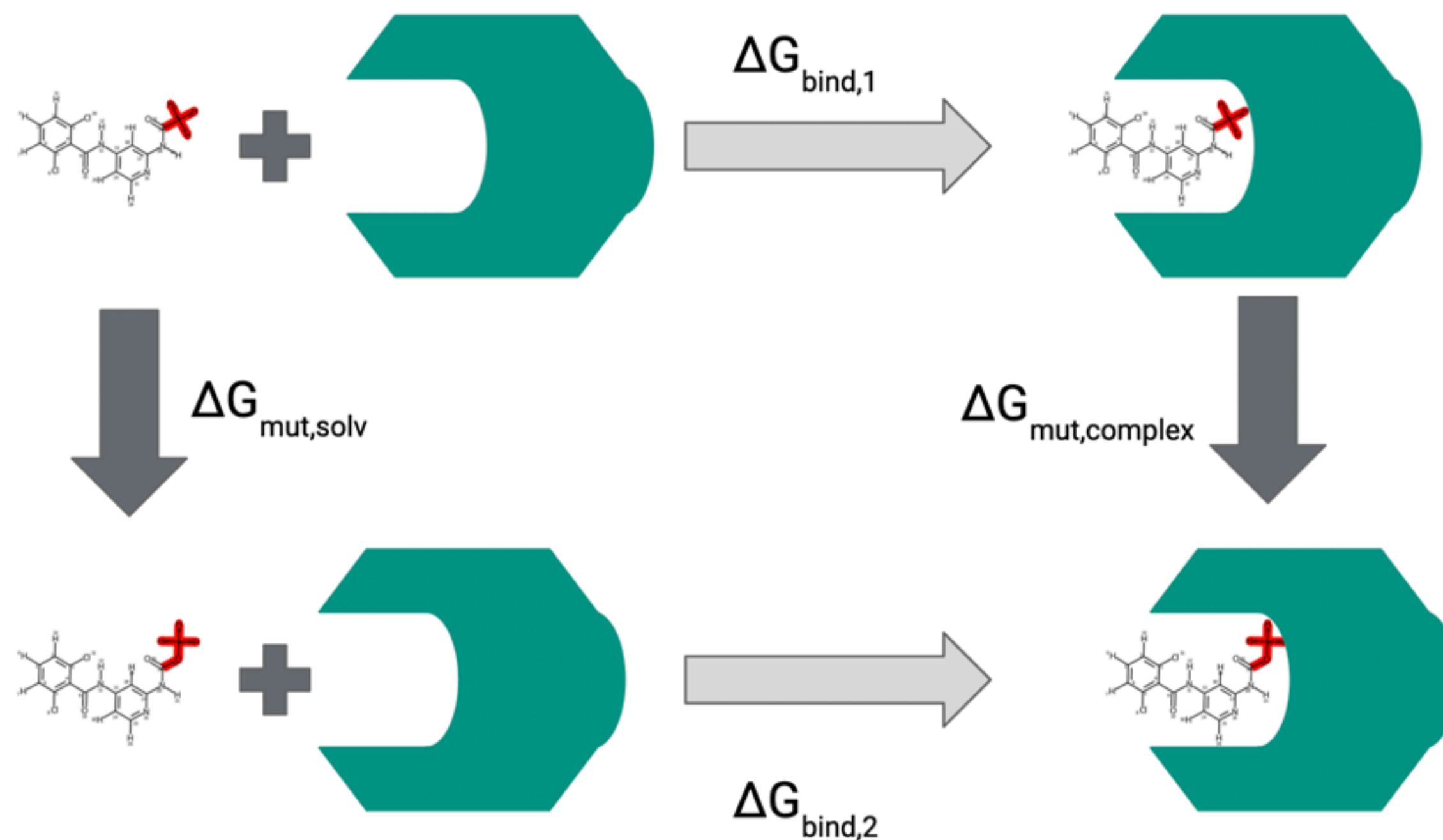


Relative Binding Free Energies

I have 2 potential drug compounds: which one is the more effective drug?



- Since this is just a thermodynamic cycle, we change which side we calculate
- This ends up being a much easier simulation.

$$\Delta\Delta G = \Delta G_{\text{mut,complex}} - \Delta G_{\text{mut,solv}}$$

Lots of sampling algorithms for this

