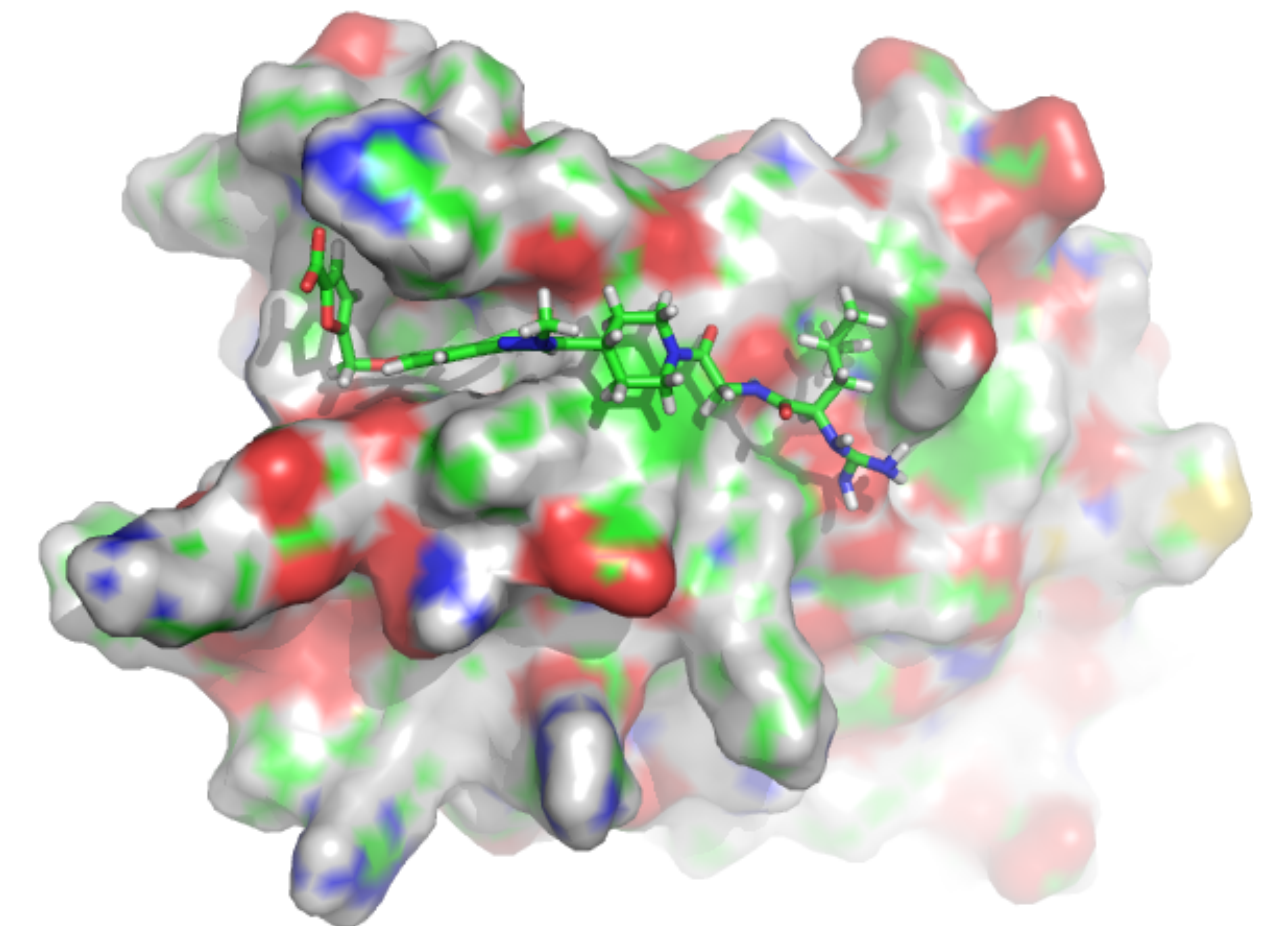


Docking approximates binding ΔG

- $\Delta G = \Delta H + T\Delta S$
- Docking score $\sim \Delta H$
- It sometimes involves
 - ad hoc ΔS based on the number of rotatable bonds
 - ΔG_{solv}
- Docking is based on “optimal” orientations



(from [1])

**How is $\Delta G/\Delta A$ calculated from
molecular simulations?**