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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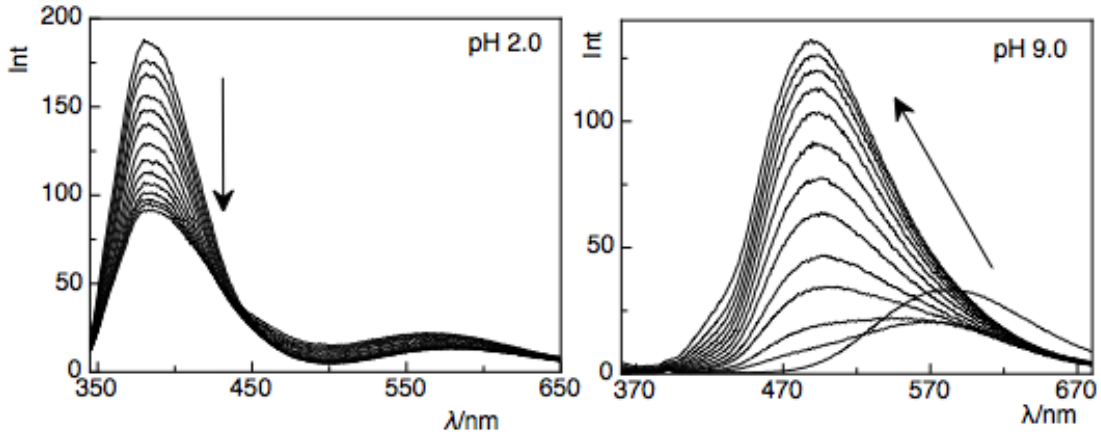

Figure S1: Fluorescence enhancement of dapoxyl dye (4μM) upon successive addition of γ-CD up to 35mM at pH 2.0 (left) and pH 9.0 (right)

