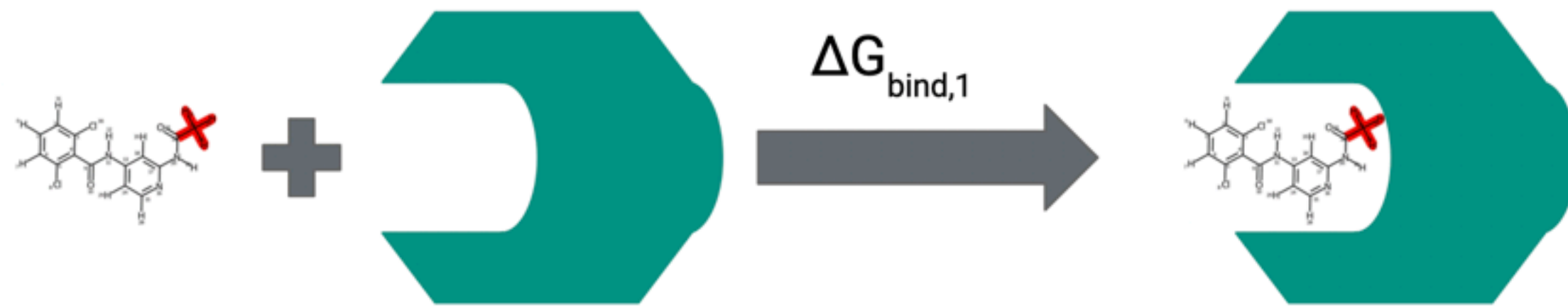# Relative Binding Free Energies

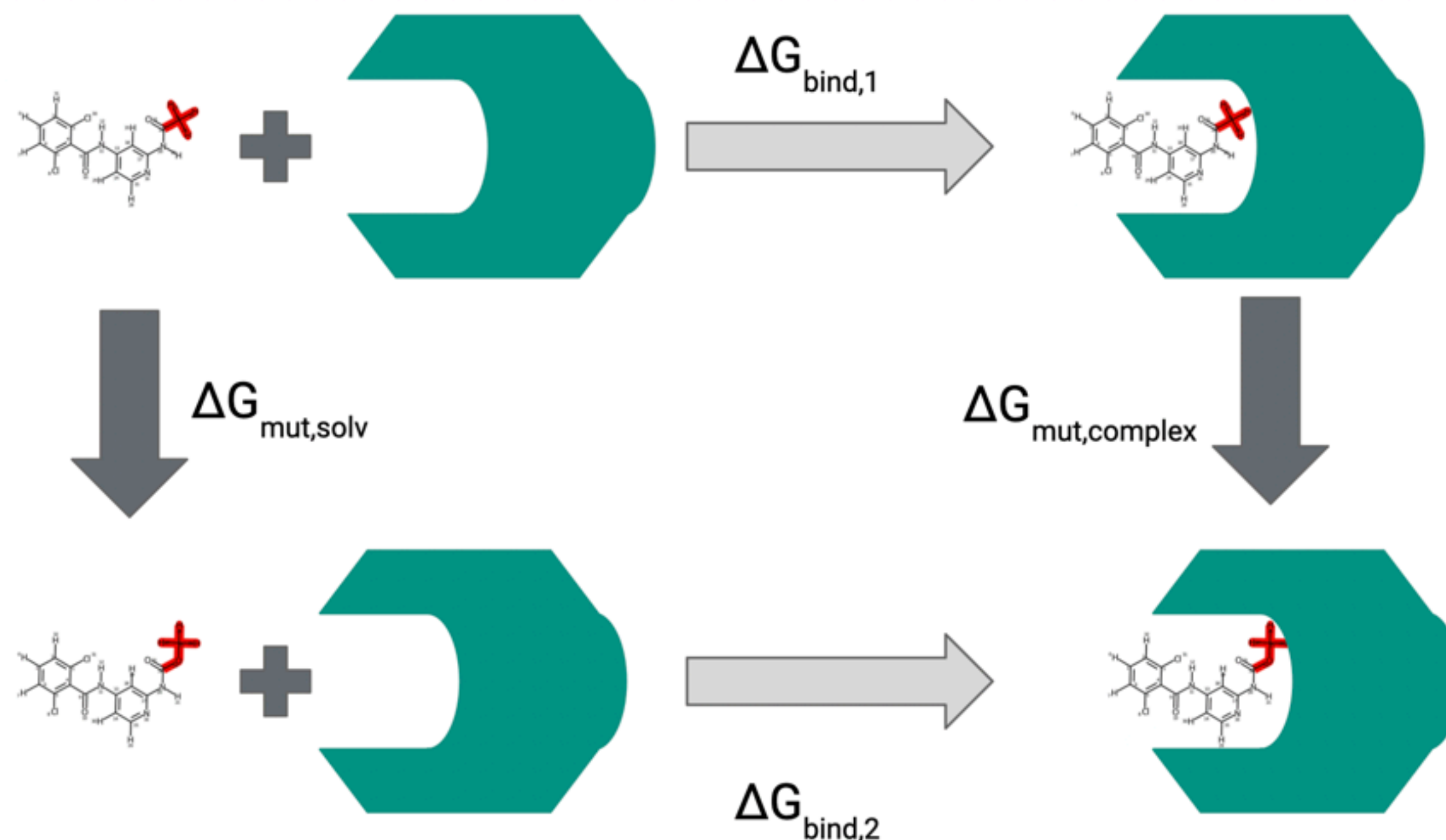I have 2 potential drug compounds: which one is the more effective drug?

- To know which ligand is better, we can look at the sign of the $\Delta\Delta G$

$$\Delta\Delta G = \Delta G_{\text{bind},2} - \Delta G_{\text{bind},1}$$

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.

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