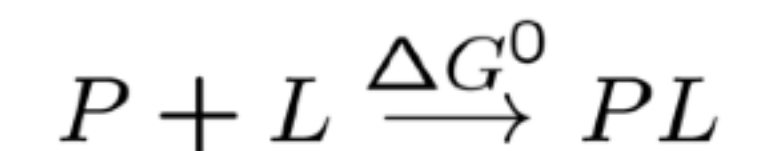
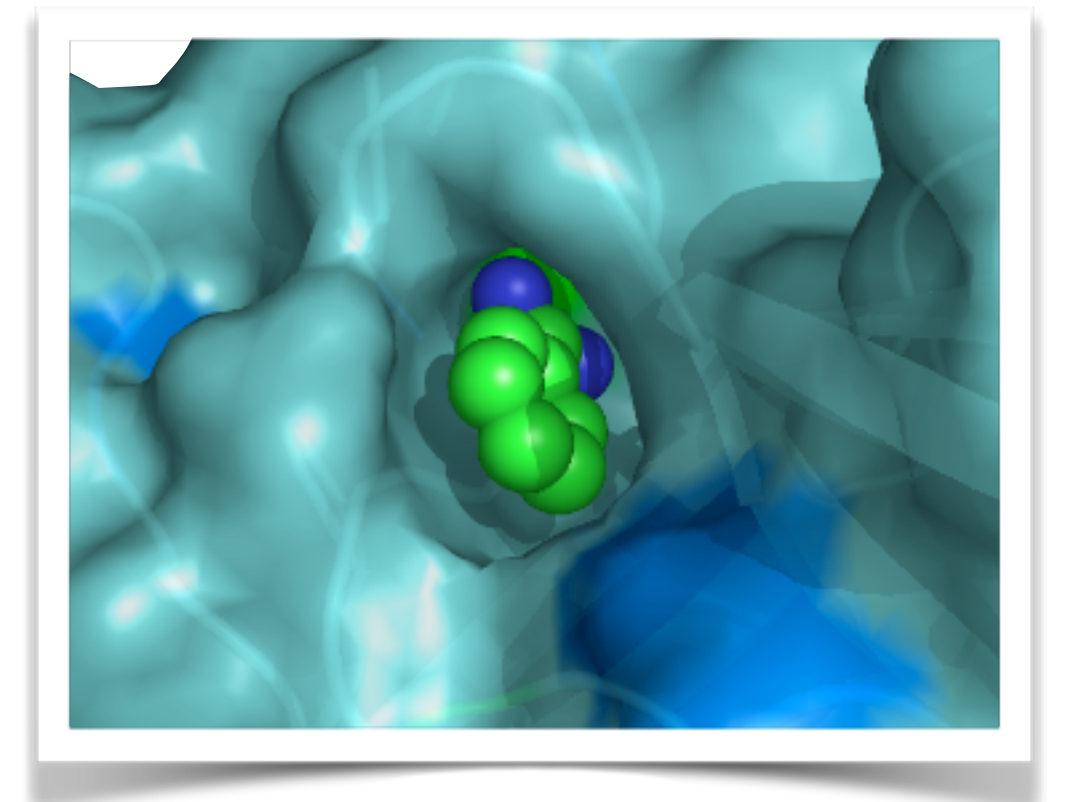


- Noncovalent binding between molecules (see [1])
 - Design molecules to manipulate protein function
 - Recognize toxins
 - Identify enzyme functions
 - Protein design: design binders to target molecule
 - Aid medicinal chemistry, guide synthesis
- Hydration free energies
 - Part of binding free energy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



(from [1])

Even modest accuracies in calculated binding free energies can have significant benefits

Hypothetical pipeline:

- Medicinal chemist suggests 100 derivatives or compounds per week
- Your job is to pick the top 10 to carry forward