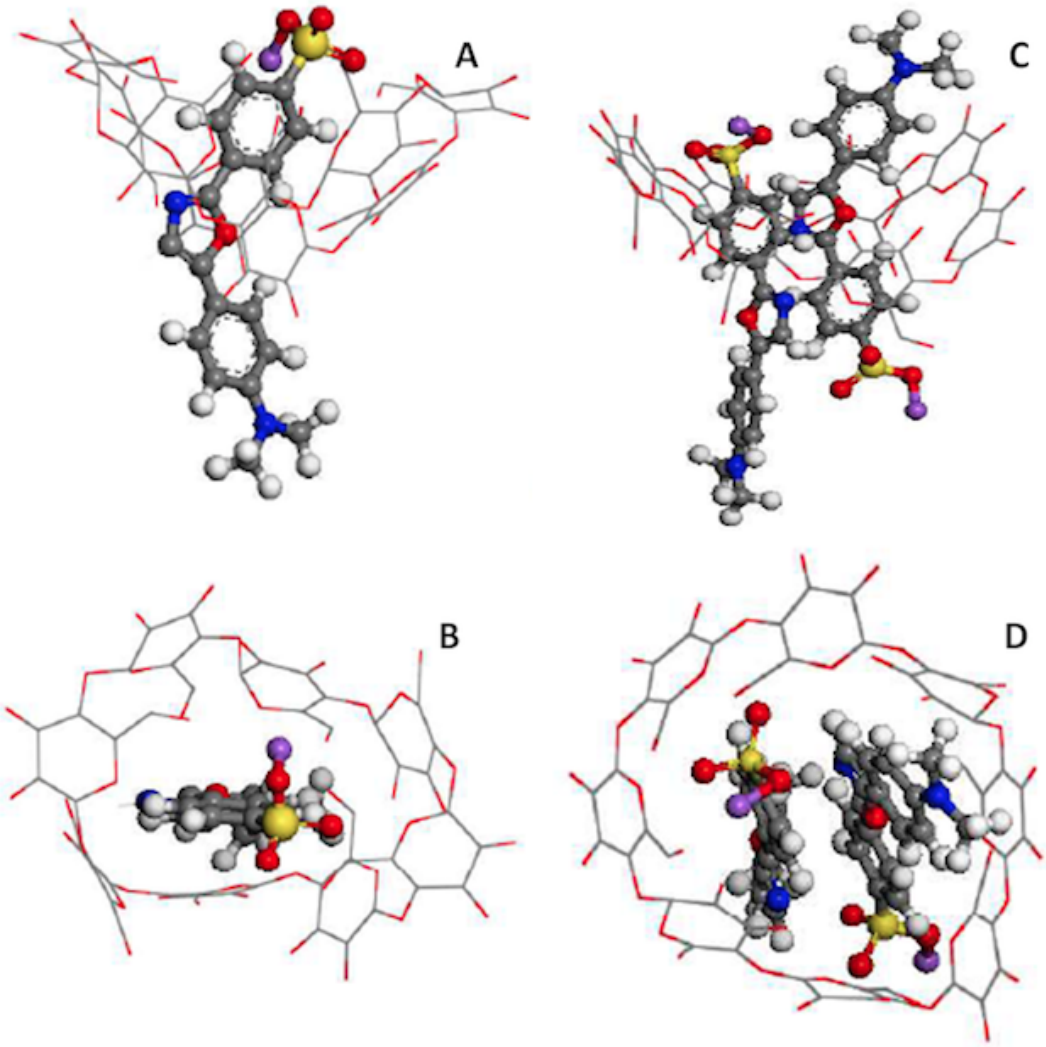

Figure S2: Energy optimized structure of DSS and *γ*-CD (a) side view, (b) top view of 1:1 complex, (c) side view and (d) top view of 1:2 complex.

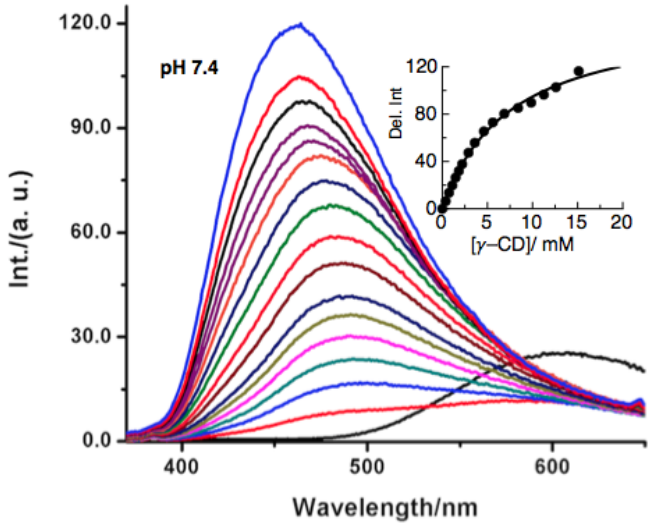

Figure S3: Fluorescence titration of DSS with γ-CD in phosphate buffer solution (100 mM) at pH 7.4 shows blue shift in the emission maxima with gradual increase in the fluorescence intensity, inset shows data fitted with 1:2 binding model having K_1K_2=2700 ± 300) M^{-2}.

