Supporting Information

Does degree of substitution on the cyclodextrin hosts impacts on their affinity towards guest binding?

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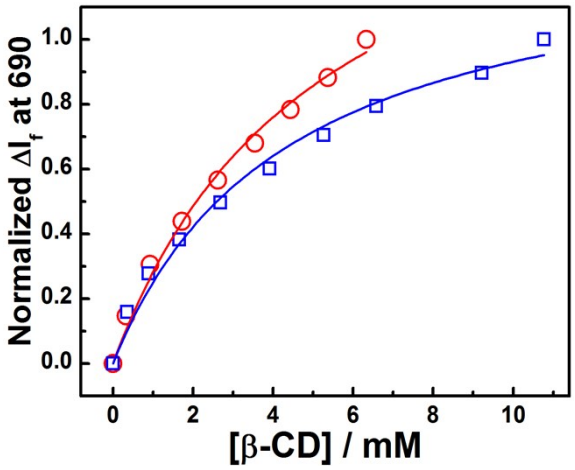

Figure S1: Binding isotherm of 3.5 μM LDS-798 with βCD in the absence of 1M NaCl (red circle) and in the presence of 1M NaCl (blue square) using 1:1 binding model.

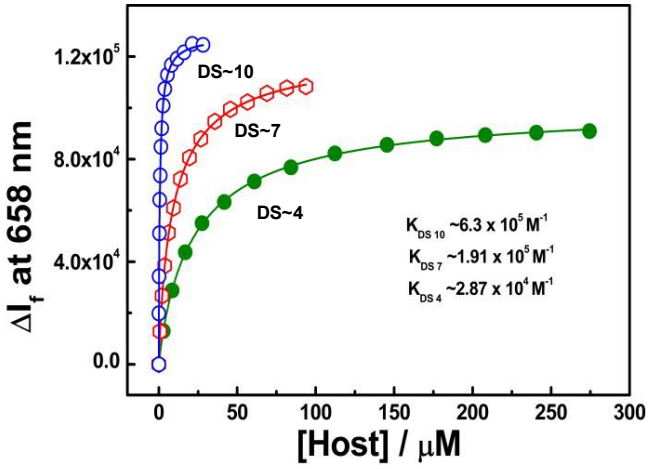

Figure S2: Binding isotherm of 1.5 μM LDS-722 with different host pH ~7, at 25 °C.

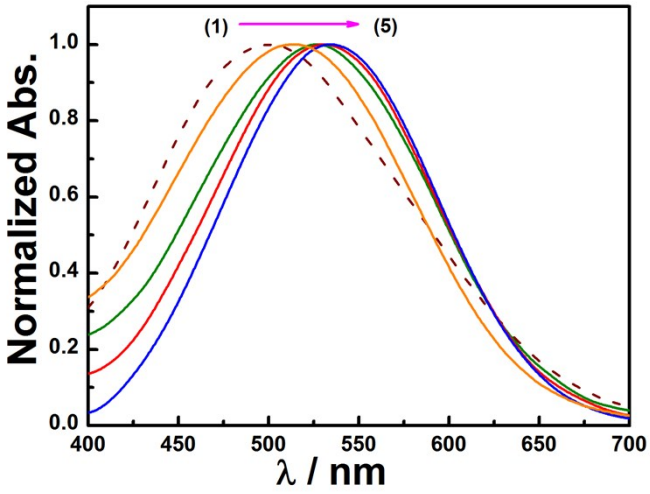

Figure S3: Normalized absorption spectra of (1) LDS-798 [λ_{max} = 500 nm] and LDS-798-cyclodextrin complexes under saturation condition; (2) β-CD [6.3 mM, λ_{max} = 513 nm], (3) DS~4 [200 μM, λ_{max} = 527 nm], (4) DS~7 [100 μM, λ_{max} = 530 nm] and (5) DS~10 [26 μM, λ_{max} = 534 nm]. [LDS-798 concentration used 3.5 μM, Temperature 25 ^{o}C, pH ~7]

Table S1. Quantum yield of different LDS-798-SBE$_n$βCD complexes.

Species	Quantum Yield[$]
LDS-798	0.002
LDS-798-βCD	0.012
LDS-798-SBE$_4$βCD	0.029
LDS-798-SBE$_7$βCD	0.034
LDS-798-SBE$_{10}$βCD	0.056

[$]Fluorescence quantum yield for LDS-798 was obtained from the literature.[1] The quantum yield values for the dye-host systems were estimated using the integrated area under the emission curve at saturated concentration of their respective binding isotherms, following comparison method.[2]

Table S2. Binding constant values for different LDS-722-SBE$_n$βCD complexes.

Complex	Binding constant (K_b) in M^{-1}
LDS-722-SBE$_4$βCD	2.87 x 10^4
LDS-722-SBE$_7$βCD	1.91 x 10^5
LDS-722-SBE$_{10}$βCD	6.3 x 10^5

Table S3. Quantum yield of different LDS-722-SBE$_n$βCD complexes.

Species	Quantum Yield[$]
LDS-722	0.01
LDS-722-SBE$_4$βCD	0.066
LDS-722-SBE$_7$βCD	0.073
LDS-722-SBE$_{10}$βCD	0.080

[$]Fluorescence quantum yield for LDS-798 was obtained from the literature[3] The quantum yield values for the dye-host systems were estimated using the integrated area under the emission curve at saturated concentration of their respective binding isotherms, following comparison method.[2]

References

1. Sarkar, P.; Luchowski, R.; Raut, S.; Sabnis, N.; Remaley, A.; Lacko, A. G.; Thamake, S.; Gryczynski, Z.; Gryczynski, I. Studies on solvatochromic properties of aminophenylstyryl-quinolinum dye, LDS 798, and its application in studying submicron lipid based structure. *Biophys. Chem.* **2010,** *153*, 61–69.

2. Lakowicz, J. R. Principles of Fluorescence Spectroscopy. 3rd Edition, Plenumm Press, Springer, New York**2006**.

3. Sola-Llano, R.; Martínez-Martínez, V.; Fujita, Y.; Gómez-Hortigüela, L.; Alfayate, A.; Uji-i, H.; Fron, E.; Pérez-Pariente, J.; López-Arbeloa, I. Formation of a Nonlinear Optical Host–Guest Hybrid Material by Tight Confinement of LDS 722 into Aluminophosphate 1D Nanochannels. *Chem. Euro. J.* **2016,** *22*, 15700-15711.