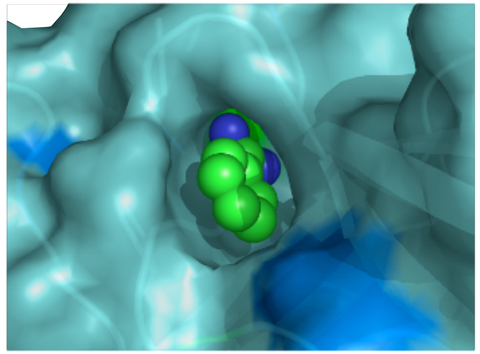
How are free energy calculations useful?

- 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



$$P + L \xrightarrow{\Delta G^0} PL$$

(from [1])