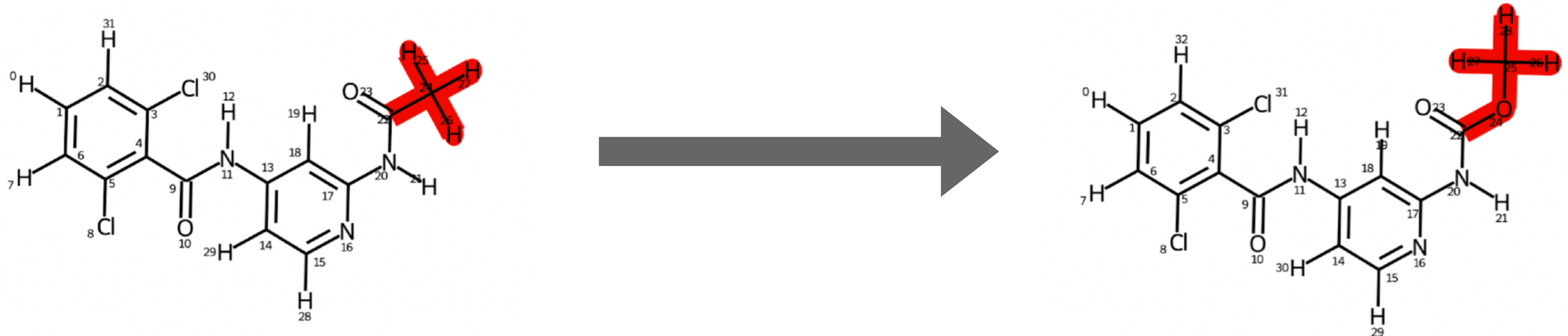


Alchemical Interpolation

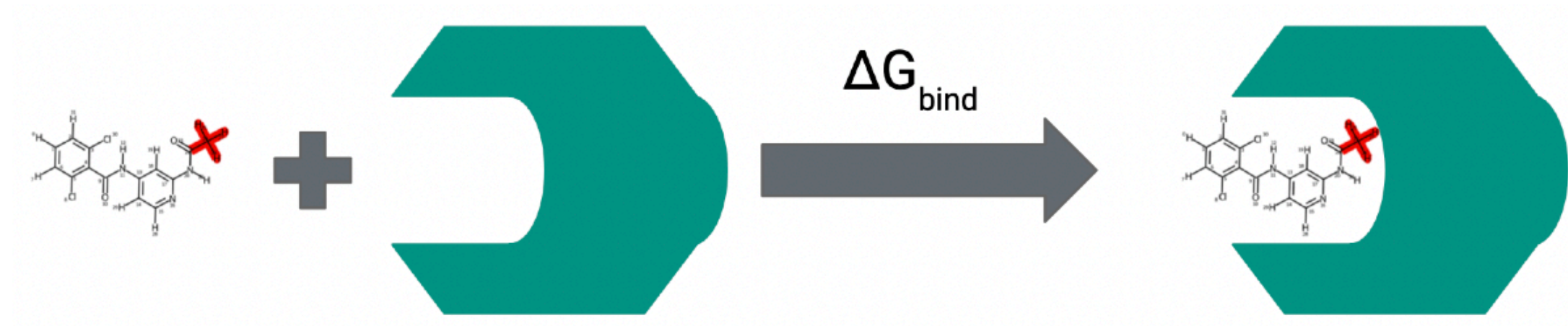


Simplest interpolation:

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

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

Absolute binding cycle



We can calculate an absolute binding free energy through a sequence of alchemical transformations

