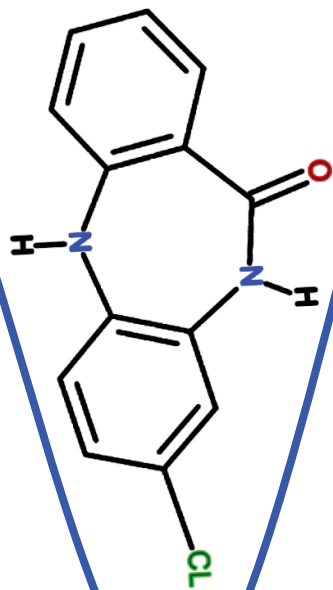


$$\Delta G_{\text{bind}} = RT \cdot \ln(K_i)$$

Multi-dimensional protein-ligand energy surface



The global energy minimum

