

$$\Delta G_{assoc}^0 = \Delta G_{interaction}^0 + \Delta G_{rot,trans}^0 \quad (4)$$

Equation 4 results in the functional form of the equation we used to calculate the association energy:

$$\Delta G_{assoc}^0 = \alpha \Delta G_{apolar}^0 + \beta \Delta G_{polar}^0 + \Delta G_{rot,trans}^0 \quad (7)$$

The coefficients α and β are dimensionless quantities used to scale the solvation energies to the observed dissociation constants. The values of α , β , and $\Delta G_{rot,trans}^0$ from Equation 7 were fit using a recursive least-squares procedure from the data in Table 2.