

Supporting information for

Preferential Molecular Encapsulation of ICT Fluorescence Probe in the Supramolecular Cage of Cucurbit[7]uril and β -Cyclodextrin: An Experimental and Theoretical Approach

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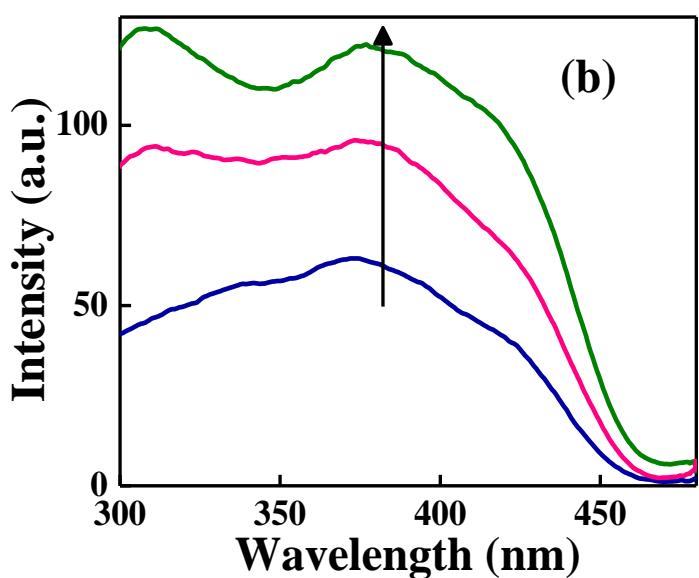
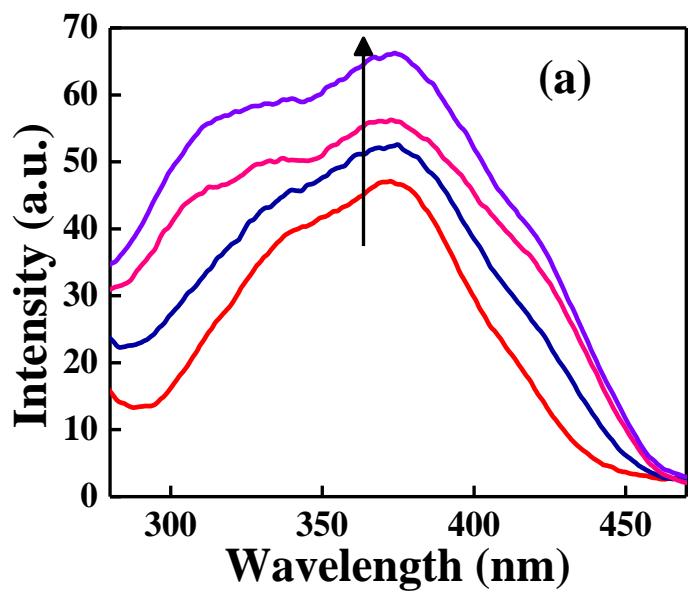


Fig. S1 Excitation spectra of DMANAN (50 μ M) monitored at the emission maxima (500 nm) with increasing concentration of (a) CB7 (0 to 0.2 mM) and (b) β -CD (0 to 6 mM).

