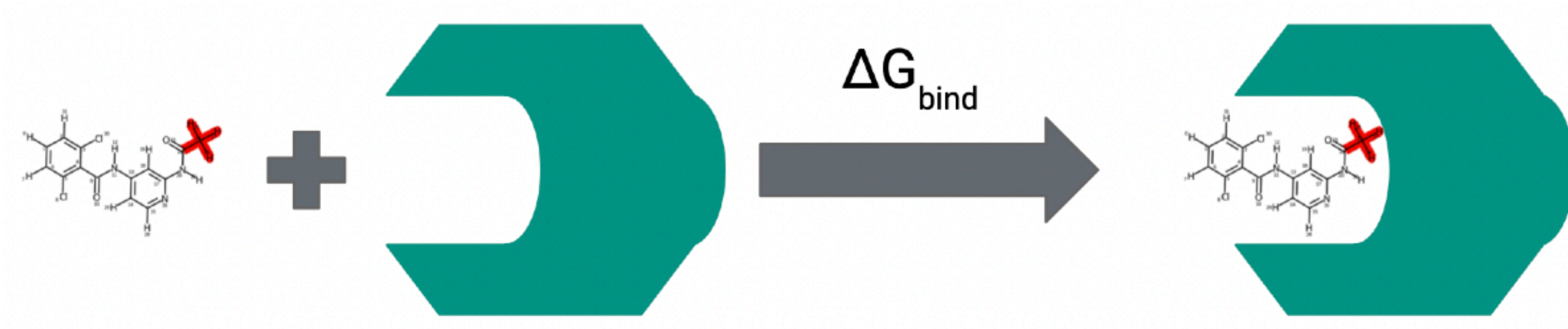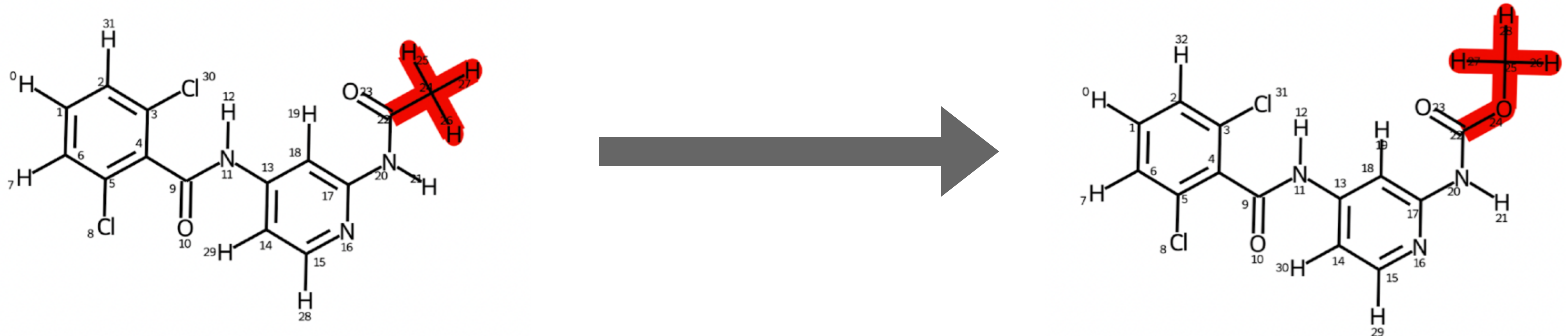# Drug design

- Most drugs are only therapeutically active when bound.

- ΔG tells us the relative probability of being bound vs. unbound.

- This makes ΔG an important metric for drug design.

Alchemical Interpolation

Simplest interpolation:

$$H_{\text{eff}}(p, q) = \lambda H_1(p, q) + (1 - \lambda)H_2(p, q)$$

(vastly oversimplified compared to real life, but this is the basic idea)