Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Contrasting interactions of DNA-intercalating dye acridine orange with hydroxypropyl derivatives of β-cyclodextrin and γ-cyclodextrin hosts

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Note-S1*: *Formulation of the binding equation for the simultaneous formation of the 1:1 and 2:1 dye to host inclusion complexes:

Complex formations in the studied systems can be represented as,

$$\mathrm{D + H \xrightleftharpoons{K_{eq(1)}} D{\bullet}H} \;;\; \mathrm{K_{eq(1)}} = \frac{\mathrm{[DH]}}{\mathrm{[D][H]}} \;; \qquad \mathrm{[DH] = K_{eq(1)}[D][H]}$$

$$\mathrm{D + DH \xrightleftharpoons{K_{eq(2)}} D_2{\bullet}H} \;;\; \mathrm{K_{eq(2)}} = \frac{\mathrm{[D_2H]}}{\mathrm{[D][DH]}} ;\; \mathrm{[D_2H] = K_{eq(2)}[D][DH] = K_{eq(1)}K_{eq(2)}[D]^2[H]}$$

For total dye concentration, we have,

$$\mathrm{[D]_0 = [D] + [DH] + 2[D_2H] = [D] + K_{eq(1)}[D][H] + 2K_{eq(1)}K_{eq(2)}[D]^2[H]}$$

Or, $$\mathrm{2K_{eq(1)}K_{eq(2)}[H][D]^2 + \left(1 + K_{eq(1)}[H]\right)[D] - [D]_0 = 0}$$

Or, $$\mathrm{[D]} = \frac{-\left(1+\mathrm{K_{eq(1)}[H]}\right) + \left(1 + 2\mathrm{K_{eq(1)}[H]} + \mathrm{K_{eq(1)}}^2\mathrm{[H]^2} + 8\mathrm{K_{eq(1)}K_{eq(2)}[H][D]_0}\right)^{1/2}}{4\mathrm{K_{eq(1)}K_{eq(2)}[H]}} \qquad (1)$$

Here [H] is the equilibrium host concentration and assumed to be the same as the total host concentration used in the solution because the host concentration is always much higher than the dye concentration used.

For the observed fluorescence intensity,

$$\mathrm{I = I_D + I_{DH} + I_{D_2H} = k_D[D] + k_{DH}[DH] + k_{D_2H}[D_2H]}$$

(Because, $\mathrm{I_0 = k_D[D]_0}$, $\mathrm{I_{DH}^{\infty} = k_{DH}[DH]_{\infty} = k_{DH}[D]_0}$, and $\mathrm{I_{D_2H}^{\infty} = k_{D_2H}[D_2H]_{\infty} = k_{D_2H}[D]_0/2}$)

So, $$\mathrm{I = I_0\frac{[D]}{[D]_0} + I_{DH}^{\infty}\frac{[DH]}{[D]_0} + 2I_{D_2H}^{\infty}\frac{[D_2H]}{[D]_0}}$$

$$\mathrm{= I_0\frac{\left([D]_0 - [DH] - 2[D_2H]\right)}{[D]_0} + I_{DH}^{\infty}\frac{[DH]}{[D]_0} + 2I_{D_2H}^{\infty}\frac{[D_2H]}{[D]_0}}$$

$$\mathrm{= I_0 + \left(I_{DH}^{\infty} - I_0\right)\frac{[DH]}{[D]_0} + 2\left(I_{D_2H}^{\infty} - I_0\right)\frac{[D_2H]}{[D]_0}}$$

Or, $$\left(I - I_0\right) = \left(I_{DH}^{\infty} - I_0\right)\frac{[DH]}{[D]_0} + 2\left(I_{D_2H}^{\infty} - I_0\right)\frac{[D_2H]}{[D]_0}$$

Or, $$\Delta I = \Delta I_{DH}^{\infty}\frac{K_{eq(1)}[D][H]}{[D]_0} + 2\Delta I_{D_2H}^{\infty}\frac{K_{eq(1)}K_{eq(2)}[D]^2[H]}{[D]_0} \qquad (2)$$

Here, [D] is to be considered as given by eq. 1.

So, working equation for fitting is,

$$\Delta I = \frac{A*C*x*[D]}{F} + \frac{2*A*B*E*x*[D]*[D]}{F} \qquad (3)$$

Here, $A = K_{eq(1)}$, $B = K_{eq(2)}$, $C = \Delta I_{DH}^{\infty}$, $E = \Delta I_{D_2H}^{\infty}$, $F = [D]_0$ and $x = [H]$.