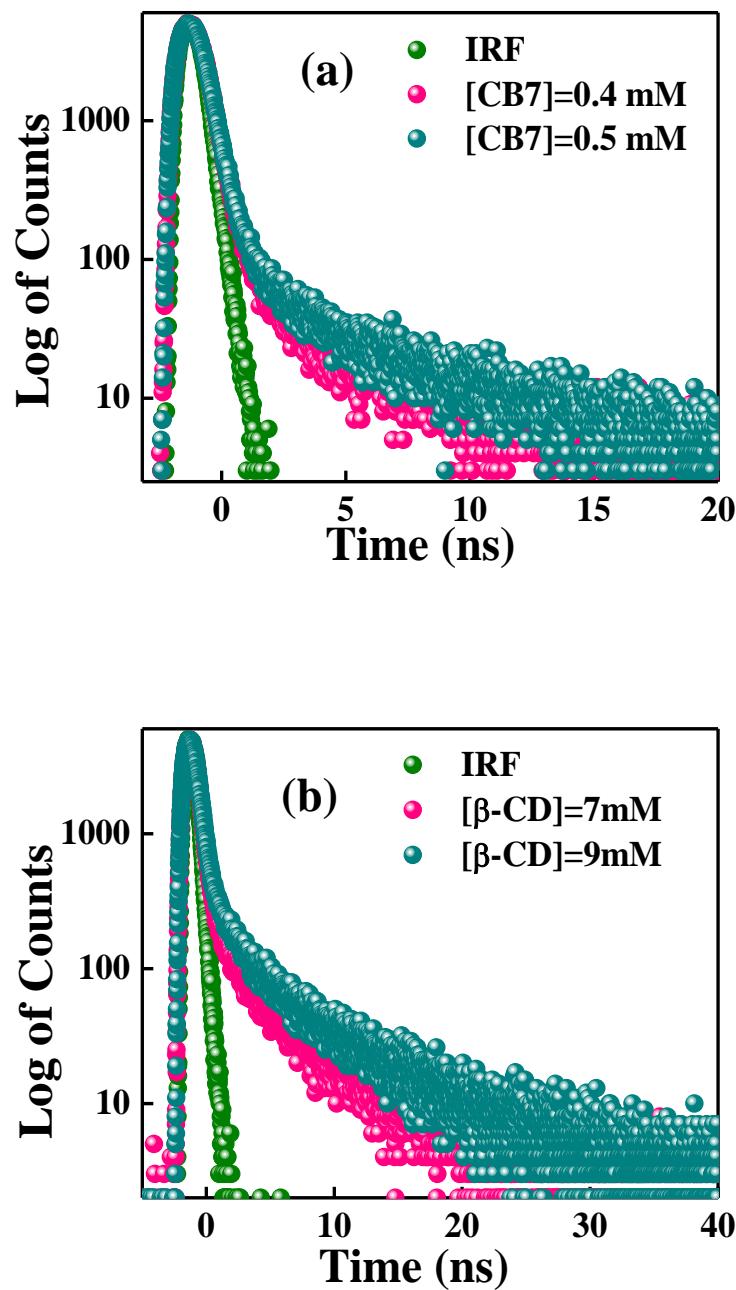


Fig. S2 Time-resolved fluorescence decay profiles ($\lambda_{\text{ex}} = 340$ nm, $\lambda_{\text{monitored}} = 415$ nm) of the probe (DMANAN) in the presence of increasing concentration of (a) CB7 and (b) β -CD.

