$$K_{a} = \frac{[H^{+}][A^{-}]}{[HA]}$$

$$pK_{a} = -logK_{a}$$

$$\Delta G = -RTlnK_{a}$$

$$pK_{a} = \frac{\Delta G}{2.303RT}$$

$$(1)$$

$$(2)$$

$$(3)$$

$$(4)$$

$$pK_a = -\log K_a \tag{2}$$

$$\Delta G = -RT ln K_a \tag{3}$$

$$pK_a = \frac{\Delta G}{2303RT} \tag{4}$$

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