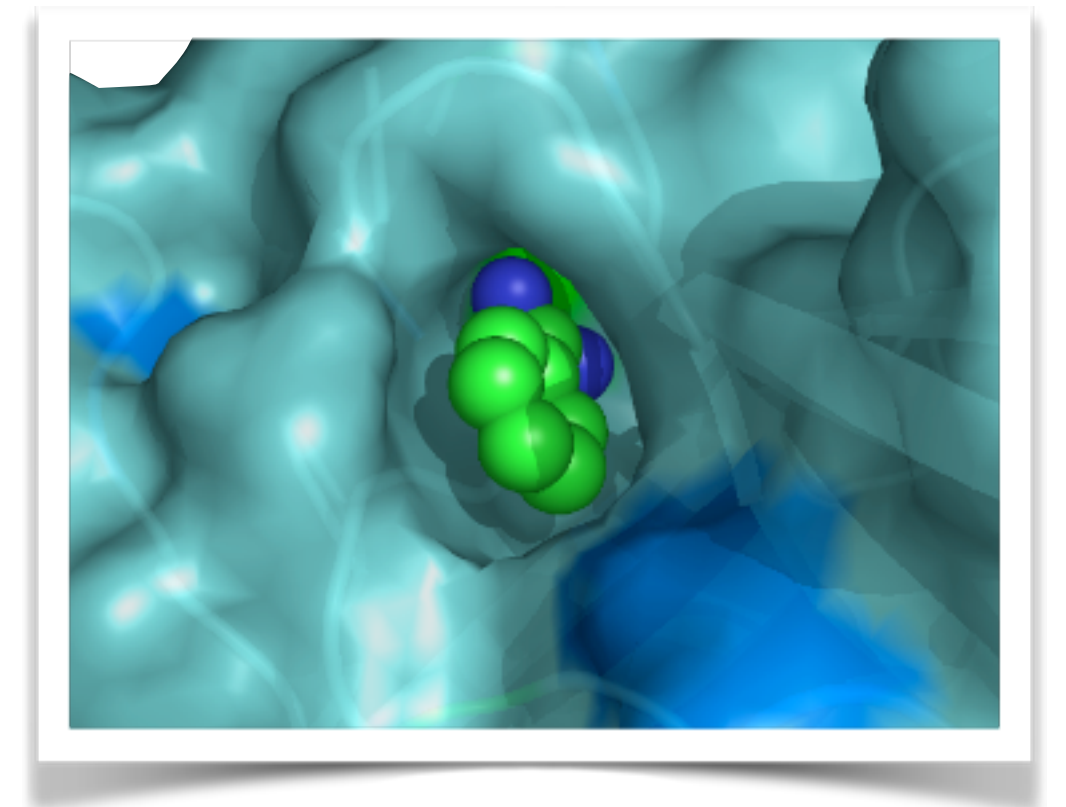


How are free energy calculations useful?

- Noncovalent binding between molecules (see [1])
 - Design molecules to manipulate protein function
 - Recognize toxins
 - Identify enzyme functions
 - Protein design: design binders to target molecule
 - Aid medicinal chemistry, guide synthesis
- Hydration free energies
 - Part of binding free energy & solubility
- Conformational free energies relevant to
 - biological mechanism
 - binding free energy



(from [1])