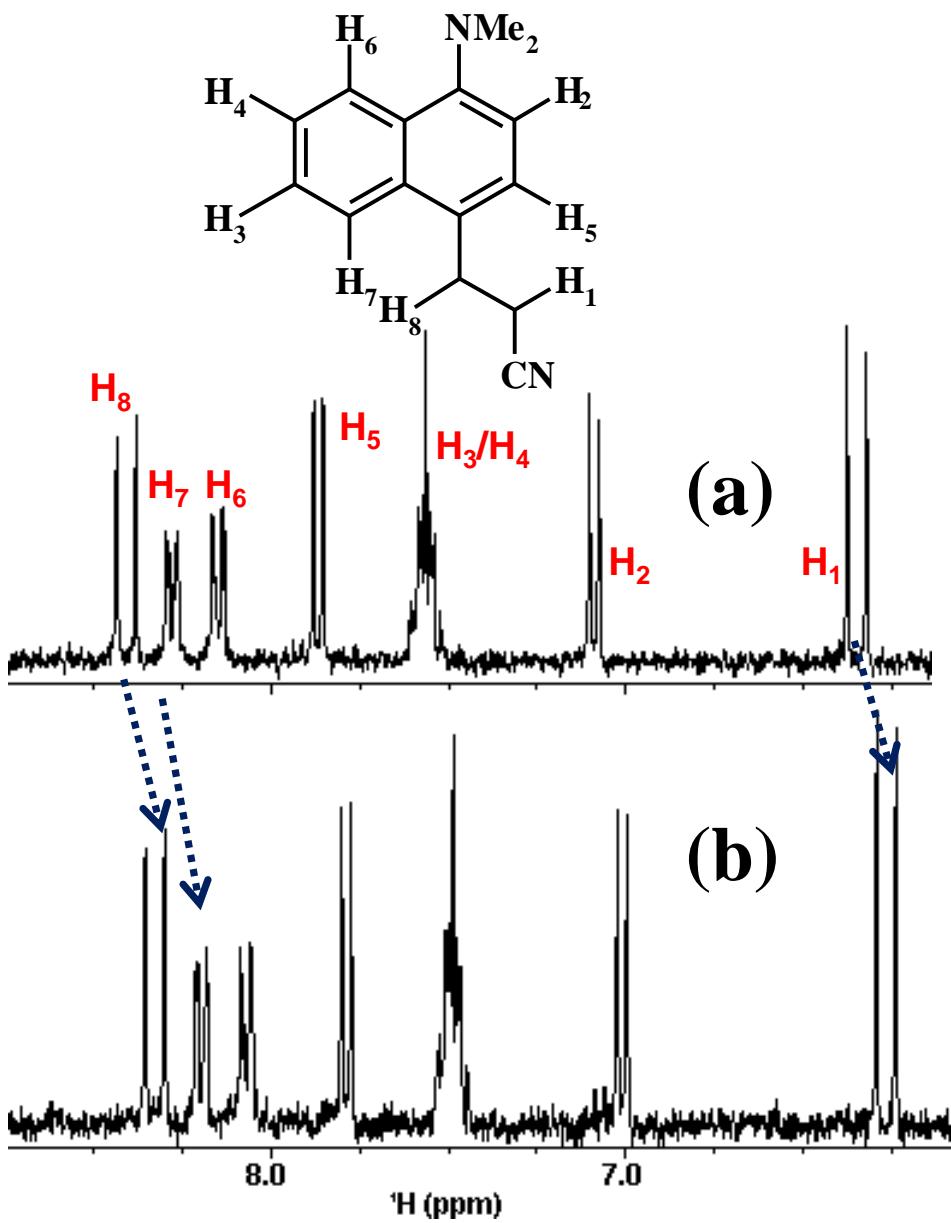


Fig. S3 ^1H NMR spectra (300 MHz) of 5 mM DMANAN (a) without any host and (b) with 5 mM β -CD in $\text{D}_2\text{O}/\text{d}_6\text{-DMSO}$ (8:2) mixed solvents. Arrows indicate characteristics spectral changes for the proton of DMANAN.

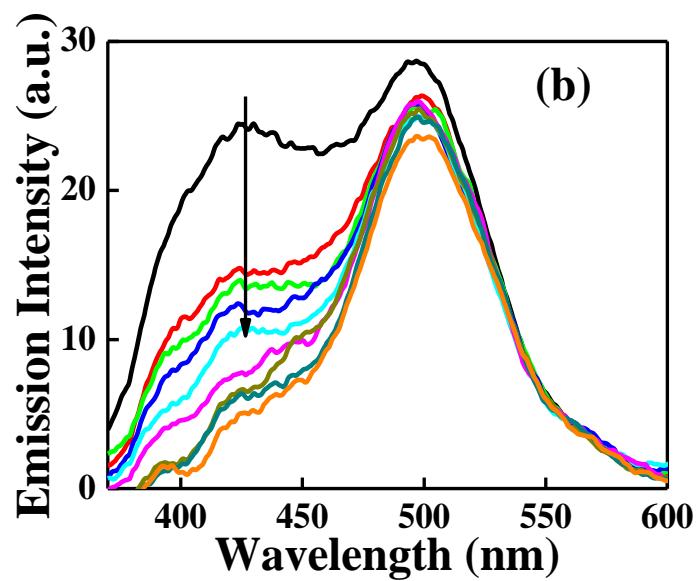
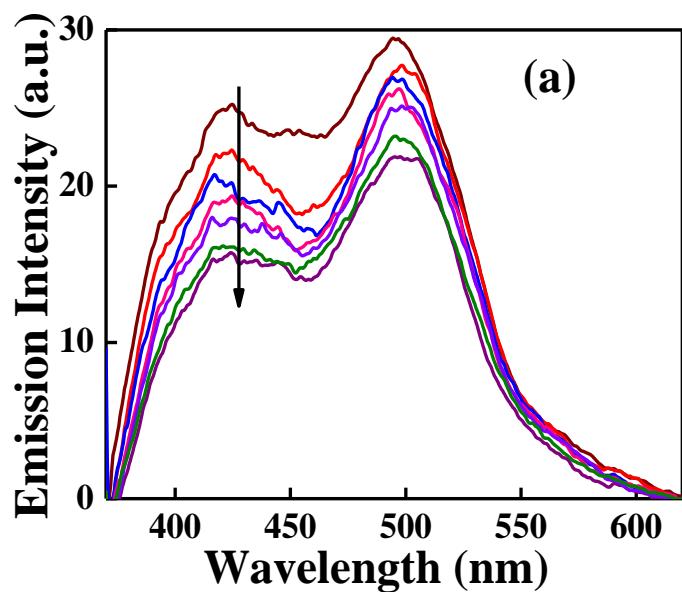