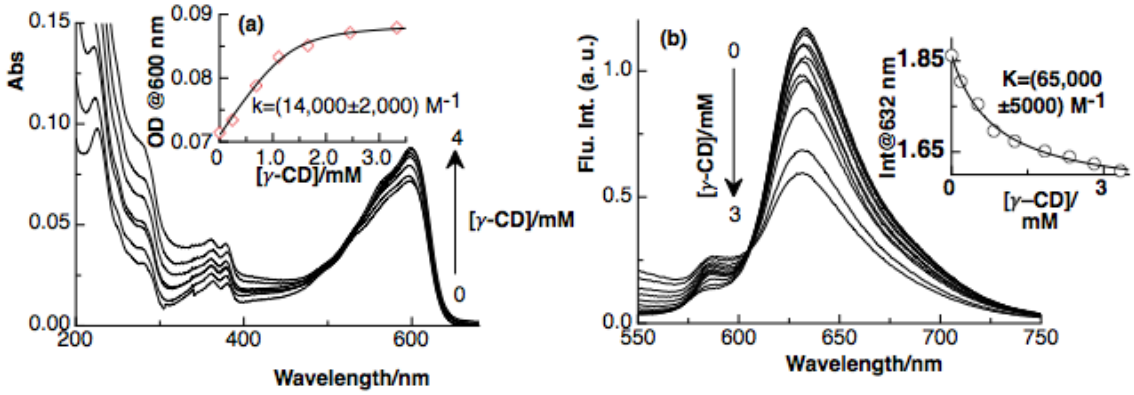

Figure S4. Binding titration plot and binding constant of Resazurin with γ-CD at pH 7.4 using (a) UV and (b) fluorescence spectroscopy. Titrations are performed with 5μM Resazurin and gradual increase of γ-CD concentration; data was fitted with 1:1 binding equation.

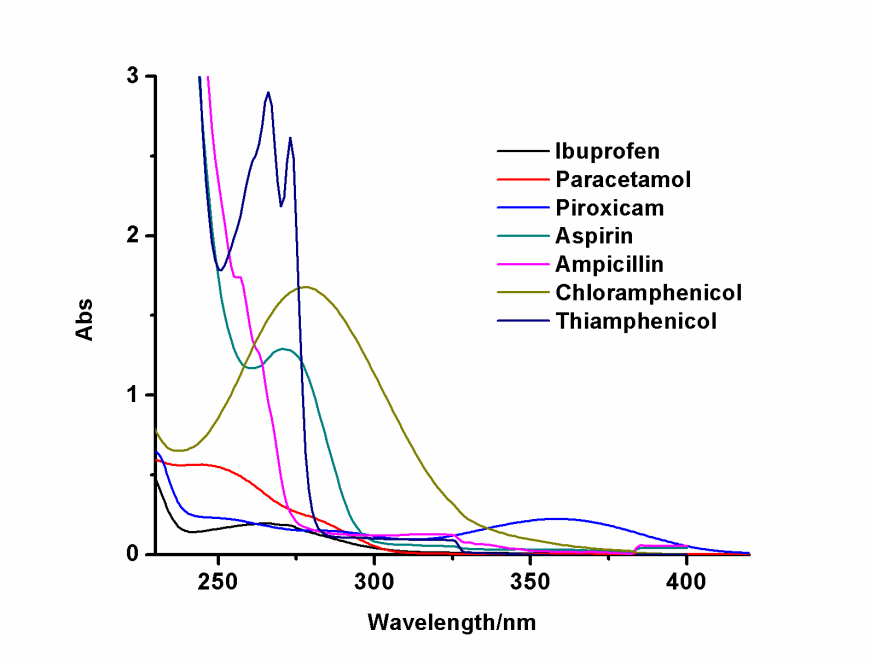

Figure S5. UV-Vis of studied drugs in water at pH 7.4

Hydrodynamic volume calculation of *γ*-CD DSS complex:

Hydrodynamic diameter of *γ*-CD =17.5 Å[1], Hydrodynamic volume of the *γ*-CD = 2800 Å^3, Molar Hydrodynamic volume of *γ*-CD ~1690 cm^3 mol^{-1}

Molar Hydrodynamic volume of phenyl group ≈ 43.4 cm^3 mol^{-1}[2]

Molar Hydrodynamic volume of isopropyl group ≈ 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 ≈ (43.4+ 30.7) cm^3 mol^{-1} ≈ 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 ≈ {volume of *γ*-CD+ (*N, N*-dimethylanilino group x2)} ≈ {1690+ (74.1x2)} cm^3 mol^{-1} ≈1838.2 cm^3 mol^{-1}

References:

[1] J. Szejtli, *Chem. Rev.* **1998**, *98*, 1743-1754.
[2] H. Bakirci, A. L. Koner, W. M. Nau, *J. Org. Chem.* **2005**, *70*, 9960-9966.