

Supplementary Material

1:2 Host:Guest Binding when Host is Transparent

In the case that the host is transparent and the guest has an absorbance at the observed wavelength, a titration is usually performed by keeping $[G]_i$ constant and incrementally increasing $[H]_i$. As a result, eqn 23 is simplified to eqn S1. By substituting eqns 19-20 into eqn S1, eqn S2 is obtained.

$$A = \epsilon_G b [G] + \epsilon_{HG} b [HG] + \epsilon_{HG_2} b [HG_2] \quad (S1)$$

$$A = \epsilon_G b [G] + \frac{\epsilon_{HG} b K_1 [G] + \epsilon_{HG_2} b K_1 K_2 [G]^2}{1 + K_1 [G] + K_1 K_2 [G]^2} [H]_i \quad (S2)$$

The script for the curve fitting thus becomes:

$$a = K_1 * K_2;$$

$$b = K_1 + 2 * K_2 * K_1 * x - K_1 * K_2 * Gt;$$

$$c = 1 + K_1 * x - K_1 * Gt;$$

$$d = -Gt;$$

for (G=x, step=1; abs(step)>1e-15; G=G-step){

$$\text{step} = (a * G * G * G + b * G * G + c * G + d) / (3 * a * G * G + 2 * b * G + c);$$

$$y = E0 * G + Ht * (E1 * K_1 * G + E2 * K_1 * K_2 * G * G) / (1 + K_1 * G + K_1 * K_2 * G * G)$$

where K_1 , K_2 , $E0$, $E1$, $E2$, Gt , x , and y represent K_1 , K_2 , $\epsilon_G b$, $\epsilon_{HG} b$, $\epsilon_{HG_2} b$, $[G]_i$, $[H]_i$, and absorbance (A), respectively. Parameters $E0$ and Gt ($\epsilon_G b$ and $[G]_i$, respectively) are known, although ϵ_G is again treated as slightly adjustable. Values for x and y are read from a standard data file by the program. Given a set of estimated initial values for K_1 , K_2 , $E1$, and $E2$, the program iteratively determines the parameter values that best fit the experimental data.