Fig. S4 Changes in the fluorescence spectra ($\lambda_{\text{ex}}=350$ nm) of DMANAN-CB7 complex ([DMANAN]=50 μM , [CB7]=100 μM) with the incremental addition of (a) NaCl ($[\text{Na}^+]$ =0 to 0.26 M) and (b) CaCl₂ ($[\text{Ca}^{2+}]$ =0 to 0.23 M).

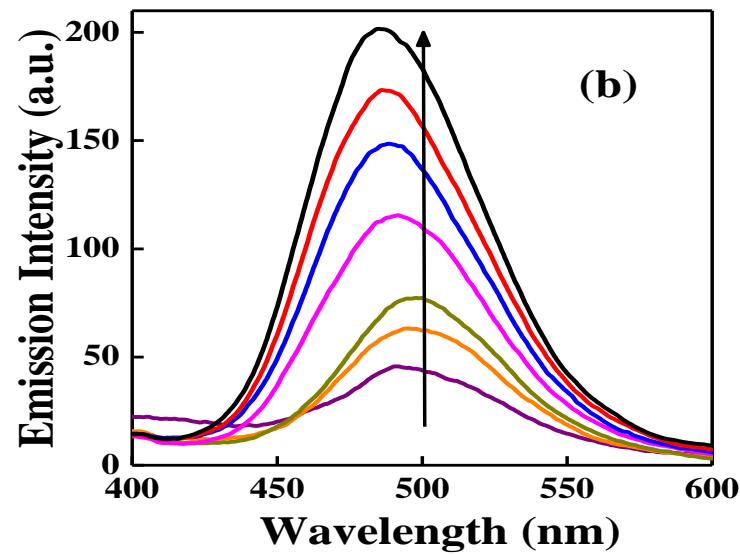
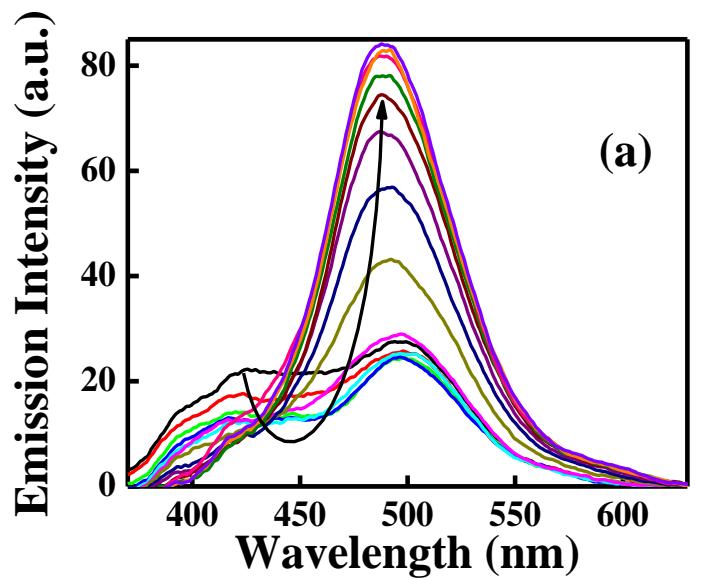


Fig. S5 Modification in the fluorescence spectra ($\lambda_{\text{ex}}=350$ nm) of (a) DMANAN-CB7 complex ([DMANAN]=50 μM , [CB7]=100 μM), and (b) DMANAN (50 μM) with gradual addition of CTAB ([CTAB]=0 to 2.5 mM).

