SUPPORTING INFORMATION

Complexation-Induced Fluorescence and Acid-Base Properties of Dapoxyl Dye with γ-cyclodextrin: A Drug-Binding Application using Displacement Assay

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Figure S1: Fluorescence enhancement of dapoxyl dye (4μM) upon successive addition of γ-CD up to 35mM at pH 2.0 (left) and pH 9.0 (right)
Figure S2: Energy optimized structure of DSS and γ-CD (a) side view, (b) top view of 1:1 complex, (c) side view and (d) top view of 1:2 complex.
**Figure S3:** Fluorescence titration of DSS with $\gamma$-CD in phosphate buffer solution (100 mM) at pH 7.4 shows blue shift in the emission maxima with gradual increase in the fluorescence intensity, inset shows data fitted with 1:2 binding model having $K_1K_2=2700 \pm 300$ M$^{-2}$.

**Figure S4.** Binding titration plot and binding constant of Resazurin with $\gamma$-CD at pH 7.4 using (a) UV and (b) fluorescence spectroscopy. Titrations are performed with 5$\mu$M Resazurin and gradual increase of $\gamma$-CD concentration; data was fitted with 1:1 binding equation.
**Figure S5.** UV-Vis of studied drugs in water at pH 7.4

**Hydrodynamic volume calculation of \(\gamma\)-CD DSS complex:**

Hydrodynamic diameter of \(\gamma\)-CD = 17.5 Å\(^{[1]}\), Hydrodynamic volume of the \(\gamma\)-CD = 2800 Å\(^3\), Molar Hydrodynamic volume of \(\gamma\)-CD \(\approx\) 1690 cm\(^3\) mol\(^{-1}\)

Molar Hydrodynamic volume of phenyl group \(\approx\) 43.4 cm\(^3\) mol\(^{-1}\)\(^{[2]}\)

Molar Hydrodynamic volume of isopropyl group \(\approx\) 30.7 cm\(^3\) mol\(^{-1}\)\(^{[2]}\) and as \(N, N\)-dimethylamino group is similar to isopropyl group we assume the same volume for \(N, N\)-dimethylamino group for our calculation.

So molar hydrodynamic volume of \(N, N\)-dimethylanilino group \(\approx\) (43.4+ 30.7) cm\(^3\) mol\(^{-1}\)

\(\approx\) 74.1 cm\(^3\) mol\(^{-1}\)

As it is a 1:2 complex and the dimethylanilino group projecting both the side, then total molar hydrodynamic volume of the complex \(\approx\) {volume of \(\gamma\)-CD+ \((N, N\)-dimethylanilino group x2)} \(\approx\) {1690+ (74.1x2)} cm\(^3\) mol\(^{-1}\) \(\approx\) 1838.2 cm\(^3\) mol\(^{-1}\)

**References:**
