

$$K_a = \frac{[H^+][A^-]}{[HA]} \quad (1)$$

$$pK_a = -\log K_a \quad (2)$$

$$\Delta G = -RT \ln K_a \quad (3)$$

$$pK_a = \frac{\Delta G}{2.303RT} \quad (4)$$

$$pK_{a,protein} - pK_{a,model} = \frac{\Delta G_{protein} - \Delta G_{model}}{2.303RT} = \frac{\Delta \Delta G}{2.303RT} \quad (5)$$