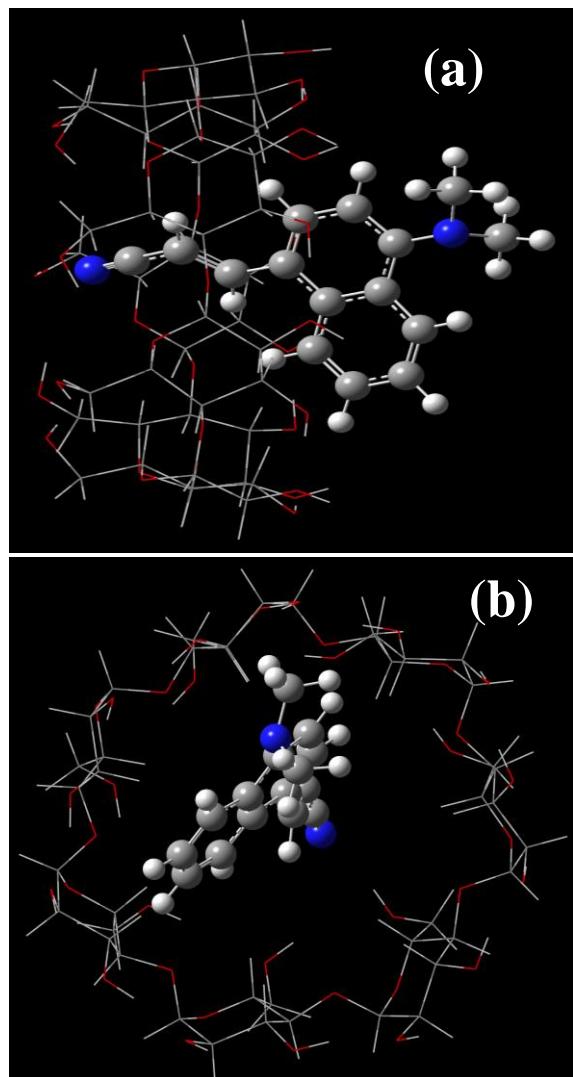
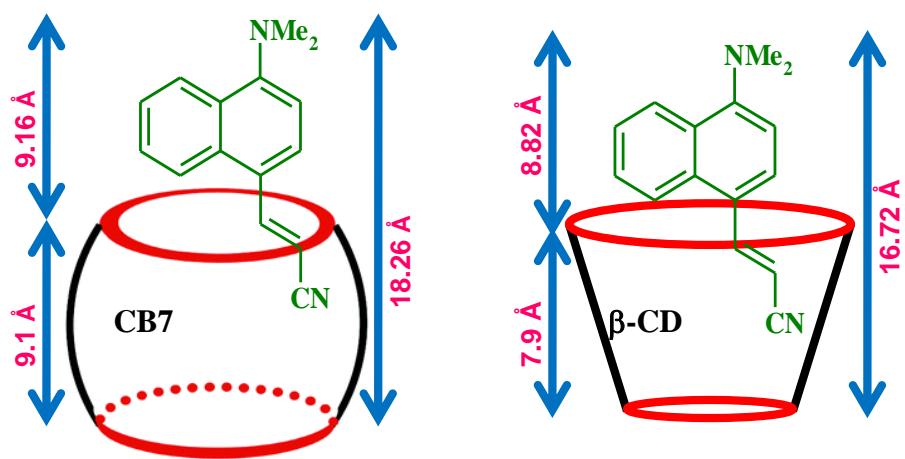


Fig. S6 Optimized ground-state structure of the host-guest complex of the probe (DMANAN) with β -CD calculated by ONIOM (B3LYP/6-31G**:PM3) level of theory. (a) side view and (b) top view are pictured here.

Table T1: Fluorescence lifetime (τ_i), their relative contribution (in parentheses), and average lifetime ($\langle \tau \rangle$) for the aqueous solution of DMANAN in the presence of CB7 and β -CD ($\lambda_{\text{ex}} = 340$ nm, $\lambda_{\text{monitored}} = 415$ nm). χ^2 and Durbin-Watson (DW) parameter represents the goodness of the fitting.

[Host]		τ_1	τ_2	τ_3	$\langle \tau \rangle$	χ^2	DW
	mM	(ns)	(ns)	(ns)	(ns)		
CB7	0.4	0.335 (0.254)	1.996 (0.004)	0.067 (0.742)	0.143	1.12	1.96
	0.5	0.384 (0.262)	2.832 (0.005)	0.108 (0.733)	0.194	1.13	2.00
β -CD	7	1.293 (0.027)	6.844 (0.004)	0.233 (0.969)	0.288	1.02	1.92
	9	1.573 (0.030)	7.590 (0.006)	0.238 (0.964)	0.322	1.02	1.87

Standard deviation for the fitting analysis is = $\pm 5\%$.



Scheme S1: Estimation of hydrodynamic diameter for the host-guest inclusion complex of DMANAN with CB7 and β -CD from time-resolved anisotropy measurements.